GPU Metaprogramming using PyCUDA: Methods & Applications

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- Nvidia Corporation

Outline

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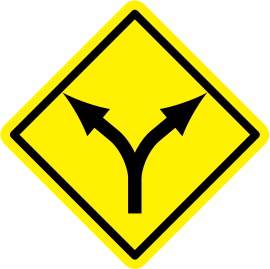
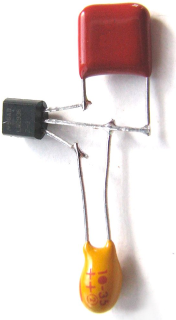
Outline

How are High-Performance Codes constructed?

- "Traditional" Construction of High-Performance Codes:
  - C/C++/Fortran
  - Libraries
- "Alternative" Construction of High-Performance Codes:
  - Scripting for 'brains'
  - GPUs for 'inner loops'
- Play to the strengths of each programming environment.



Scripting: Means

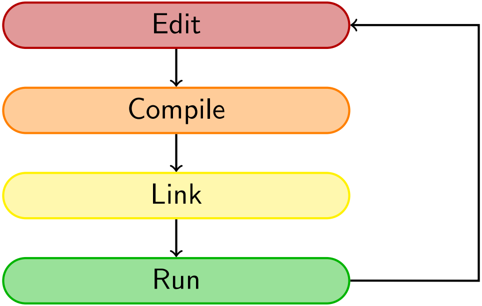


A scripting language...

- is discoverable and interactive.
- has comprehensive built-in functionality.
- manages resources automatically.
- is dynamically typed.
- works well for “gluing” lower-level blocks together.

Scripting: Interpreted, not Compiled

Program creation workflow:



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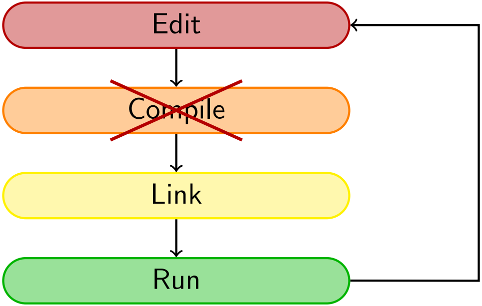

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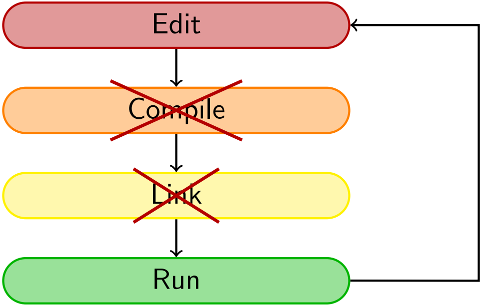

Scripting: Python

One example of a scripting language: Python

- Mature
- Large and active community
- Emphasizes readability
- Written in widely-portable C
- A ‘multi-paradigm’ language

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Why do Scripting for GPUs?

- GPUs are everything that scripting languages are not.
  - Highly parallel
  - Very architecture-sensitive
  - Built for maximum FP/memory throughput

$\rightarrow$ complement each other

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  - Scripting fast enough

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  $\rightarrow$ complement each other
- CPU: largely restricted to control tasks ($\sim$1000/sec)
  - Scripting fast enough
- Python + CUDA = **PyCUDA**

Outline

Whetting your appetite

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

a = numpy.random.randn(4,4).astype(numpy.float32)
a_gpu = cuda.mem_alloc(a.nbytes)
cuda.memcpy_htod(a_gpu, a)
```

[This is `examples/demo.py` in the PyCUDA distribution.]

Whetting your appetite

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

func = mod.get_function("twice")
func(a_gpu, block=(4,4,1))

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

Whetting your appetite

```
mod = cuda.SourceModule("""
    __global__ void twice(float *a)
    {
      int idx = threadIdx.x + threadIdx.y*4;
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```

Compute kernel

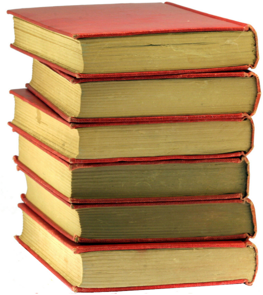
Whetting your appetite, Part II

Did somebody say "Abstraction is good"?

Whetting your appetite, Part II

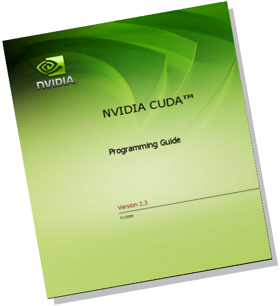
```
import numpy
import pycuda.autoinit
import pycuda.gpuarray as gpuarray

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
```

PyCUDA Philosophy



- Provide complete access
- Automatically manage resources
- Provide abstractions
- Allow interactive use
- Check for and report errors automatically
- Integrate tightly with `numpy`

PyCUDA: Completeness



PyCUDA exposes *all* of CUDA.

