High-Productivity Supercomputing: Metaprogramming GPUs

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Applied Mathematics, Brown University

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Thanks

- Jan Hesthaven (Brown)
- Tim Warburton (Rice)
- Nico Gödel (HSU Hamburg)
- Lucas Wilcox (UT Austin)
- Akil Narayan (Brown)
- PyCuda contributors

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Outline

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Scripting: Goals

Scripting languages aim to reduce the load on the programmer:

- Reduce required knowledge

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Think about the tools you use.

Use the right tool for the job.

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- Encourage abstraction wherever possible
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> Think about the tools you use.
>
> Use the right tool for the job.

How are these goals achieved?

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Scripting: Means

A scripting language...

- is discoverable and interactive.

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A scripting language...

- is discoverable and interactive.
- is interpreted, not compiled.
- has comprehensive built-in functionality.
- manages resources automatically.
- is dynamically typed.
- works well for "gluing" lower-level blocks together.

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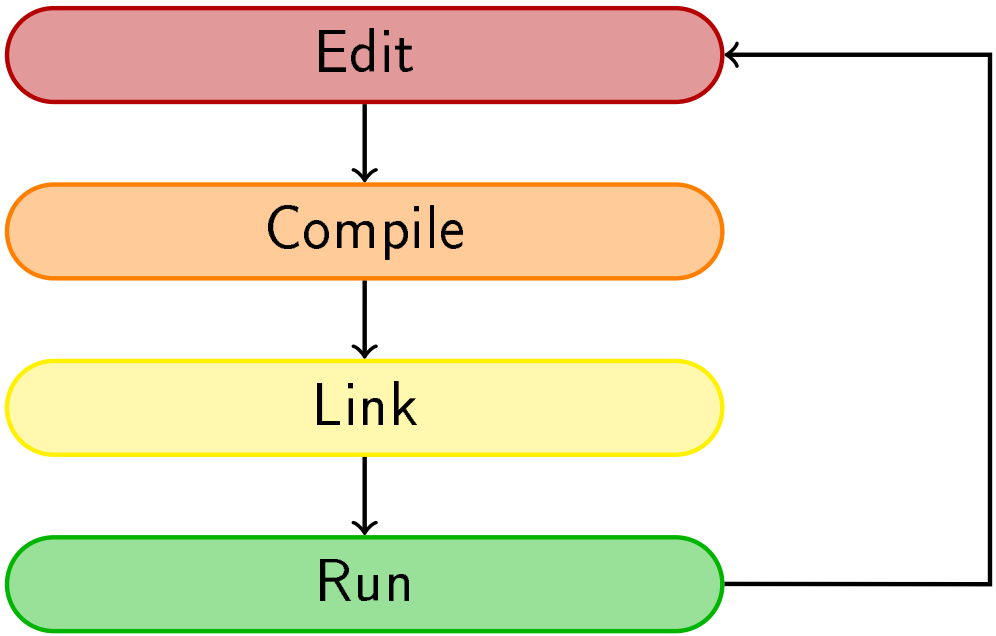
Scripting: Interpreted, not Compiled

Program creation workflow:



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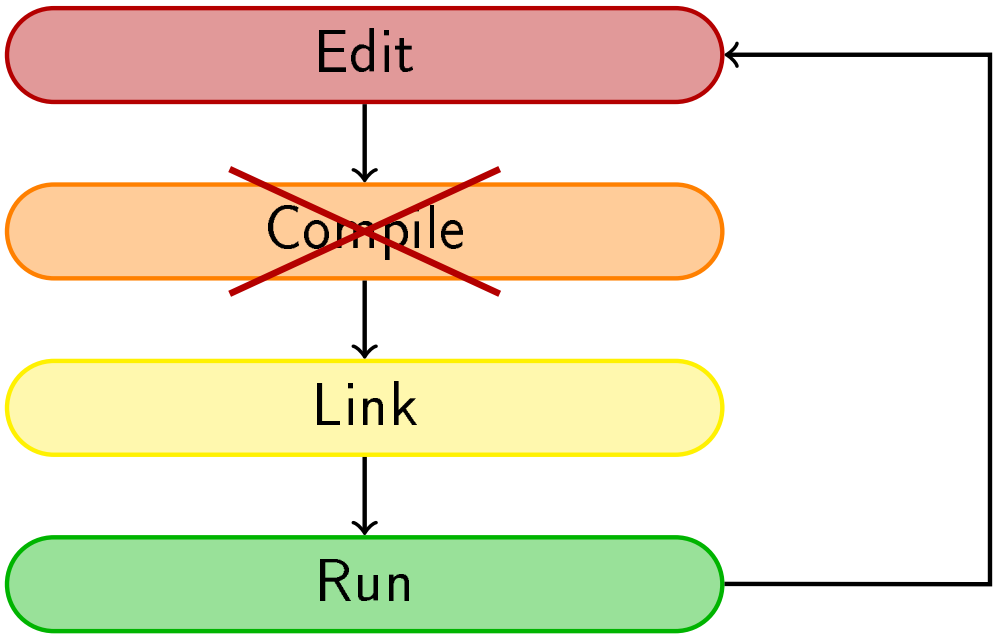

