# The PyCUDA Module

Will Landau
Prof. Jarad Niemi

October 7, 2012

# Outline

# hello_gpu.py I

```
import pycuda.autoinit
import pycuda.driver as drv
import numpy

from pycuda.compiler import SourceModule
mod = SourceModule("""
__global__ void multiply_them(float *dest, float *a,
    float *b)
{
  const int i = threadIdx.x;
  dest[i] = a[i] * b[i];
}
""")

multiply_them = mod.get_function("multiply_them")

a = numpy.random.randn(400).astype(numpy.float32)
b = numpy.random.randn(400).astype(numpy.float32)

dest = numpy.zeros_like(a)
multiply_them(
        drv.Out(dest), drv.In(a), drv.In(b),
```

# hello_gpu.py II

```
        block=(400,1,1), grid=(1,1))

print dest-a*b
```

# demo.py

Import and initialize PyCUDA:

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

Initial data: a $4 \times 4$ array of numbers:

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

Apparently, most NVIDIA cards only support single precision:

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

# demo.py

Allocate device memory:

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

Send data to the device:

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

Define a kernel to multiply each array entry by 2:

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

# demo.py

Turn our CUDA C kernel into a callable Python function:

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

Call the kernel with:

- 1 grid
- 1 block
- 4 threads in the x direction
- 4 threads in the y direction
- 1 thread in the z direction

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

# demo.py

Make a NumPy array to store the results:

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

Copy the results to the host:

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

Print arrays:

```
print a_doubled
print a
```

# Example output

```
[landau@impact1 PyCUDA_sandbox]$ python demo.py
[[-1.29063177  0.82264316  0.02254304  2.0740006 ]
 [ 1.40431428  1.95245779 -1.84627843 -1.5800966 ]
 [-2.77298713  0.99803442  1.85154581  0.63633269]
 [ 0.55860651 -0.50091052 -1.465307    4.12601614]]
[[-0.64531589  0.41132158  0.01127152  1.0370003 ]
 [ 0.70215714  0.97622889 -0.92313921 -0.7900483 ]
 [-1.38649356  0.49901721  0.92577291  0.31816635]
 [ 0.27930325 -0.25045526 -0.7326535   2.06300807]]
```

# Simplifying memory transfer

There are three function argument handlers that take care of memory transfer for the user:

- `pycuda.driver.In`
- `pycuda.driver.Out`
- `pycuda.driver.InOut`

# demohandler.py I

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

import numpy

a = numpy.random.randn(4,4)
a = a.astype(numpy.float32)
print "Original array:"
print a

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

func = mod.get_function("doublify")
func(cuda.InOut(a), block=(4, 4, 1))
```

# demohandler.py II

```
print "Doubled array:"
print a
```

# Example output

```
[landau@impact1 PyCUDA_sandbox]$ python demohandler.py
Original array:
[[-0.35754886 -0.08118289  1.42489266  0.6799224 ]
 [ 0.54355925 -2.00721192 -0.6814152  -0.88118494]
 [ 1.29756403  1.37618589  0.78046876 -0.93179333]
 [-0.96092844  0.5301944  -0.36968505  1.54017532]]
Doubled array:
[[-0.71509773 -0.16236578  2.84978533  1.3598448 ]
 [ 1.08711851 -4.01442385 -1.3628304  -1.76236987]
 [ 2.59512806  2.75237179  1.56093752 -1.86358666]
 [-1.92185688  1.0603888  -0.73937011  3.08035064]]
[landau@impact1 PyCUDA_sandbox]$
```

# demoshort.py

Use a `pycuda.gpuarray.GPUArray` to shorten the code even more:

```
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
```

The output is analogous.

# Outline

# functiontemplates.py I

Let's try something a little more complicated:

```
import pycuda.gpuarray as gpuarray
import pycuda.driver as drv
import pycuda.autoinit
import numpy as np

from pycuda.compiler import SourceModule
func_mod = SourceModule("""
template <class T>
__device__ T incr(T x) {
    return (x + 1.0);
}

// Needed to avoid name mangling so that PyCUDA can
// find the kernel function:
extern "C" {
    __global__ void func(float *a, int N)
    {
        int idx = threadIdx.x;
        if (idx < N)
            a[idx] = incr(a[idx]);
    }
```

# functiontemplates.py II

```
}
""", no_extern_c=1)

func = func_mod.get_function('func')