For example:

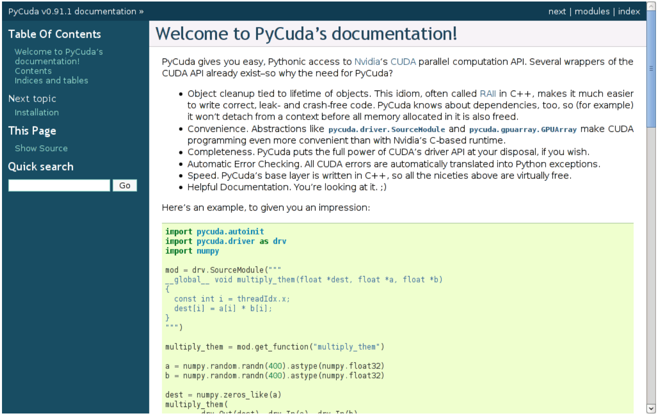
- Arrays and Textures
- Pagelocked host memory
- Memory transfers (asynchronous, structured)
- Streams and Events
- Device queries
- GL Interop

PyCUDA: Completeness

PyCUDA supports every OS that CUDA supports.

- Linux
- Windows
- OS X

PyCUDA: Documentation



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Welcome to PyCuda's documentation!

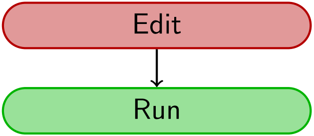
PyCuda gives you easy, Pythonic access to Nvidia's CUDA parallel computation API. Several wrappers of the CUDA API already exist–so why the need for PyCuda?

- Object cleanup tied to lifetime of objects. This idiom, often called RAII in C++, makes it much easier to write correct, leak- and crash-free code. PyCuda knows about dependencies, too, so (for example) it won't detach from a context before all memory allocated in it is also freed.
- Convenience. Abstractions like `pycuda.driver.SourceModule` and `pycuda.gpuarray.GPUArray` make CUDA programming even more convenient than with Nvidia's C-based runtime.
- Completeness. PyCuda puts the full power of CUDA's driver API at your disposal, if you wish.
- Automatic Error Checking. All CUDA errors are automatically translated into Python exceptions.
- Speed. PyCuda's base layer is written in C++, so all the niceties above are virtually free.
- Helpful Documentation. You're looking at it. ;)

Here's an example, to given you an impression:

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

mod = drv.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),
```

PyCUDA: Workflow



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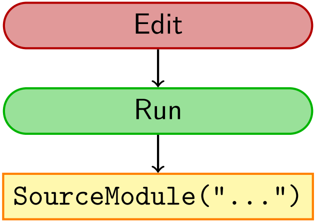

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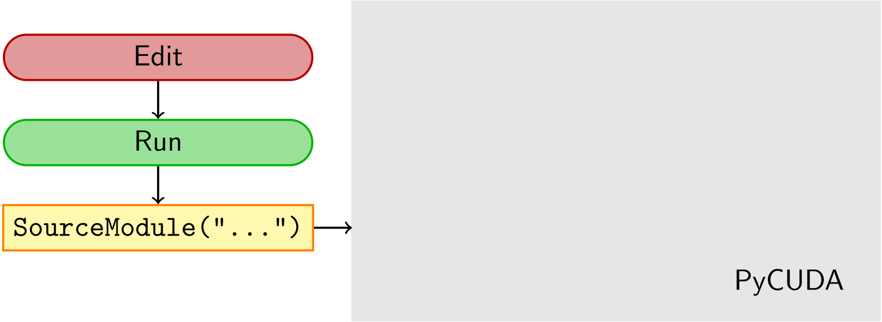

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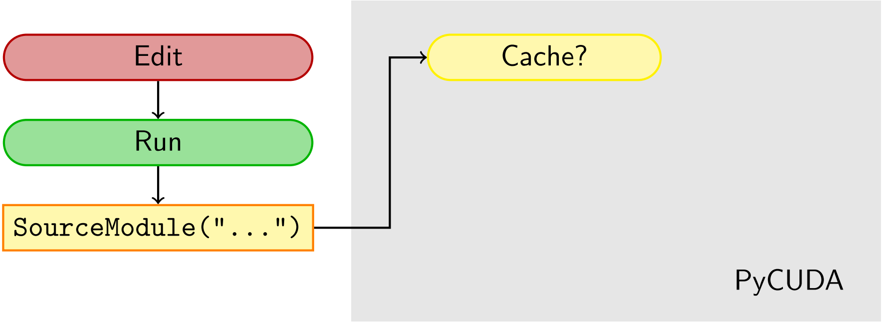

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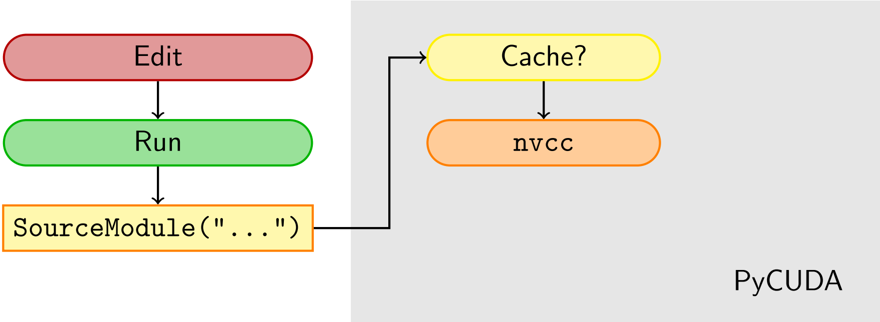

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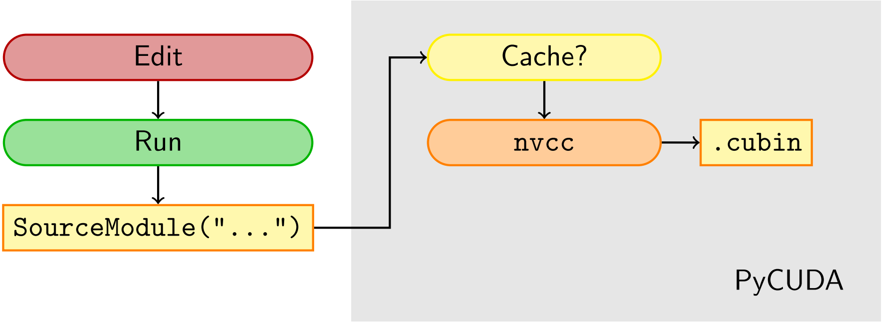

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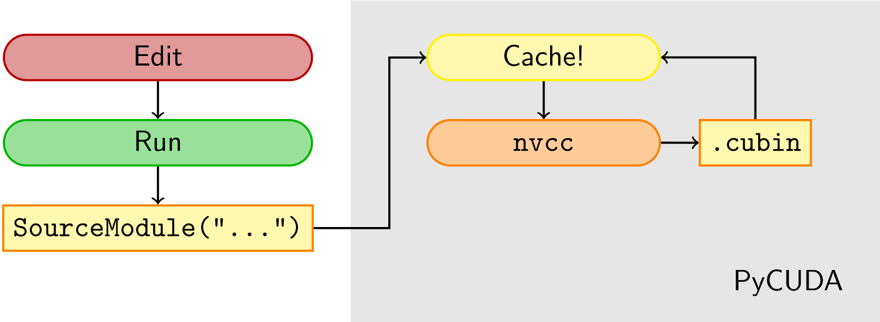

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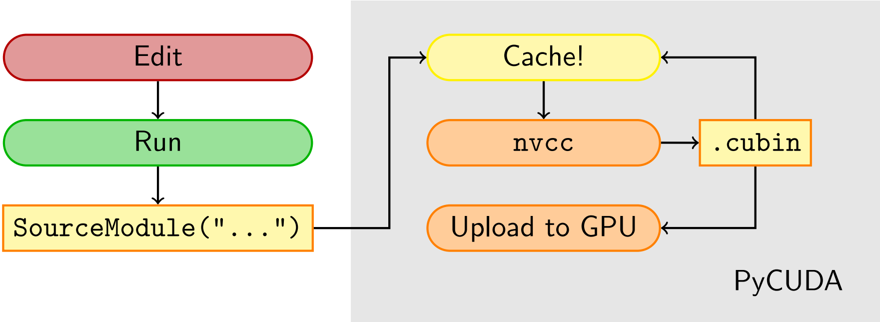

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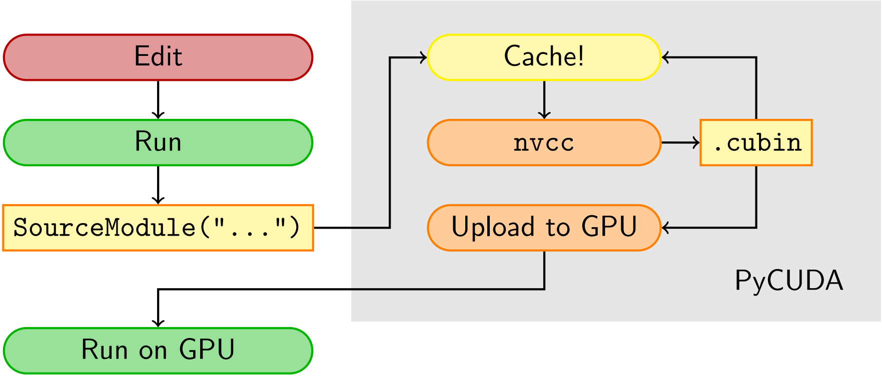
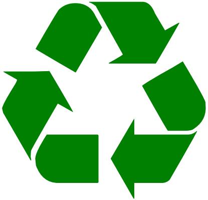


Automatic Cleanup

- Reachable objects (memory, streams, ...) are never destroyed.
- Once unreachable, released at an unspecified future time.
- Scarce resources (memory) can be explicitly freed. (`obj.free()`)
- Correctly deals with multiple contexts and dependencies.



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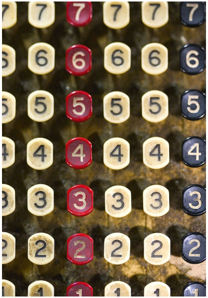
gpuarray: Simple Linear Algebra

pycuda.gpuarray:

- Meant to look and feel just like numpy.
  - gpuarray.to_gpu(numpy_array)
  - numpy_array = gpuarray.get()
- +, -, ∗, /, fill, sin, exp, rand, basic indexing, norm, inner product, . . .
- Mixed types (int32 + float32 = float64)
- print gpuarray for debugging.
- Allows access to raw bits
  - Use as kernel arguments, textures, etc.



gpuarray: Elementwise expressions

Avoiding extra store-fetch cycles for elementwise math:

```
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]")

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

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

gpuarray: Reduction made easy

Example: A scalar product calculation

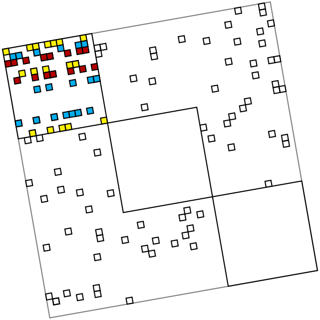
```
from pycuda.reduction import ReductionKernel
dot = ReductionKernel(dtype_out=numpy.float32, neutral="0",
        reduce_expr="a+b", map_expr="x[i]*y[i]",
        arguments="const float *x, const float *y")

from pycuda.curandom import rand as curand
x = curand((1000*1000), dtype=numpy.float32)
y = curand((1000*1000), dtype=numpy.float32)

x_dot_y = dot(x, y).get()
x_dot_y_cpu = numpy.dot(x.get(), y.get())
```

Sparse Matrix-Vector on the GPU

- In development version: Sparse matrix-vector multiplication
- Uses “packeted format” by Garland and Bell (also includes parts of their code)
- Integrates with `scipy.sparse`.
- Optimized conjugate-gradients solver included



PyCUDA: Vital Information

- `http://mathema.tician.de/software/pycuda`
- Complete documentation
- X Consortium License (no warranty, free for all use)
- Requires: numpy, Boost C++, Python 2.4+.
- Support via mailing list.

Outline

Metaprogramming

In GPU scripting,
GPU code does
not need to be
a compile-time
constant.

Metaprogramming

In GPU scripting, GPU code does *not* need to be a compile-time constant.

(Key: Code is data–it *wants* to be reasoned about at run time)

Metaprogramming

Idea

In GPU scripting,
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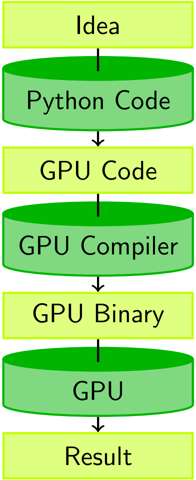
Metaprogramming



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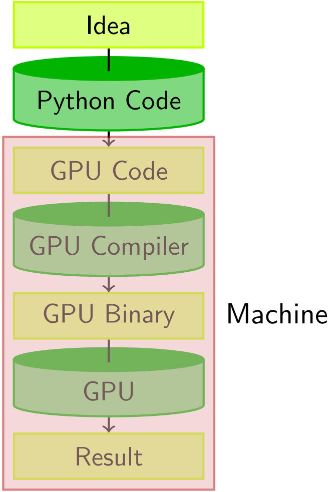
Metaprogramming



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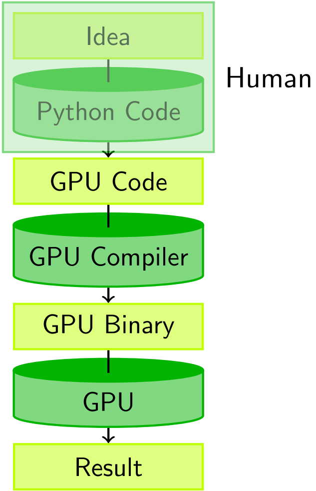

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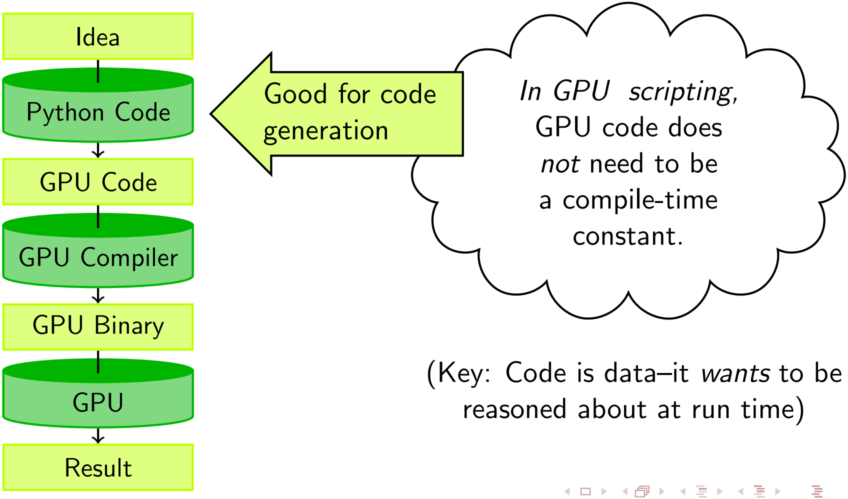

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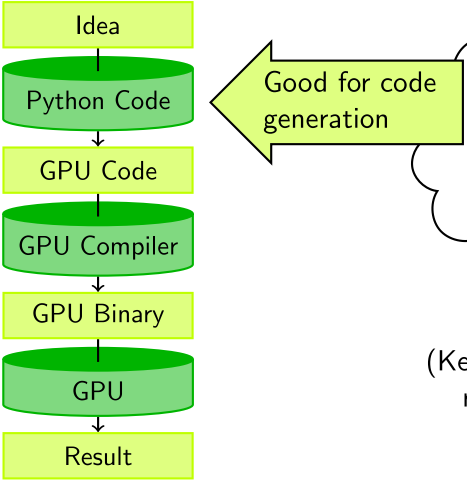
Metaprogramming



In PyCUDA
GPU code does *not* need to be a compile-time constant.