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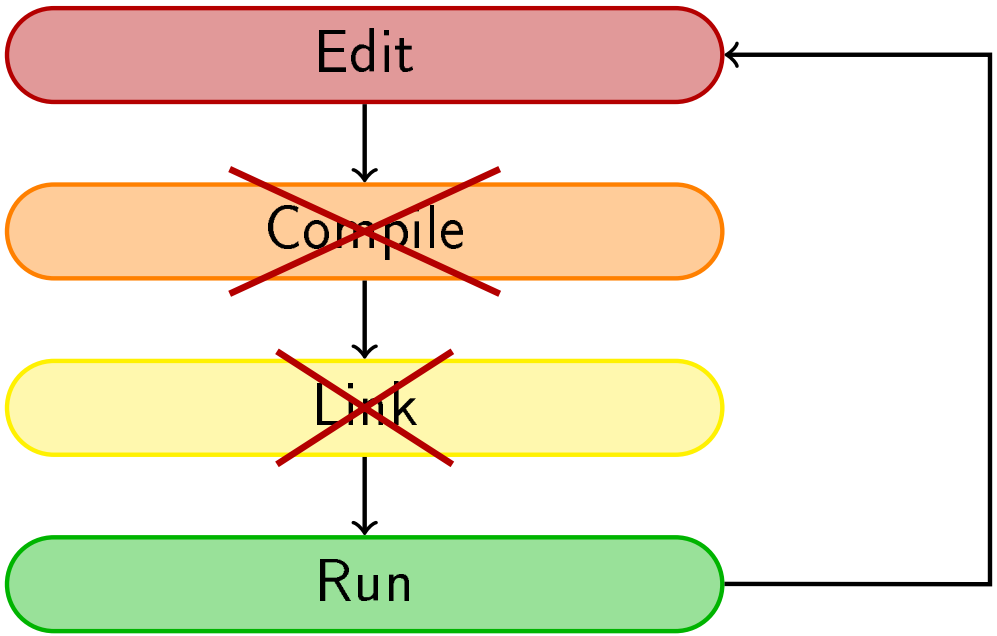

Batteries Included

Scripting languages come with "batteries included" (or easily available):

- Data structures: Lists, Sets, Dictionaries
- Linear algebra: Vectors, Matrices
- OS Interface: Files, Networks, Databases
- Persistence: Store, send and retrieve objects
- Defined, usable C interface

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Scripting: Run-Time Typing

Typing Discipline

"If it walks like a duck and quacks like a duck, it *is* a duck."

```
def print_all(iterable):
    for i in iterable:
        print i

print_all([6, 7, 19])
print_all({1: "a", 2: "b", 3: "c"})
```

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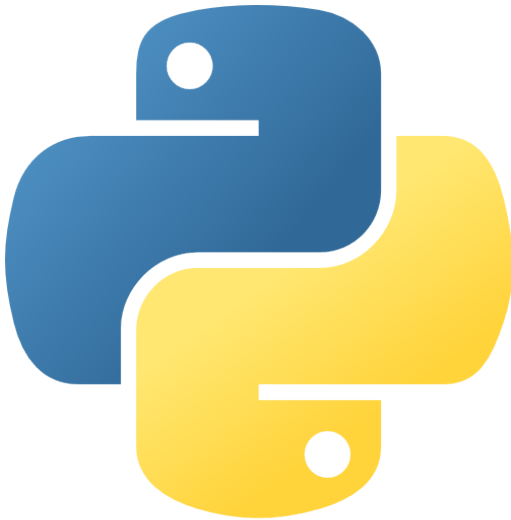
Scripting: Python

For this talk, Python is the scripting language of choice.



