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Best Practices II: Testing, Documenting And Packaging Of Code

Day 4

Advanced Scientific Programming with Python

Visualization

- Data visualisation is an important part of data analysis
- There are multiple data visualisation and plotting packages for Python.
- Among the most popular are `plotly`, `plotnine` (aka ggplot) and `Altair`
- Despite its many quirks the most widely used is still `matplotlib` which I'll briefly demonstrate.

Matplotlib Notebook

SciPy

- The scipy package contains various toolboxes dedicated to common issues in scientific computing.
- Its different submodules correspond to different applications, such as interpolation, integration, optimization, image processing, statistics, special functions, etc.
- scipy can be compared to other standard scientific-computing libraries, such as the GSL (GNU Scientific Library for C and C++), or Matlab's toolboxes.
- scipy is the core package for scientific routines in Python; it is meant to operate efficiently on numpy arrays, so that numpy and scipy work hand in hand.

Why SciPy?

- Before implementing a routine, it is worth checking if the desired data processing is not already implemented in SciPy.
- As non-professional programmers, scientists often tend to re-invent the wheel, which leads to buggy, non-optimal, difficult-to-share and unmaintainable code.
- By contrast, SciPy's routines are optimized and tested, and should therefore be used when possible.

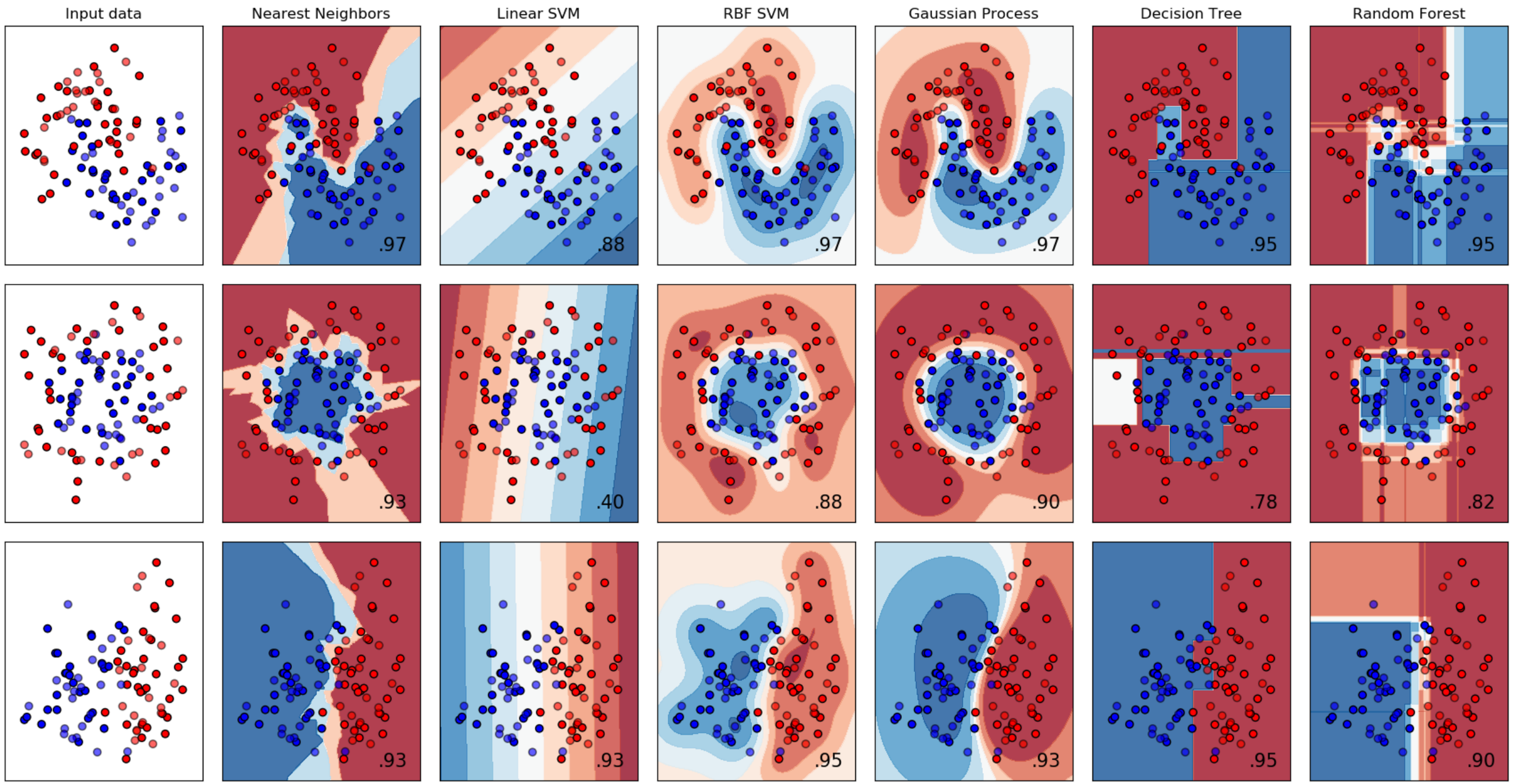
What's In SciPy?

- Clustering package (scipy.cluster)
- Constants (scipy.constants)
- Discrete Fourier transforms (scipy.fftpack)
- Integration and ODEs (scipy.integrate)
- Interpolation (scipy.interpolate)
- Input and output (scipy.io)
- Linear algebra (scipy.linalg)
- Miscellaneous routines (scipy.misc)
- Multi-dimensional image processing (scipy.ndimage)
- Orthogonal distance regression (scipy.odr)
- Optimization and root finding (scipy.optimize)
- Signal processing (scipy.signal)
- Sparse matrices (scipy.sparse)
- Sparse linear algebra (scipy.sparse.linalg)
- Compressed Sparse Graph Routines (scipy.sparse.csgraph)
- Spatial algorithms and data structures (scipy.spatial)
- Special functions (scipy.special)
- Statistical functions (scipy.stats)
- Statistical functions for masked arrays (scipy.stats.mstats)
- Low-level callback functions