(Key: Code is data–it *wants* to be reasoned about at run time)

Machine-generated Code

Why machine-generate code?

- Automated Tuning
  (cf. ATLAS, FFTW)
- Data types
- Specialize code for given problem
- Constants faster than variables
  ($\rightarrow$ register pressure)
- Loop Unrolling

PyCUDA: Support for Metaprogramming

- Access properties of compiled code:
  `func.{num_regs,shared_size_bytes,local_size_bytes}`
- Exact GPU timing via events
- Can calculate hardware-dependent MP occupancy
- `codepy`:
  - Build C syntax trees from Python
  - Generates readable, indented C
- Or use a templating engine (many available)

RTCG via Templates

```
from jinja2 import Template
tpl = Template("""
    __global__ void twice({{ type_name }} *tgt)
    {
      int idx = threadIdx.x +
        {{ thread_block_size }} * {{block_size}}
        * blockIdx.x;

      {% for i in range( block_size ) %}
          {% set offset = i* thread_block_size %}
          tgt[idx + {{ offset }}] *= 2;
      {% endfor %}
    }""")

rendered_tpl = tpl.render(
    type_name="float", block_size=block_size,
    thread_block_size=thread_block_size)

smod = SourceModule(rendered_tpl)
```

RTCG via AST Generation

```
from codepy.cgen import *
from codepy.cgen.cuda import CudaGlobal

mod = Module([
    FunctionBody(
        CudaGlobal(FunctionDeclaration(
            Value("void", "twice"),
             arg_decls=[Pointer(POD(dtype, "tgt"))])),
        Block([
             Initializer(POD(numpy.int32, "idx"),
                "threadIdx.x + %d*blockIdx.x"
                % (thread_block_size * block_size)),
            ]+[
            Assign("tgt[idx+%d]" % (o*thread_block_size),
                "2*tgt[idx+%d]" % (o*thread_block_size))
            for o in range(block_size)])])])

smod = SourceModule(mod)
```

Outline

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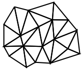
Discontinuous Galerkin Method

Let $\Omega := \bigcup_i D_k \subset \mathbb{R}^d$. 

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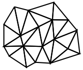
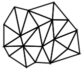
Let $\Omega := \bigcup_i D_k \subset \mathbb{R}^d$. 

Goal

Solve a *conservation law* on Ω: $u_t + \nabla \cdot F(u) = 0$

Discontinuous Galerkin Method

Let $\Omega := \bigcup_i \mathrm{D}_k \subset \mathbb{R}^d$. 

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Example

Maxwell's Equations: EM field: $E(x,t)$, $H(x,t)$ on Ω governed by

$$\partial_t E - \frac{1}{\varepsilon}\nabla \times H = -\frac{j}{\varepsilon}, \qquad \partial_t H + \frac{1}{\mu}\nabla \times E = 0,$$

$$\nabla \cdot E = \frac{\rho}{\varepsilon}, \qquad \nabla \cdot H = 0.$$

Discontinuous Galerkin Method

Multiply by test function, integrate by parts:

$$
\begin{aligned}
0 &= \int_{\mathrm{D}_k} u_t \varphi + [\nabla \cdot F(u)]\varphi \, \mathrm{d}x \\
&= \int_{\mathrm{D}_k} u_t \varphi - F(u) \cdot \nabla \varphi \, \mathrm{d}x + \int_{\partial \mathrm{D}_k} (\hat{n} \cdot F)^* \varphi \, \mathrm{d}S_x,
\end{aligned}
$$

Integrate by parts again, subsitute in basis functions, introduce elementwise differentiation and "lifting" matrices D, L:

$$
\partial_t u^k = -\sum_{\nu} D^{\partial_\nu, k}[F(u^k)] + L^k[\hat{n} \cdot F - (\hat{n} \cdot F)^*]|_{A \subset \partial \mathrm{D}_k}.
$$

For straight-sided simplicial elements:
Reduce D^{∂_ν} and L to reference matrices.