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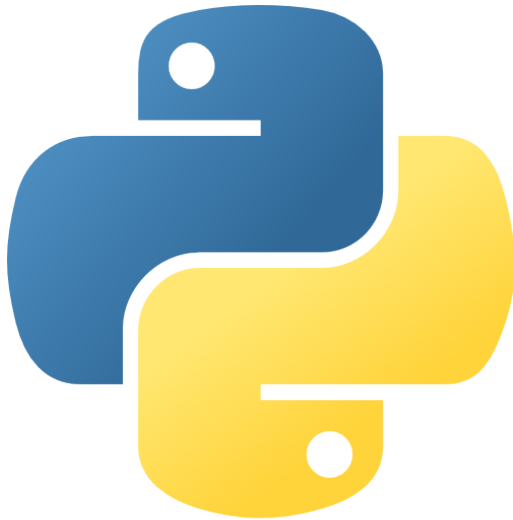

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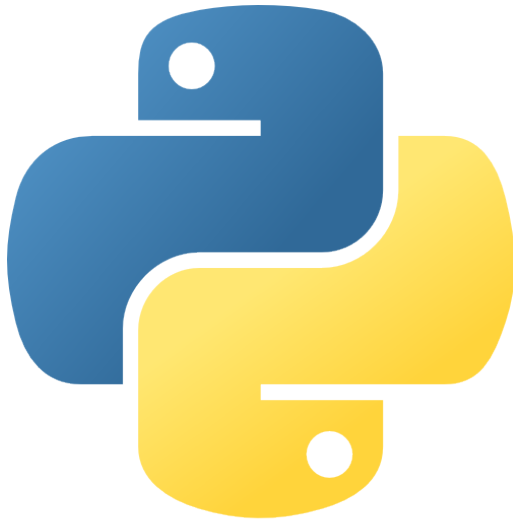

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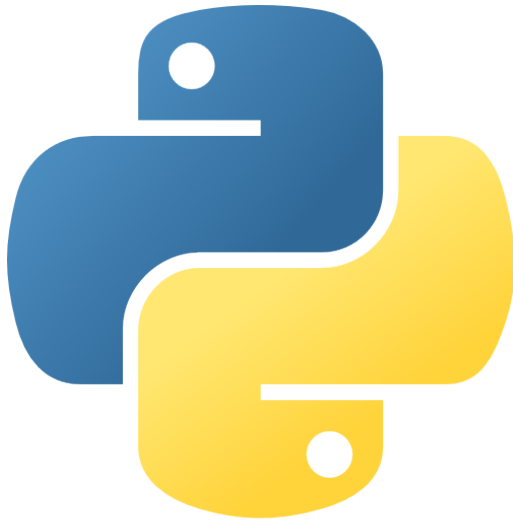

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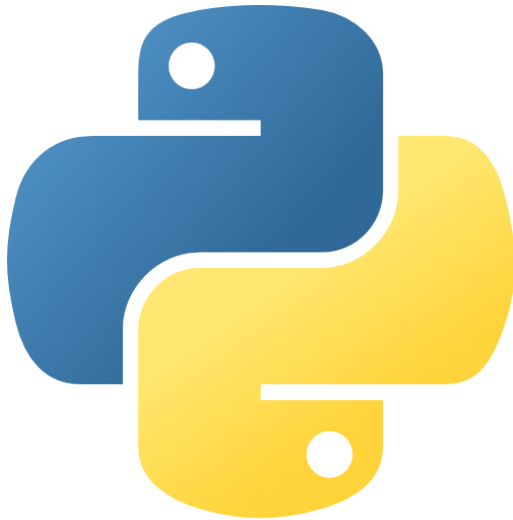

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Scripting: Python

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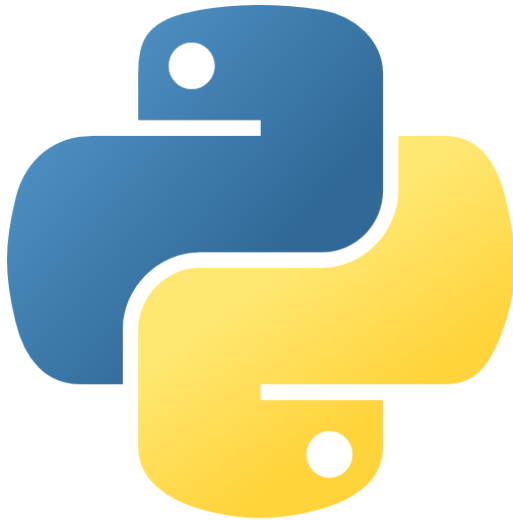
- Mature language
- Has a large and active community
- Emphasizes readability
- Written in widely-portable C
- A 'multi-paradigm' language



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Python + CUDA hybrids?