N = 5
x = np.asarray(np.random.rand(N), np.float32)
x_orig = x.copy()
x_gpu = gpuarray.to_gpu(x)

func(x_gpu.gpudata, np.uint32(N), block=(N, 1, 1))
print 'x:         ', x
print 'incr(x): ', x_gpu.get()
```

# Example output:

```
[landau@impact1 PyCUDA_sandbox]$ python
    functiontemplates.py
x:          [ 0.79577702  0.73002166  0.19413722
    0.30437419  0.24752268]
incr(x):    [ 1.79577708  1.73002172  1.19413722
    1.30437422  1.24752271]
[landau@impact1 PyCUDA_sandbox]$
```

# pycurand.py

We can use CURAND with PyCUDA:

```
import pycuda.gpuarray as gpuarray
import pycuda.autoinit
import numpy
from pycuda.curandom import rand as curand

a_gpu = curand((50,))
b_gpu = curand((50,))

from pycuda.elementwise import ElementwiseKernel
lin_comb = ElementwiseKernel(
        "float a, float *x, float b, float *y, float *
            z",
        "z[i] = a*x[i] + b*y[i]",
        "linear_combination")

c_gpu = gpuarray.empty_like(a_gpu)
lin_comb(5, a_gpu, 6, b_gpu, c_gpu)

import numpy.linalg as la
assert la.norm((c_gpu - (5*a_gpu+6*b_gpu)).get()) < 1e
    -5
```

# DumpProperties.py

PyCUDA can extract hardware information:

```
import pycuda.driver as drv

drv.init()
print "%d device(s) found." % drv.Device.count()

for ordinal in range(drv.Device.count()):
    dev = drv.Device(ordinal)
    print "Device #%d: %s" % (ordinal, dev.name())
    print "  Compute Capability: %d.%d" % dev.
        compute_capability()
    print "  Total Memory: %s KB" % (dev.total_memory
        ()//(1024))
    atts = [(str(att), value)
            for att, value in dev.get_attributes().
                iteritems()]
    atts.sort()

    for att, value in atts:
        print "  %s: %s" % (att, value)
```

# MatmulSimple.py I

```
#!/usr/bin/env python
# -*- coding: utf-8 -*-

"""
Multiples two square matrices together using a *single
    * block of threads and
global memory only. Each thread computes one element
    of the resulting matrix.
"""

import numpy as np
from pycuda import driver, compiler, gpuarray, tools

# -- initialize the device
import pycuda.autoinit

kernel_code_template = """
__global__ void MatrixMulKernel(float *a, float *b,
    float *c)
{
    // 2D Thread ID (assuming that only *one* block
        will be executed)
```

# MatmulSimple.py II

```
    int tx = threadIdx.x;
    int ty = threadIdx.y;

    // Pvalue is used to store the element of the
        matrix
    // that is computed by the thread
    float Pvalue = 0;

    // Each thread loads one row of M and one column
        of N,
    //   to produce one element of P.
    for (int k = 0; k < %(MATRIX_SIZE)s; ++k) {
        float Aelement = a[ty * %(MATRIX_SIZE)s + k];
        float Belement = b[k * %(MATRIX_SIZE)s + tx];
        Pvalue += Aelement * Belement;
    }

    // Write the matrix to device memory;
    // each thread writes one element
    c[ty * %(MATRIX_SIZE)s + tx] = Pvalue;
}
"""
```

# MatmulSimple.py III

```
# define the (square) matrix size
#  note that we'll only use *one* block of threads
     here
#  as a consequence this number (squared) can't exceed
      max_threads,
#  see http://documen.tician.de/pycuda/util.html#
     pycuda.tools.DeviceData
#  for more information on how to get this number for
     your device
MATRIX_SIZE = 2

# create two random square matrices
a_cpu = np.random.randn(MATRIX_SIZE, MATRIX_SIZE).
     astype(np.float32)
b_cpu = np.random.randn(MATRIX_SIZE, MATRIX_SIZE).
     astype(np.float32)

# compute reference on the CPU to verify GPU
     computation
c_cpu = np.dot(a_cpu, b_cpu)

# transfer host (CPU) memory to device (GPU) memory
a_gpu = gpuarray.to_gpu(a_cpu)
```

# MatmulSimple.py IV

```
b_gpu = gpuarray.to_gpu(b_cpu)

# create empty gpu array for the result (C = A * B)
c_gpu = gpuarray.empty((MATRIX_SIZE, MATRIX_SIZE), np.
    float32)

# get the kernel code from the template
# by specifying the constant MATRIX_SIZE
kernel_code = kernel_code_template % {
    'MATRIX_SIZE': MATRIX_SIZE
    }