SciPy Notebook

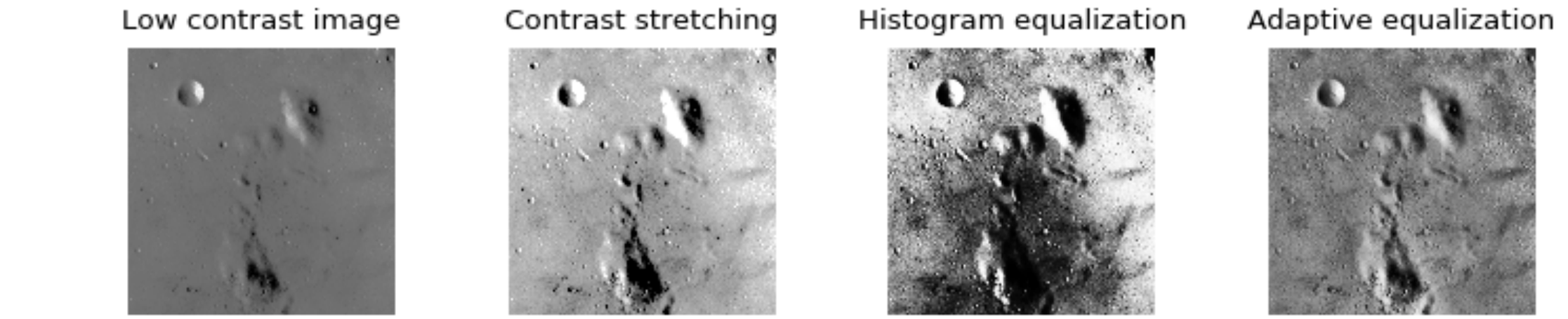
Beyond Numpy And Scipy

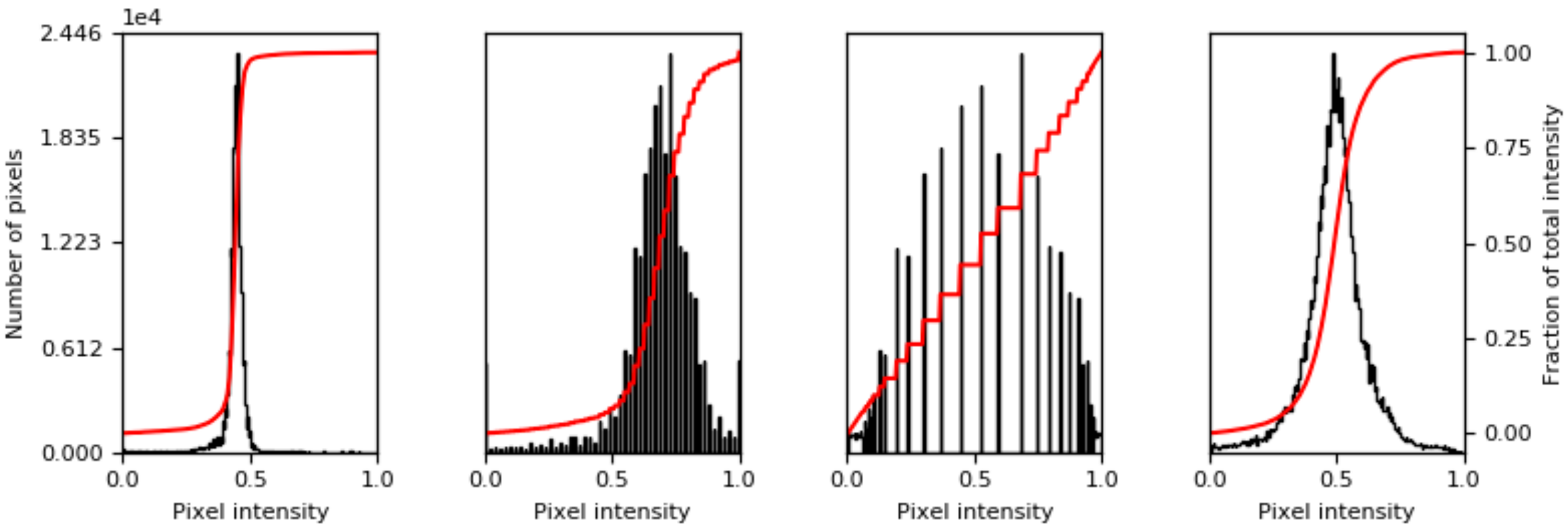
- scikit-learn - Simple Machine Learning in Python



Beyond Numpy And Scipy

- scikit-image - Image Processing in Python





Basics Of Cython

- The fundamental nature of Cython can be summed up as follows: Cython is Python with C data types.
- Almost any piece of Python code is also valid Cython code. The Cython compiler will convert it into C code which makes equivalent calls to the Python/C API.
- But Cython is much more than that, because parameters and variables can be declared to have C data types.
- Code which manipulates Python values and C values can be freely intermixed, with conversions occurring automatically wherever possible.
- Reference count maintenance and error checking of Python operations is also automatic, and the full power of Python's exception handling facilities, including the try-except and try-finally statements, is available to you – even in the midst of manipulating C data.

Cython Hello World

- As Cython can accept almost any valid python source file, one of the hardest things in getting started is just figuring out how to compile your extension.
- So lets start with the canonical python hello world. We'll save it under **helloworld.pyx**:

```
print("Hello World")
```

- Now we need to create a **setup.py** to compile this:

```
from distutils.core import setup
from Cython.Build import cythonize

setup(
    ext_modules = cythonize("helloworld.pyx")
)
```

- To now build your Cython file do:

```
$ python setup.py build_ext --inplace
```

- Which will leave a file in your local directory called helloworld.so in unix or helloworld.pyd in Windows.

Cython Hello World

- Now to use this file: start the python interpreter and simply import it as if it was a regular python module:

```
>>> import helloworld
Hello World
```

- Congratulations! You now know how to build a Cython extension.

- But so far this example doesn't really give a feeling why one would ever want to use Cython, so lets create a more realistic example.

Cython Primes

primes.py

```
import numpy

"""
 Calculates first kmax primes
"""
def primes(kmax):
    p = numpy.zeros((1000),dtype=numpy.int)
    result = []
    if kmax > 1000:
        kmax = 1000
    k = 0
    n = 2
    while k < kmax:
        i = 0
        while i < k and n % p[i] != 0:
            i = i + 1
        if i == k:
            p[k] = n
            k = k + 1
            result.append(n)
        n = n + 1
    return result
```

cy_primes.pyx

```
def primes(int kmax):
    cdef int n, k, i
    cdef int p[1000]
    result = []
    if kmax > 1000:
        kmax = 1000
    k = 0
    n = 2
    while k < kmax:
        i = 0
        while i < k and n % p[i] != 0:
            i = i + 1
        if i == k:
            p[k] = n
            k = k + 1
            result.append(n)
        n = n + 1
    return result
```

Cython Primes

```
In [1]: import primes

In [2]: import cy_primes

In [3]: %timeit primes.primes(2000)
1 loop, best of 3: 704 ms per loop

In [4]: %timeit cy_primes.primes(2000)
100 loops, best of 3: 1.92 ms per loop
```

For certain code Cython give massive performance gains!