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- It does matter for inner loops.
- One solution: hybrid ("glued") code.

Python + CUDA hybrids? **PyCuda!**

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Questions?

?

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Whetting your appetite

```
1  import pycuda.driver as cuda
2  import pycuda.autoinit
3  import numpy
4
5  a = numpy.random.randn(4,4).astype(numpy.float32)
6  a_gpu = cuda.mem_alloc(a.size * a.dtype.itemsize)
7  cuda.memcpy_htod(a_gpu, a)
```

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

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Whetting your appetite

```
 9  mod = cuda.SourceModule("""
10      __global__ void doublify(float *a)
11      {
12        int idx = threadIdx.x + threadIdx.y*4;
13        a[idx] *= 2;
14      }
15      """)
16
17  func = mod.get_function("doublify")
18  func(a_gpu, block=(4,4,1))
19
20  a_doubled = numpy.empty_like(a)
21  cuda.memcpy_dtoh(a_doubled, a_gpu)
22  print a_doubled
23  print a
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Compute kernel

Whetting your appetite, Part II

Did somebody say "Abstraction is good"?

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Whetting your appetite, Part II

```
1  import numpy
2  import pycuda.autoinit
3  import pycuda.gpuarray as gpuarray
4
5  a_gpu = gpuarray.to_gpu(