# compile the kernel code
mod = compiler.SourceModule(kernel_code)

# get the kernel function from the compiled module
matrixmul = mod.get_function("MatrixMulKernel")

# call the kernel on the card
matrixmul(
    # inputs
    a_gpu, b_gpu,
    # output
```

# MatmulSimple.py V

```
    c_gpu,
    # (only one) block of MATRIX_SIZE x MATRIX_SIZE
        threads
    block = (MATRIX_SIZE, MATRIX_SIZE, 1),
    )

# print the results
print "-" * 80
print "Matrix A (GPU):"
print a_gpu.get()

print "-" * 80
print "Matrix B (GPU):"
print b_gpu.get()

print "-" * 80
print "Matrix C (GPU):"
print c_gpu.get()

print "-" * 80
print "CPU-GPU difference:"
print c_cpu - c_gpu.get()
```

# MatmulSimple.py VI

```
np.allclose(c_cpu, c_gpu.get())
```

# Example output:

```
[landau@impact1 PyCUDA_sandbox]$ python MatmulSimple.
    py
```

```
Matrix A (GPU):
[[ 0.46055064 -0.85658211]
 [ 0.57233274  2.47072577]]
```

```
Matrix B (GPU):
[[ 1.76631308  0.0654699 ]
 [-0.13310859  0.73874539]]
```

```
Matrix C (GPU):
[[ 0.92749506 -0.60264391]
 [ 0.68204403  1.86270785]]
```

```
CPU-GPU difference:
[[ 0.  0.]
 [ 0.  0.]]
[landau@impact1 PyCUDA_sandbox]$
```

# Measuring performance: I

```
#! /usr/bin/env python
import pycuda.autoinit
import pycuda.driver as drv
import pycuda.curandom as curandom
import numpy
import numpy.linalg as la
from pytools import Table



def main():
    import pycuda.gpuarray as gpuarray

    sizes = []
    times = []
    flops = []
    flopsCPU = []
    timesCPU = []

    for power in range(10, 25): # 24
        size = 1<<power
```

# Measuring performance: II

```
        print size
        sizes.append(size)
        a = gpuarray.zeros((size,), dtype=numpy.
            float32)

        if power > 20:
            count = 100
        else:
            count = 1000

        #start timer
        start = drv.Event()
        end = drv.Event()
        start.record()

        #cuda operation which fills the array with
            random numbers
        for i in range(count):
            curandom.rand((size, ))

        #stop timer
        end.record()
        end.synchronize()
```

# Measuring performance: III

```
        #calculate used time
        secs = start.time_till(end)*1e-3

        times.append(secs/count)
        flops.append(size)

        #cpu operations which fills teh array with
            random data
        a = numpy.array((size,), dtype=numpy.float32)

        #start timer
        start = drv.Event()
        end = drv.Event()
        start.record()

        #cpu operation which fills the array with
            random data
        for i in range(count):
            numpy.random.rand(size).astype(numpy.
                float32)

        #stop timer
```

# Measuring performance: IV

```
        end.record()
        end.synchronize()

        #calculate used time
        secs = start.time_till(end)*1e-3

        #add results to variable
        timesCPU.append(secs/count)
        flopsCPU.append(size)


    #calculate pseudo flops
    flops = [f/t for f, t in zip(flops,times)]
    flopsCPU = [f/t for f, t in zip(flopsCPU,timesCPU)
        ]