Do you have any examples from your research where Cython could be useful?

Adapted from:

http://materials.jeremybejarano.com/MPIwithPython/introMPI.html

https://mpi4py.readthedocs.io/en/stable/intro.html#what-is-mpi

MPI

- MPI, the Message Passing Interface, is a standardized and portable message-passing system designed to function on a wide variety of parallel computers.
- The standard defines the syntax and semantics of library routines and allows users to write portable programs in the main scientific programming languages (Fortran, C, or C++).
- Since its release, the MPI specification has become the leading standard for message-passing libraries for parallel computers.
- Implementations are available from vendors of high-performance computers and from well known open source projects like MPICH, Open MPI or LAM.

Introduction to MPI

- As tradition has it, we will introduce you to MPI programming using a variation on the standard hello world program.
- Our first MPI python program will be the Hello World program for multiple processes. The source code is as follows:

```
#hello.py
from mpi4py import MPI
comm = MPI.COMM_WORLD
rank = comm.Get_rank()
print("hello world from process ", rank)
```

- After saving this text as hello.py, it is executed using the following command-line syntax, run from the file's directory:

```
$ mpiexec  -n 5 python  hello.py
```

- The above command will execute five python processes which can all communicate with each other.

Introduction to MPI

- When each program runs, it will print hello, and tell you its rank:

```
hello world from process 0
hello world from process 1
hello world from process 3
hello world from process 2
hello world from process 4
```

- Notice that when you try this on your own, they do not necessarily print in order. This is because 5 separate processes are running on different processors, and we cannot know beforehand which one will execute its print statement first.
- If the processes are being scheduled on the same processor instead of multiple processors, then it is up to the operating system to schedule the processes, and it has no preference of any one of our processes over any other process of ours. In essence, each process executes autonomously.

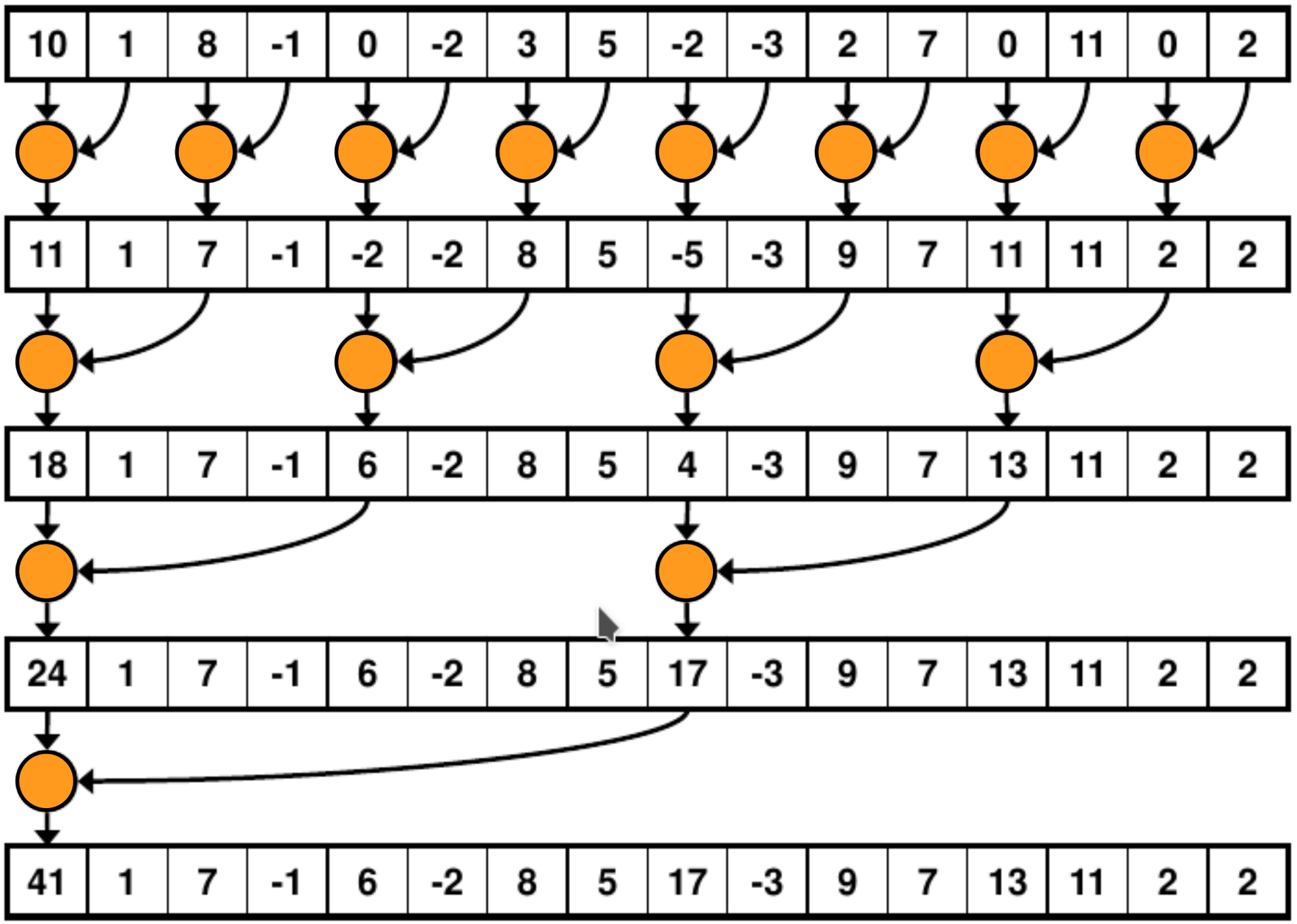
Point To Point Communication

- The simplest message passing involves two processes: a sender and a receiver.
- Let's make two processes. One will draw a random number and then send it to the other.
- We will do this using the routines Comm.Send and Comm.Recv:

```
#passRandomDraw.py
import numpy
from mpi4py import MPI
comm = MPI.COMM_WORLD
rank = comm.Get_rank()

randNum = numpy.zeros(1)

if rank == 1:
        randNum = numpy.random.random_sample(1)
        print "Process", rank, "drew the number", randNum[0]
        comm.Send(randNum, dest=0)

if rank == 0:
        print "Process", rank, "before receiving has the number", randNum[0]
        comm.Recv(randNum, source=1)
        print "Process", rank, "received the number", randNum[0]
```

Collective Communication

- Suppose we have eight processes, each with a number to be summed.
- What's the best way to do the sum while minimising communication?