Metaprogramming for GPU-DG

- Specialize code for user-given problem:
  - Flux Terms

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Metaprogramming DG: Flux Terms

$$0 = \int_{\mathrm{D}_k} u_t \varphi + [\nabla \cdot F(u)]\varphi \,\mathrm{d}x - \underbrace{\int_{\partial \mathrm{D}_k} [\hat{n} \cdot F - (\hat{n} \cdot F)^*]\varphi \,\mathrm{d}S_x}_{\text{Flux term}}$$

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Flux terms:

- vary by problem
- expression specified by user
- evaluated pointwise

Metaprogramming DG: Flux Terms Example

Example: Fluxes for Maxwell's Equations

$$\hat{n} \cdot (F - F^*)_E := \frac{1}{2} [\hat{n} \times ([\![H]\!] - \alpha \hat{n} \times [\![E]\!])]$$

Metaprogramming DG: Flux Terms Example

Example: Fluxes for Maxwell's Equations

$$\hat{n} \cdot (F - F^*)_E := \frac{1}{2}\left[\hat{n} \times \left(\llbracket H \rrbracket - \alpha \hat{n} \times \llbracket E \rrbracket\right)\right]$$

User writes: Vectorial statement in math. notation

```
flux = 1/2*cross(normal, h.int-h.ext
        -alpha*cross(normal, e.int-e.ext))
```

Metaprogramming DG: Flux Terms Example

Example: Fluxes for Maxwell's Equations

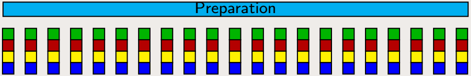
$$\hat{n} \cdot (F - F^*)_E := \frac{1}{2} [\hat{n} \times ([\![H]\!] - \alpha \hat{n} \times [\![E]\!])]$$

We generate: Scalar evaluator in C ($6\times$)

```
a_flux += (
    ((( val_a_field5 - val_b_field5 )* fpair->normal[2]
      - ( val_a_field4 - val_b_field4 )* fpair->normal[0])
     + val_a_field0 - val_b_field0 )* fpair->normal[0]
    - ((( val_a_field4 - val_b_field4 ) * fpair->normal[1]
        - ( val_a_field1 - val_b_field1 )* fpair->normal[2])
      + val_a_field3 - val_b_field3 ) * fpair->normal[1]
    )*value_type (0.5);
```

Loop Slicing on the GPU: A Pattern

Setting: N independent work units + preparation



Question: How should one assign work units to threads?

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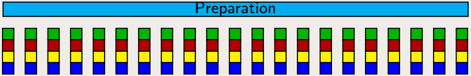

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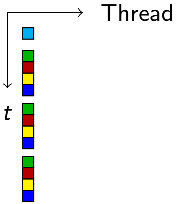
w_s: in sequence



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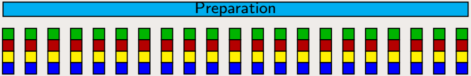

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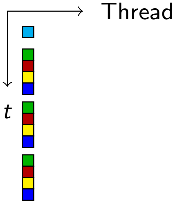
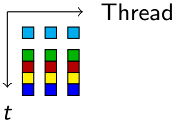


w_p: in parallel



Loop Slicing on the GPU: A Pattern

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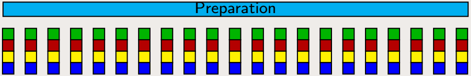

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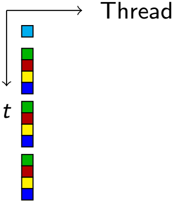
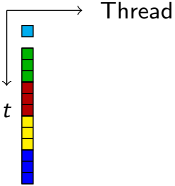
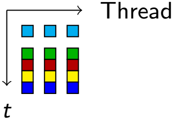


w_i: "inline-parallel"



w_p: in parallel



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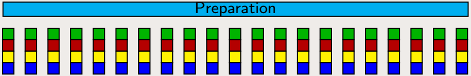

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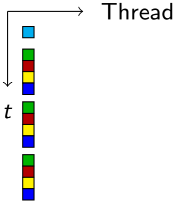

(amortize preparation)

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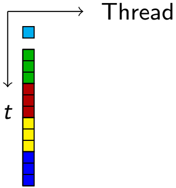
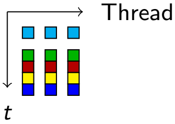


w_p: in parallel



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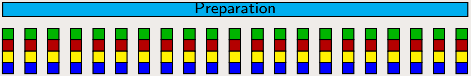

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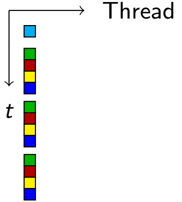
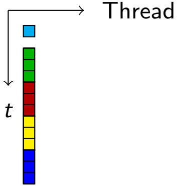


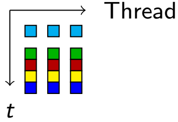
(amortize preparation)

w_i: "inline-parallel"

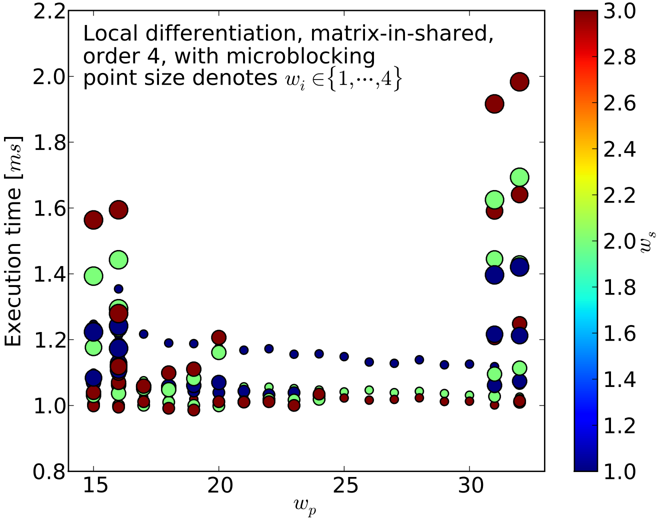


(exploit register space)