    #print the data out
    tbl = Table()
    tbl.add_row(("Size", "Time GPU", "Size/Time GPU",
        "Time CPU","Size/Time CPU","GPU vs CPU speedup
        "))
    for s, t, f,tCpu,fCpu in zip(sizes, times, flops,
        timesCPU,flopsCPU):
```

# Measuring performance: V

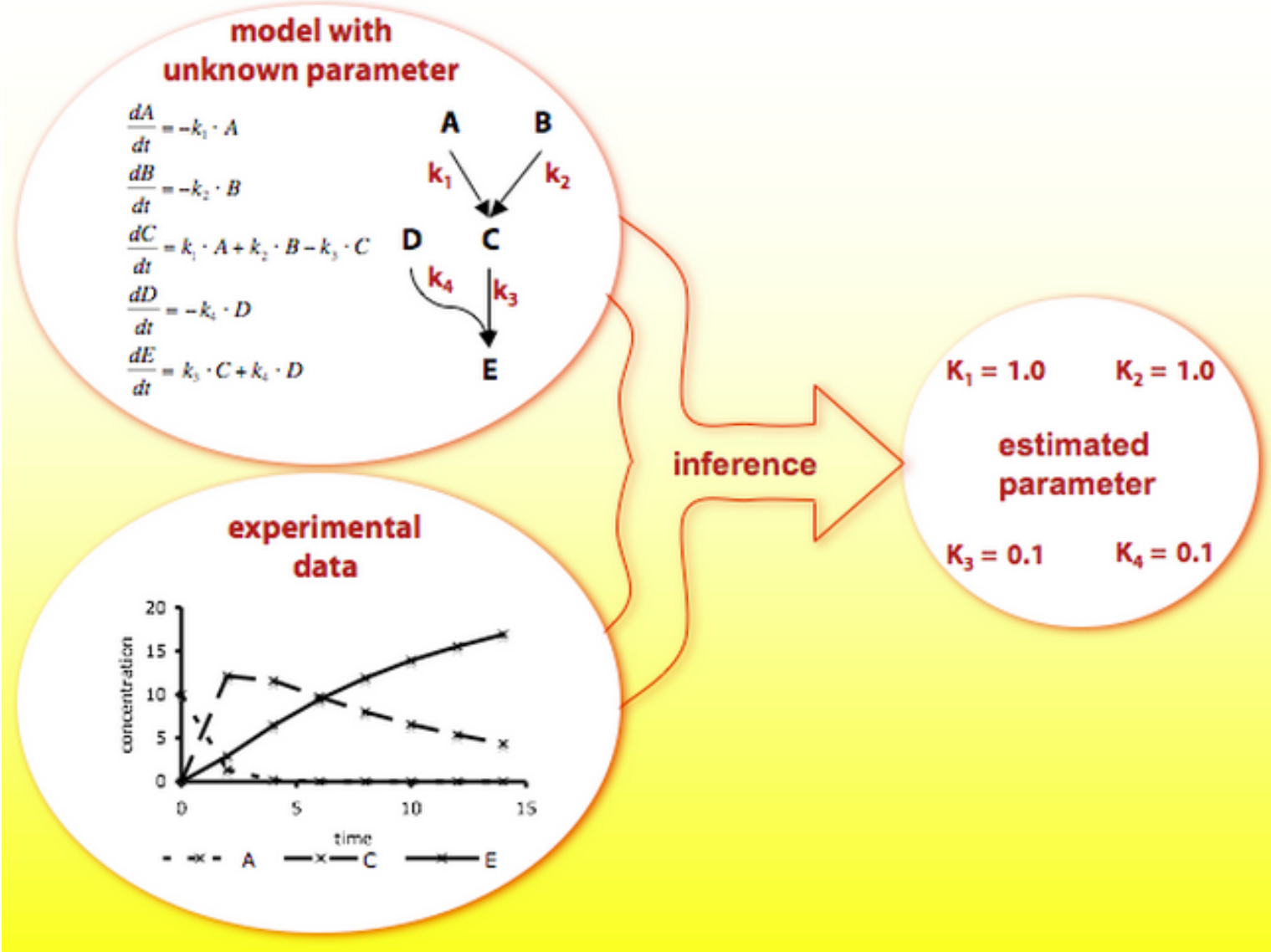
```
            tbl.add_row((s,t,f,tCpu,fCpu,f/fCpu))
        print tbl