Collective Communication

```
#collective.py
#example to run: mpiexec -n 4 python collective.py 10000
import numpy
import sys
from mpi4py import MPI

comm = MPI.COMM_WORLD
rank = comm.Get_rank()
size = comm.Get_size()

n = int(sys.argv[1])
x = numpy.linspace(start=float(rank)/size, stop=float(1+rank)/size, num=n/size,
endpoint=False)
cosx = numpy.cos(x)

#initializing variables. mpi4py requires that we pass numpy objects.
integral = numpy.zeros(1)
total = numpy.zeros(1)

# perform local computation. Each process integrates its own interval
integral[0] = numpy.sum(cosx)*1.0/n
print("Estimate of integral of cos(x) from %f to %f is %f" % (float(rank)/size,
float(1+rank)/size, integral))
```

Collective Communication

```
# communication
# root node receives results with a collective "reduce"
comm.Reduce(integral, total, op=MPI.SUM, root=0)

# root process prints results
if comm.rank == 0:
    print("With n=%d our estimate of the integral from 0 to 1 of cos(x)
is %f" % (n, total))
    print("Exact integral (sin(1)) is %f" % (numpy.sin(1.0)))
```

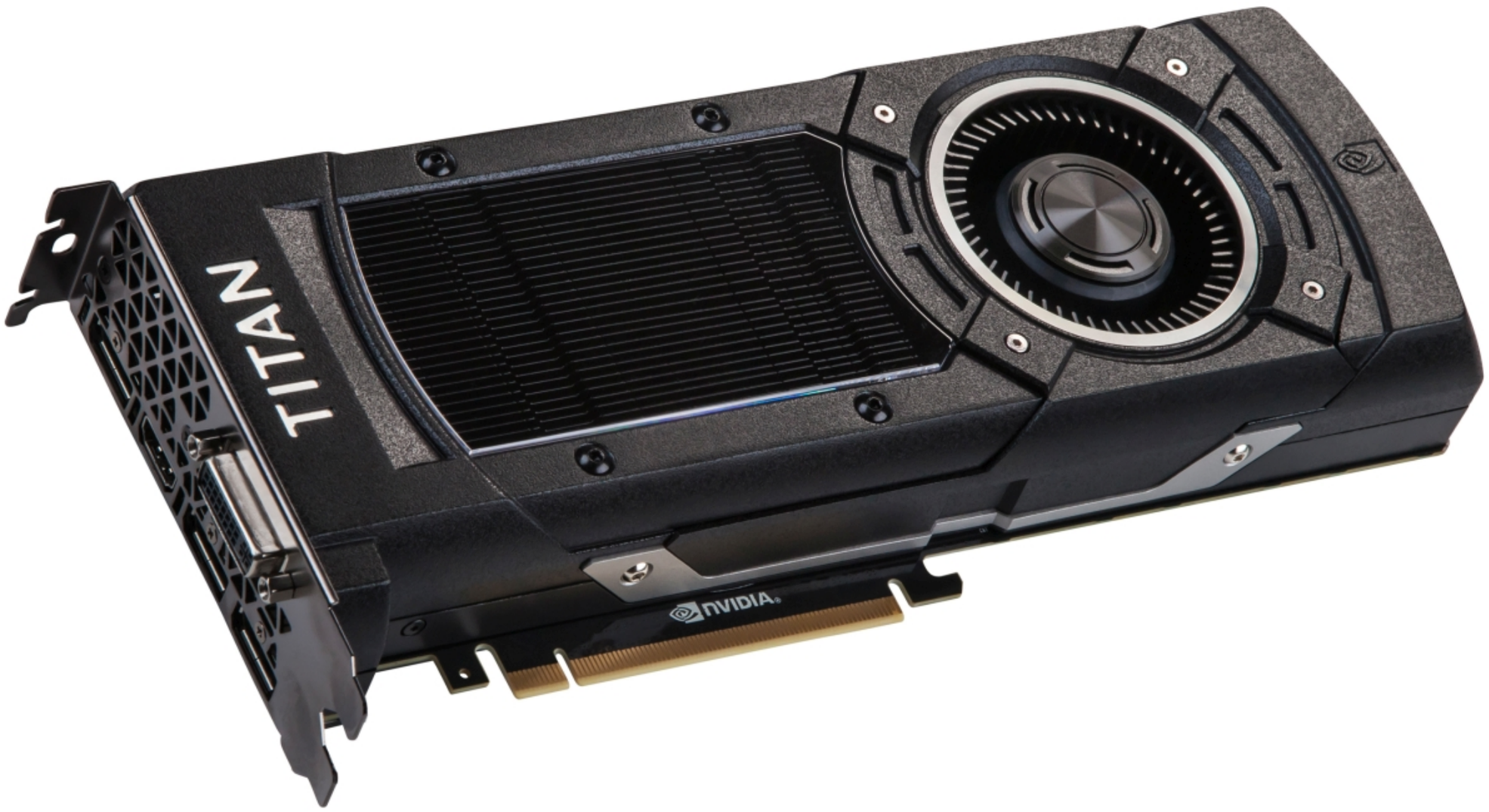
More on MPI

- There is a wealth of resources about MPI and the subject is too vast for one lecture
- Just be aware that you ca use it from Python with mpi4py
- For more information about MPI in general check:

  http://mpitutorial.com/

- And for mpi4py in particular check the documentation at:

  https://mpi4py.readthedocs.io/en/stable/index.html

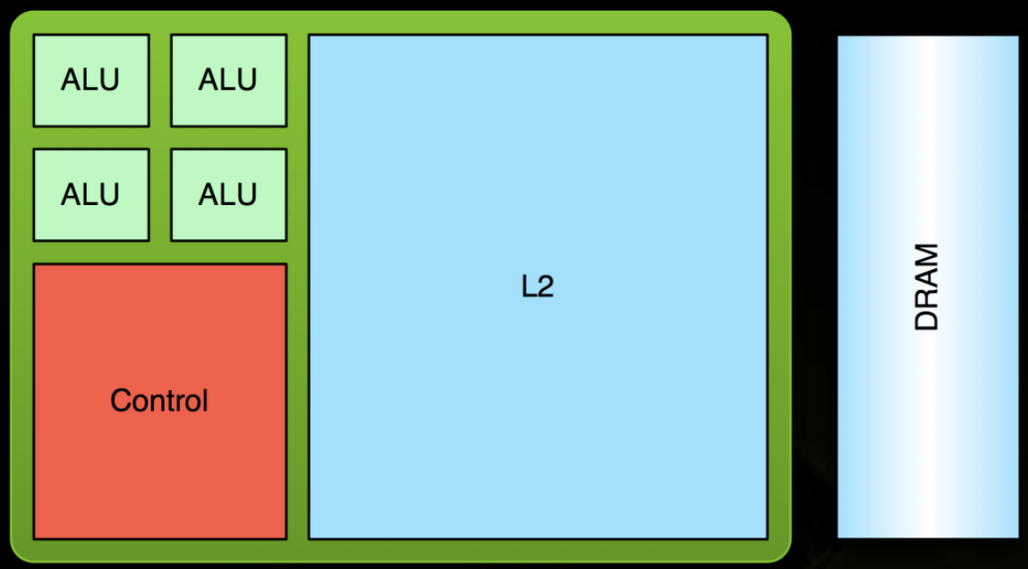


Adapted from:
http://www.cc.gatech.edu/~vetter/keeneland/tutorial-2011-04-14/02-cuda-overview.pdf
https://documen.tician.de/pycuda/tutorial.html

GPU Acceleration

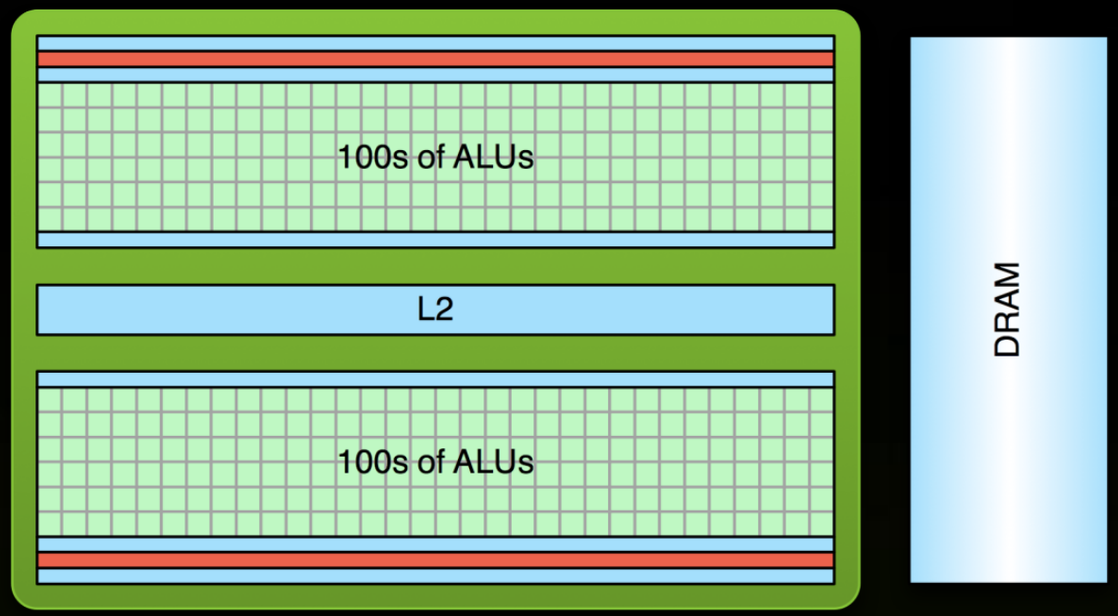
- Another way to obtain large gains in performance is to use GPUs to carry out a large fraction of the calculations
- GPUs have enormous computing power. For example an NVIDIA RTX 2090 is capable of 36 TFLOPS in single precision for $1500.
- For comparison an AMD Epic 7742 (a top of the line $5000 CPU) reaches only 3.4 TFLOPS
- The two main languages to program GPUs are OpenCL and CUDA
- You can use them from Python using the packages `PyCuda` and `PyOpenCL`, but this requires knowledge CUDA and OpenCL respectively.
- Another way to take advantage of them is to use libraries to do their computations in GPUs.
- An example is `arrayfire-python` which provides a range of numerical algorithms.

Low Latency or High Throughput?



CPU

- Optimized for low-latency access to cached data sets
- Control logic for out-of-order and speculative execution