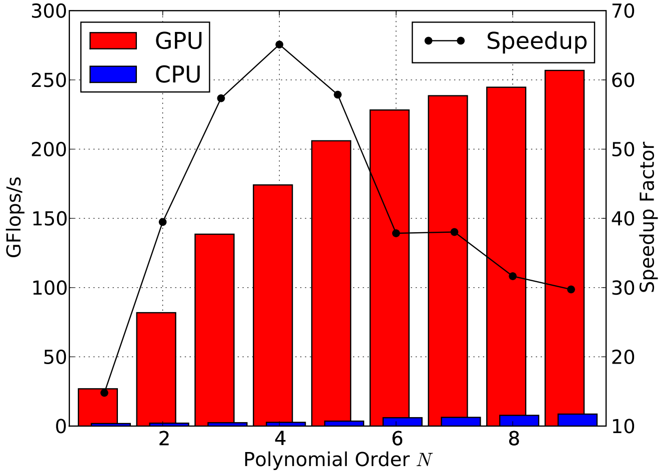
w_p: in parallel



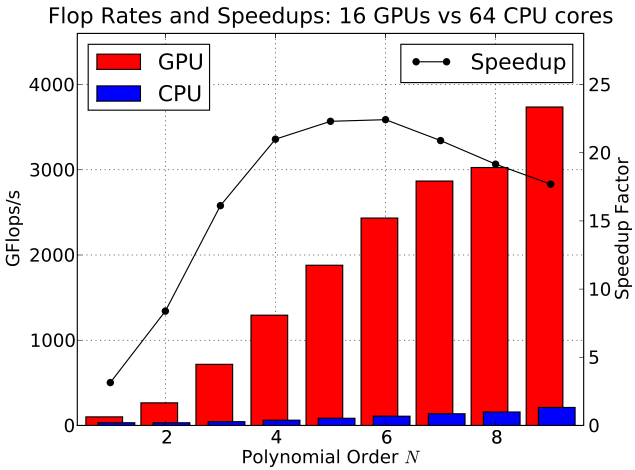
Loop Slicing for Differentiation



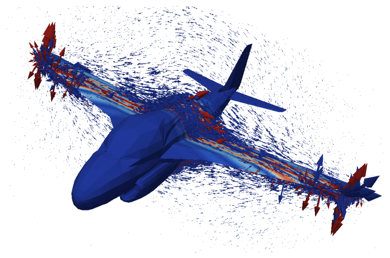
Nvidia GTX280 vs. single core of Intel Core 2 Duo E8400