if __name__ == "__main__":
        main()
```

# Outline

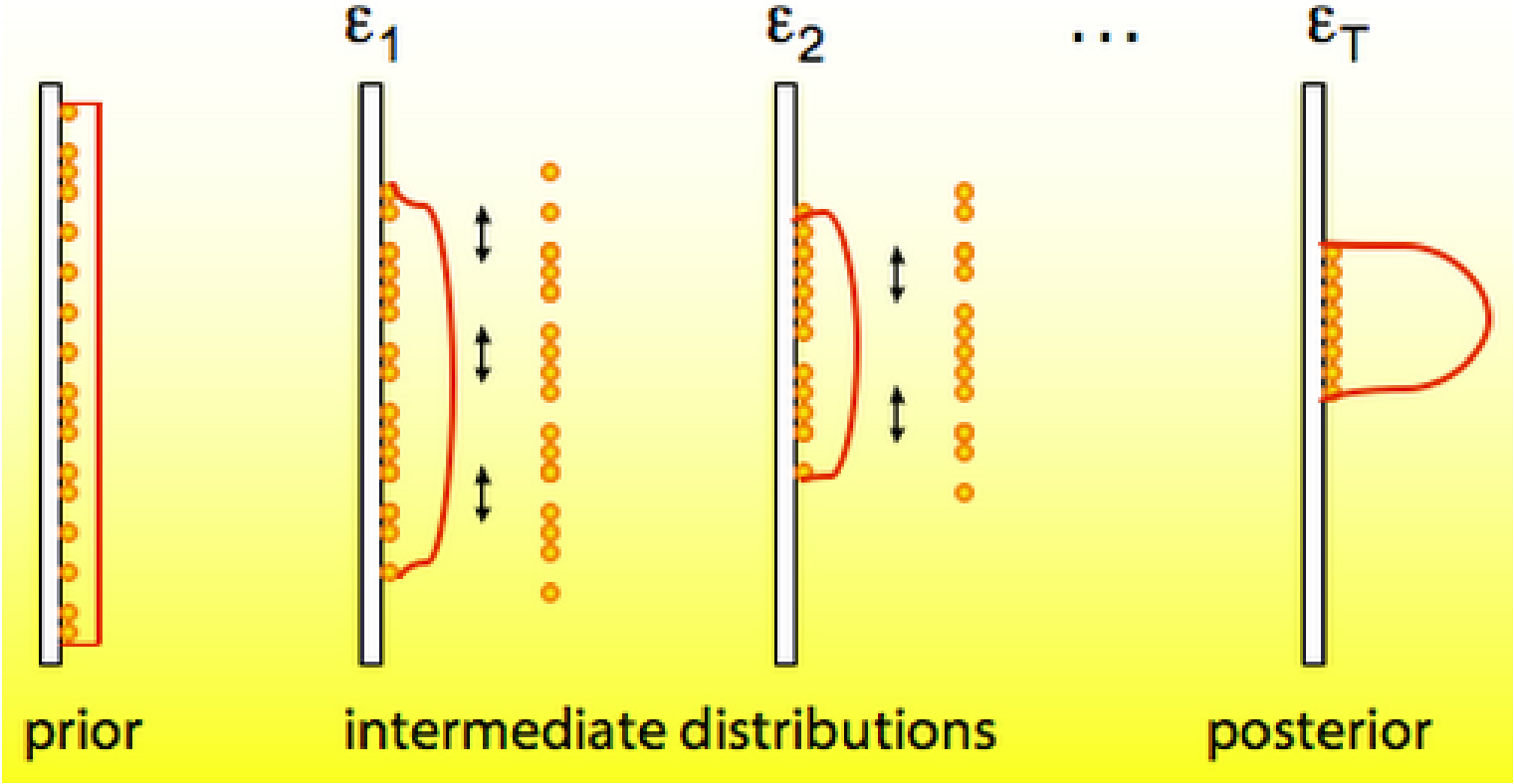
# ABC-SysBio: a PyCUDA-implemented toolkit

GPU-accelerated approximate Bayesian for parameter estimation in dynamical systems



Methods:

- ABC rejection sampler
- ABC SMC for parameter inference
- ABC SMC for model selection



- ABC-SysBio is ready to use on impact1.
  - `import abcsysbio` (Python script)
  - `abc-sysbio-sbml-sum` (command line)
  - `run-abc-sysbio` (command line)
- For more information, visit:
  - http://www.theosysbio.bio.ic.ac.uk/resources/abc-sysbio
  - http://bioinformatics.oxfordjournals.org/content/26/14/1797.full?keytype=ref&ijkey=AVSfAhR7XFxjrMj
- For the input files in the online examples, visit:
  - https://github.com/wlandau/gpu/tree/master/Code/Python/ABC-SysBio

# Sources



Kloeckner A.
Examples of pycuda usage.
http://wiki.tiker.net/PyCuda/Examples, May 2012.


Kloeckner A.
Pycuda 2012.1 documentation.
http://documen.tician.de/pycuda/index.html, June 2012.


C. Barnes, J. Liepe, E. Cule, S. Filippi, D. Rolando, S. McMahon, B. Lisowska, P. Kirk, K. Erguler, T. Toni, and M. Stumpf.
Abc-sysbio: A tool for parameter inference and model selection.
http://www.theosysbio.bio.ic.ac.uk/resources/abc-sysbio, 2011.


J. Liepe, C. Barnes, E. Cule, K. Erguler, P. Kirk, T. Toni, and M. Stumpf.
Abc-sysbio-approximate bayesian computation in python with gpu support.
*Bioinformatics*, 26(14):1797–1799, May 2010.