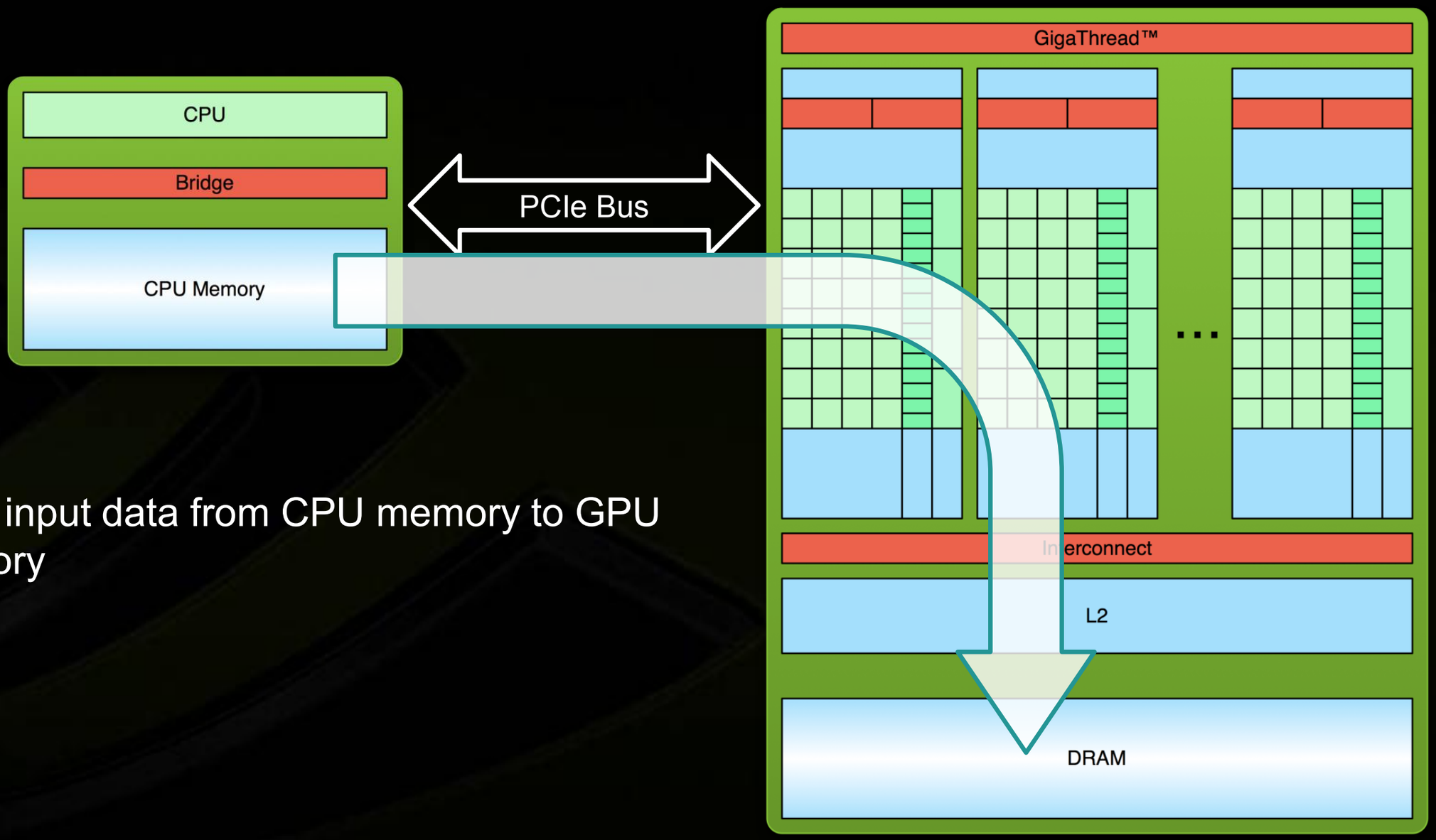


GPU

- Optimized for data-parallel, throughput computation
- Architecture tolerant of memory latency
- More transistors dedicated to computation