16 T10s vs. $64 = 8 \times 2 \times 4$ Xeon E5472

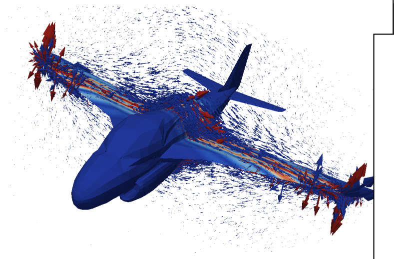


GPU DG Showcase

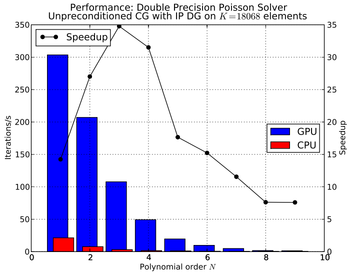


Eletromagnetism

GPU DG Showcase

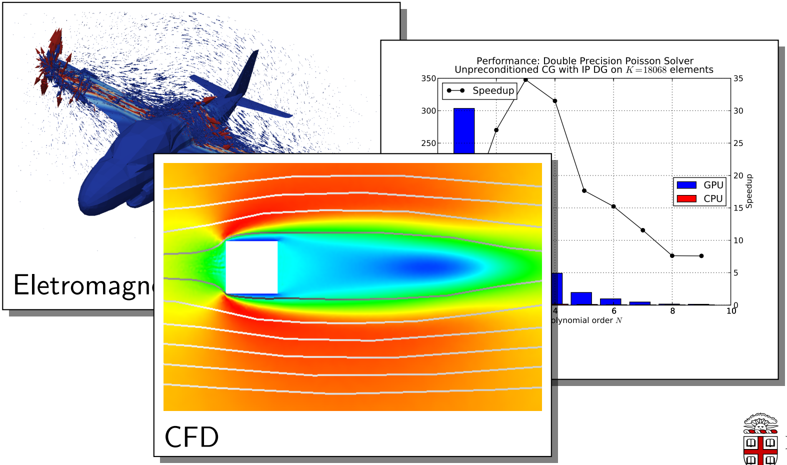


Eletromagnetism

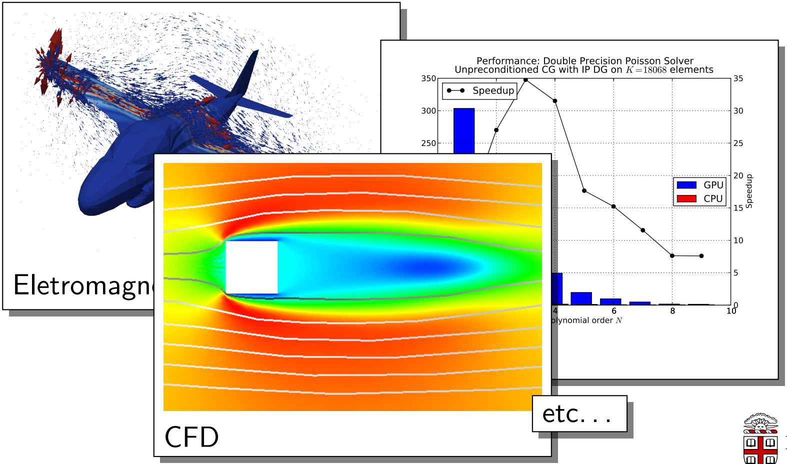


Poisson

GPU DG Showcase



GPU DG Showcase



etc. . .

Outline

Introducing... PyOpenCL

- PyOpenCL is "PyCUDA for OpenCL"
- Complete, mature API wrapper
- Features like PyCUDA: not yet
- Tested on all available Implementations, OSs
- `http://mathema.tician.de/software/pyopencl`

OpenCL

Introducing... PyOpenCL

Same flavor, different recipe:

```
ctx = cl.create_context_from_type(cl.device_type.ALL)
queue = cl.CommandQueue(ctx)

a = numpy.random.rand(50000).astype(numpy.float32)
a_buf = cl.Buffer(ctx, cl.mem_flags.COPY_HOST_PTR, hostbuf=a)

prg = cl.Program(ctx, """
    __kernel void twice( __global float *x)
    { x[get_global_id(0)] *= 2; }""").build()
prg.twice(queue, a.shape, a_buf)

twice_a = numpy.empty_like(a)
cl.enqueue_read_buffer(queue, a_buf, twice_a).wait()
```

Automating GPU Programming

GPU programming can be time-consuming, unintuitive and error-prone.

- Obvious idea: Let the computer do it.
- One way: Smart compilers

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GPU programming can be time-consuming, unintuitive and error-prone.

- Obvious idea: Let the computer do it.
- One way: Smart compilers
  - GPU programming requires complex tradeoffs
  - Tradeoffs require heuristics
  - Heuristics are fragile
- Another way: Dumb enumeration
  - Enumerate loop slicings
  - Enumerate prefetch options
  - Choose by running resulting code on actual hardware

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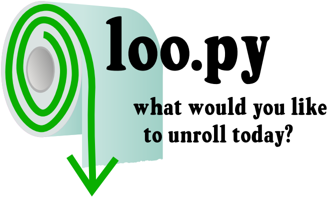
Loo.py Example

Empirical GPU loop optimization:

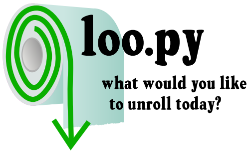
```
a, b, c, i, j, k = [var(s) for s in "abcijk"]
n = 500
k = make_loop_kernel([
    LoopDimension("i", n),
    LoopDimension("j", n),
    LoopDimension("k", n),
    ], [
    (c[i+n*j], a[i+n*k]*b[k+n*j])
    ])

gen_kwargs = {
        "min_threads": 128,
        "min_blocks": 32,
        }
```



→ Ideal case: Finds 160 GF/s kernel without human intervention.

Loo.py Status

- Limited scope:
  - Require input/output separation
  - Kernels must be expressible using "loopy" model
    (i.e. indices decompose into "output" and "reduction")
  - Enough for DG, LA, FD, . . .



Loo.py Status

- Limited scope:
  - Require input/output separation
  - Kernels must be expressible using "loopy" model
    (i.e. indices decompose into "output" and "reduction")
  - Enough for DG, LA, FD, ...
- Kernel compilation limits trial rate
- Non-Goal: Peak performance
- Good results currently for dense linear algebra and (some) DG subkernels

loo.py
what would you like to unroll today?

Conclusions

- Fun time to be in computational science

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- Use Python and PyCUDA to have even more fun :-)
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Conclusions

- Fun time to be in computational science
- Use Python and PyCUDA to have even more fun :-)
  - With no compromise in performance
- GPUs and scripting work well together
  - Enable Metaprogramming
- Further work in GPU-DG:
  - Other equations (Euler, Navier-Stokes)
  - Curvilinear Elements
  - Local Time Stepping

Where to from here?

More at...

→ `http://mathema.tician.de/`

CUDA-DG

AK, T. Warburton, J. Bridge, J.S. Hesthaven, *"Nodal Discontinuous Galerkin Methods on Graphics Processors"*, J. Comp. Phys., 2009.

GPU RTCG

AK, N. Pinto et al. *PyCUDA: GPU Run-Time Code Generation for High-Performance Computing*, in prep.

Questions?

?

Thank you for your attention!

`http://mathema.tician.de/`

image credits

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