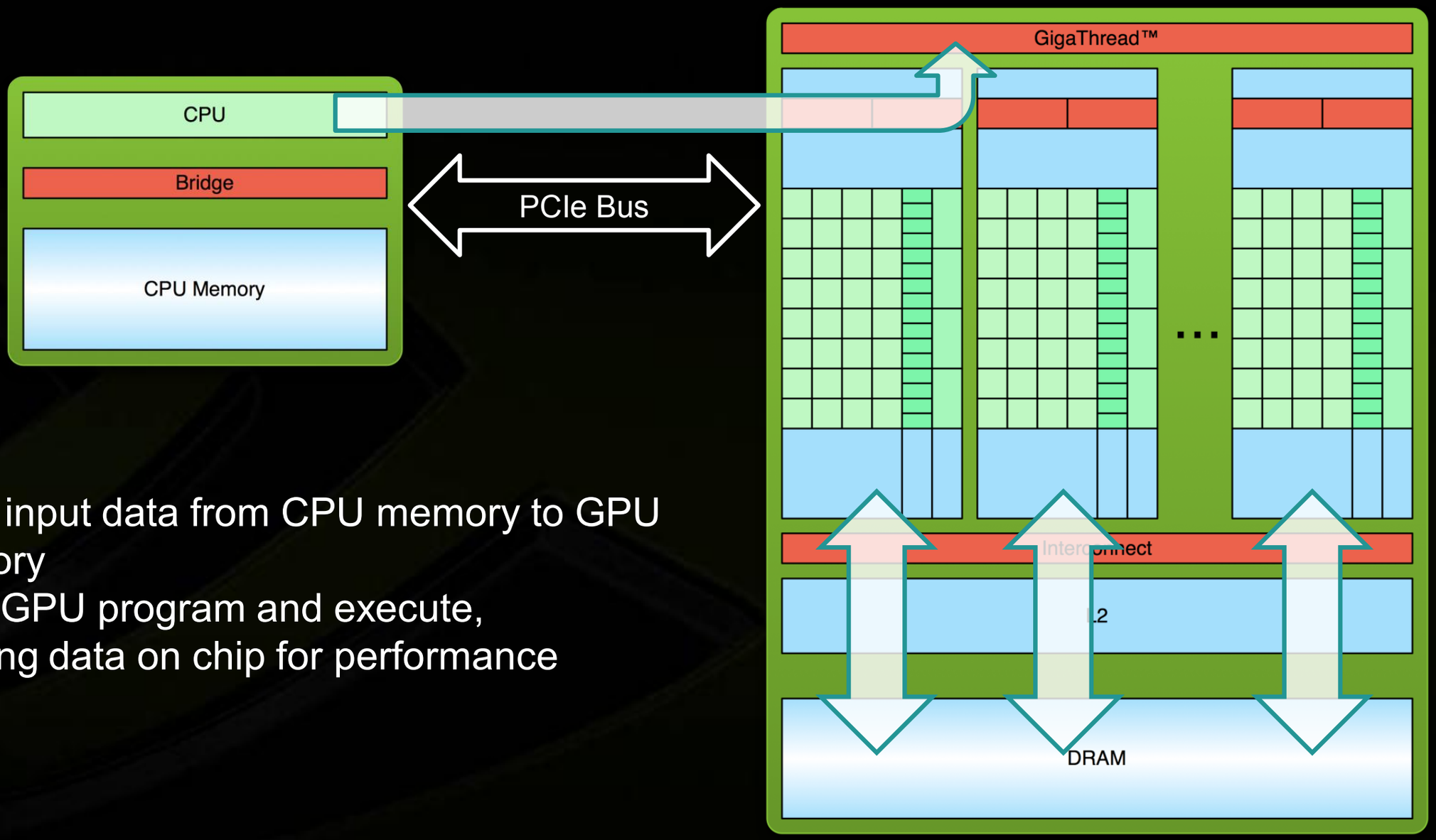
GPU Acceleration

Processing Flow



1. Copy input data from CPU memory to GPU memory

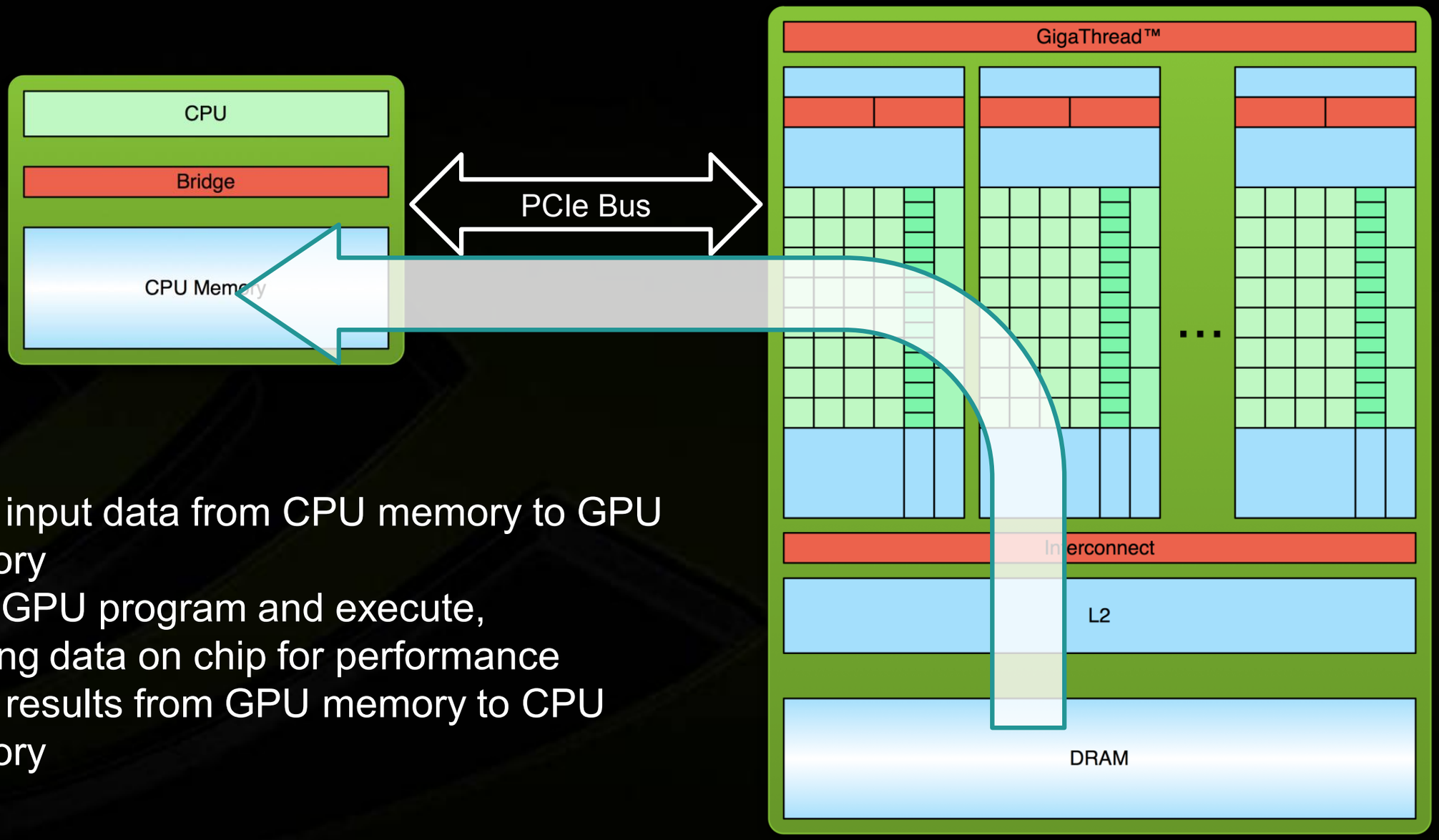
Processing Flow



1. Copy input data from CPU memory to GPU memory
2. Load GPU program and execute, caching data on chip for performance

GPU Acceleration

Processing Flow



1. Copy input data from CPU memory to GPU memory
2. Load GPU program and execute, caching data on chip for performance
3. Copy results from GPU memory to CPU memory

PyCUDA example

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

import numpy
# Let's make a 4x4 array of random numbers
a = numpy.random.randn(4,4)

# But wait, a consists of double precision numbers,
# but most nVidia devices only support single precision:
a = a.astype(numpy.float32)

# Finally, we need somewhere to transfer data to,
# so we need to allocate memory on the device
a_gpu = cuda.mem_alloc(a.nbytes)

# As a last step, we need to transfer the data to the GPU:
cuda.memcpy_htod(a_gpu, a)

# Kernel to double each entry in an array
# which is compiled by SourceModule
mod = SourceModule("""
  __global__ void doublify(float *a)
  {
    int idx = threadIdx.x + threadIdx.y*4;
    a[idx] *= 2;
  }
  """)
```

PyCUDA example

```
# Grab the compiled function
func = mod.get_function("doublify")

# Execute the function on the GPU
# Using one block with 4x4 threads
func(a_gpu, block=(4,4,1))

# Finally, we fetch the data back from the GPU and
# display it, together with the original a

a_doubled = numpy.empty_like(a)
cuda.memcpy_dtoh(a_doubled, a_gpu)
print(a_doubled)
print(a)
```

```
[[ 0.51360393  1.40589952  2.25009012  3.02563429]
 [-0.75841576 -1.18757617  2.72269917  3.12156057]
 [ 0.28826082 -2.92448163  1.21624792  2.86353827]
 [ 1.57651746  0.63500965  2.21570683 -0.44537592]]
[[ 0.25680196  0.70294976  1.12504506  1.51281714]
 [-0.37920788 -0.59378809  1.36134958  1.56078029]
 [ 0.14413041 -1.46224082  0.60812396  1.43176913]
 [ 0.78825873  0.31750482  1.10785341 -0.22268796]]
```

PyCUDA example

- Now lets do it the easy way!
- PyCUDA has some support for NumPy arrays so you don't need to write kernels for many things!

```
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).astype(numpy.float32))
a_doubled = (2*a_gpu).get()
print a_doubled
print a_gpu
```

- For more information check the **pycuda.gpuarray.GPUArray** class

ArrayFire

- ArrayFire is a general-purpose library that simplifies the process of developing software that targets parallel and massively-parallel architectures including CPUs, GPUs, and other hardware acceleration devices.
- Developers write code which performs operations on ArrayFire arrays which, in turn, are automatically translated into near-optimal kernels that execute on the computational device.
- ArrayFire runs on CPUs from all major vendors (Intel, AMD, ARM), GPUs from the prominent manufacturers (NVIDIA, AMD, and Qualcomm), as well as a variety of other accelerator devices on Windows, Mac, and Linux.
- And **most importantly** it's Open Source and available on GitHub!
  https://github.com/arrayfire/arrayfire

GitHub

arrayfire-python example

Arrayfire pi.py

```
import arrayfire as af

# Monte Carlo estimation of pi
def calc_pi_device(samples):
    x = af.randu(samples)
    y = af.randu(samples)
    within_unit_circle = (x * x + y * y) < 1
    return 4 * af.count(within_unit_circle) / samples
```

NumPy np_pi.py

```
import numpy as np

# Monte Carlo estimation of pi
def calc_pi_device(samples):
    x = np.random.random(size=samples)
    y = np.random.random(size=samples)
    within_unit_circle = (x * x + y * y) < 1.0
    return 4.0 * sum(within_unit_circle) / samples
```

```
In [7]: %timeit np_pi.calc_pi_device(100000)
10 loops, best of 3: 90.2 ms per loop

In [8]: %timeit pi.calc_pi_device(100000)
The slowest run took 80.80 times longer than the fastest. This could mean that an
intermediate result is being cached.
1000 loops, best of 3: 859 µs per loop
```

CuPy

- ArrayFire is very useful but has one important downside: **it's API is very different from NumPy!**
- NVIDIA aimed to address this problem by supporting the development of **CuPy**, a NumPy-compatible array library accelerated by CUDA.
- Like Arrayfire this library is also Open Source (https://github.com/cupy/cupy) but unlike Arrayfire, **only supports CUDA**.

CuPy cupy_pi.py

```
import cupy as np

# Monte Carlo estimation of pi
def calc_pi_device(samples):
    x = np.random.random(size=samples)
    y = np.random.random(size=samples)
    within_unit_circle = (x * x + y * y) < 1.0
    return 4.0 * np.sum(within_unit_circle) / samples
```

```
In [11]: %timeit cupy_pi.calc_pi_device(100000)
323 µs ± 20.8 µs per loop (mean ± std. dev. of 7 runs, 1000 loops each)
```

For what kind of tasks are GPUs better suited than CPUs? What about MPI?

pytest

Adapted from:
https://jacobian.org/writing/getting-started-with-pytest/

Testing

- Testing is crucial to high quality software!
- It's important to make testing as automated as possible to make sure it's done!
- Python as several packages that provide **test frameworks**: `unittest`, `nose/nose2`, `py.test`
- There are also services that automatically build your code and run tests every time you `push` your code.
- A few of these **Continuous Integration** services are Travis CI (travis-ci.org), GitLab (gitlab.com), CircleCI (circleci.com) and CodeShip (codeship.com) as well as GitHub through GitHub Actions.
- In this course we'll focus on `py.test` and **Travis CI**.

py.test in action

```python
# fib.py
def fib(n):
    """Return the first Fibonacci number above n."""
    a = 0
    b = 1
    while b < n:
        a, b = b, a + b
    return b
```

- Lets test our code above. The file with the tests should start with `test_`:

```python
# test_fib.py
import fib

# the name of the testing function should
# also start with test_
def test_fib():
    assert fib(0) == 1
```

- Now to run the test we simply do:

```
$ py.test
```

py.test in action

```
$ py.test
============================= test session starts ==============================
platform darwin -- Python 3.5.1, pytest-2.9.0, py-1.4.31, pluggy-0.3.1
rootdir: /Users/filipe/Documents/Teaching/Advanced Scientific Programming with Python/
python-course/day4-bestpractices-2/code/pytest, inifile:
collected 1 items

test_fib.py F

=================================== FAILURES ===================================
_____________________________________ test_fib _____________________________________

    def test_fib():
>       assert fib(0) == 1
E       TypeError: 'module' object is not callable

test_fib.py:4: TypeError
=========================== 1 failed in 0.01 seconds ===========================
```

As you can see you can also have bugs in your tests!

py.test in action

- And after fixing the silly error:

```
$ py.test
============================= test session starts ==============================
platform darwin -- Python 3.5.1, pytest-2.9.0, py-1.4.31, pluggy-0.3.1
rootdir: /Users/filipe/Documents/Teaching/Advanced Scientific Programming with Python/
python-course/day4-bestpractices-2/code/pytest, inifile:
collected 1 items

test_fib.py .

=========================== 1 passed in 0.01 seconds ===========================
```

- This is the most important feature of **`py.test`**, but it can do much more!
- Check pytest.org and py.test --help for more information.
- Lets do a slightly more advanced example now…

py.test in action

- Multiple test parameters with one function:

```
# test_fib_params.py
import fib
import pytest

# Fibonacci Sequence
# 0, 1, 1, 2, 3, 5, 8, 13, 21, 34, ...
@pytest.mark.parametrize("n, expected", [
    (0, 1),
    (1, 2),
    (3, 5)
])
def test_fib_parametrized(n, expected):
    assert fib.fib(n) == expected
```

- Lets try this again:

```
$ py.test
```

py.test in action

```
$ py.test
============================= test session starts ==============================
platform darwin -- Python 3.5.1, pytest-2.9.0, py-1.4.31, pluggy-0.3.1
rootdir: /Users/filipe/Documents/Teaching/Advanced Scientific Programming with Python/python-
course/day4-bestpractices-2/code/pytest, inifile:
collected 4 items

test_fib.py .
test_fib_params.py .FF

=================================== FAILURES ===================================
_____________________________ test_fib_parametrized[1-2] _____________________________

n = 1, expected = 2

    @pytest.mark.parametrize("n, expected", [
        (0, 1),
        (1, 2),
        (3, 5)
    ])
    def test_fib_parametrized(n, expected):
>       assert fib.fib(n) == expected
E       assert 1 == 2
E        +  where 1 = <function fib at 0x107876840>(1)
E        +    where <function fib at 0x107876840> = fib.fib

test_fib_params.py:11: AssertionError
```

py.test in action

```
_____________________________ test_fib_parametrized[3-5] ______________________________

n = 3, expected = 5

    @pytest.mark.parametrize("n, expected", [
        (0, 1),
        (1, 2),
        (3, 5)
    ])
    def test_fib_parametrized(n, expected):
>       assert fib.fib(n) == expected
E       assert 3 == 5
E        +  where 3 = <function fib at 0x107876840>(3)
E        +    where <function fib at 0x107876840> = fib.fib

test_fib_params.py:11: AssertionError
====================== 2 failed, 2 passed in 0.02 seconds ======================
```

Conclusion: Our “simple” function does not do what it claims!

What does it really do...?