6      numpy.random.randn(4,4).astype(numpy.float32))
7  a_doubled = (2*a_gpu).get()
8  print a_doubled
9  print a_gpu
```

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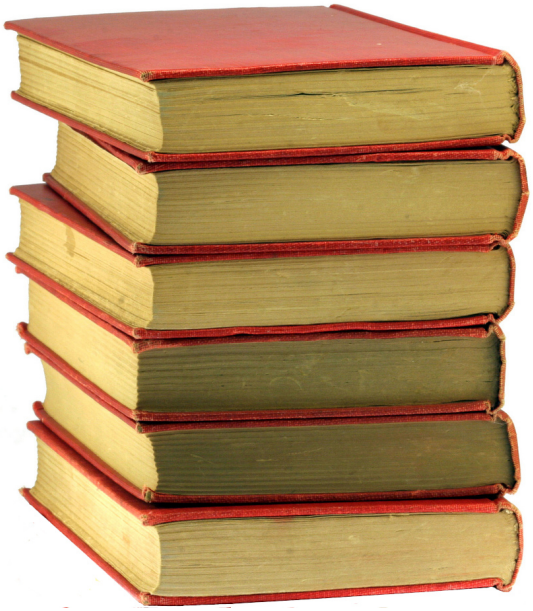
PyCuda Philosophy



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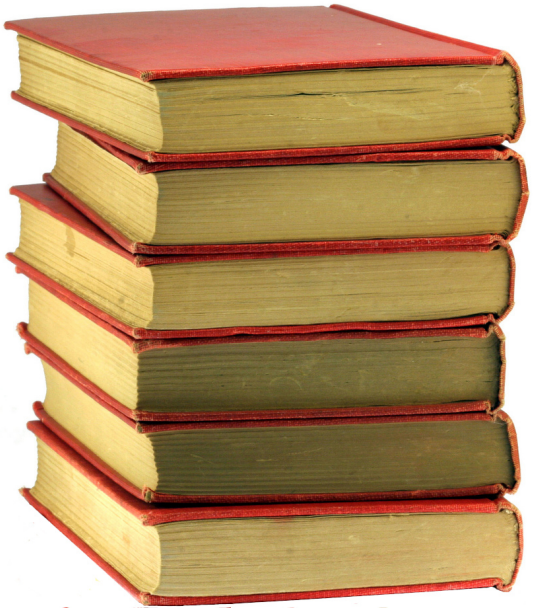
PyCuda Philosophy



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- Automatically manage resources

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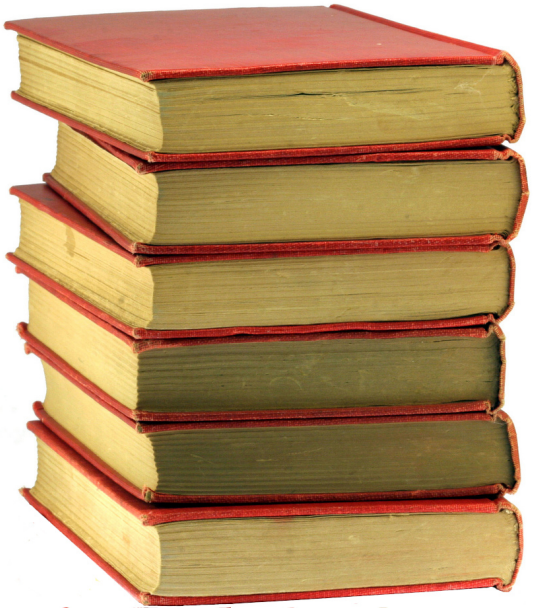

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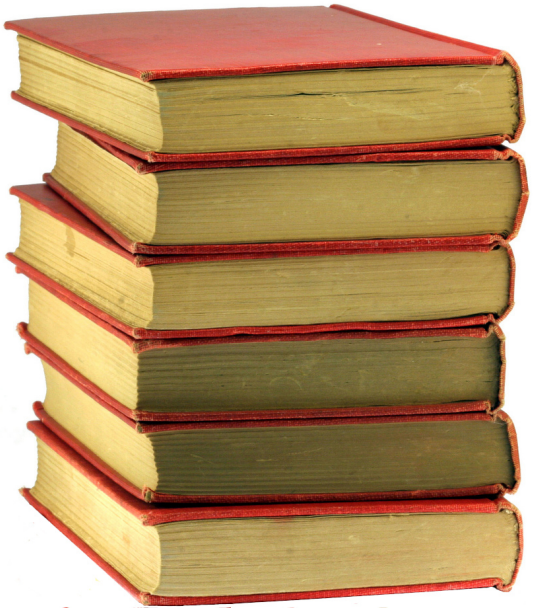

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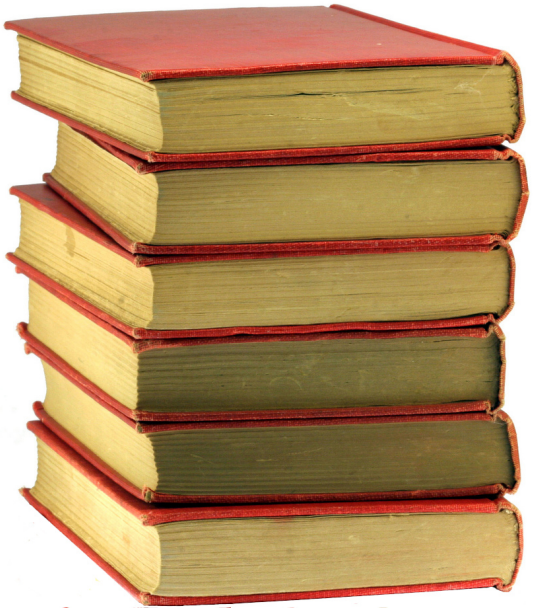

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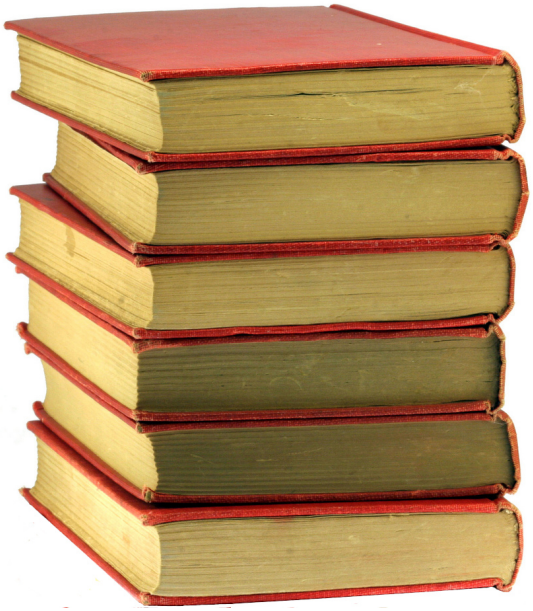

- Provide complete access
- Automatically manage resources
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- Check for and report errors automatically
- Integrate tightly with `numpy`

PyCuda: Completeness

PyCuda exposes *all* of CUDA.

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For example:

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

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PyCuda: Completeness

PyCuda supports every OS that CUDA supports.

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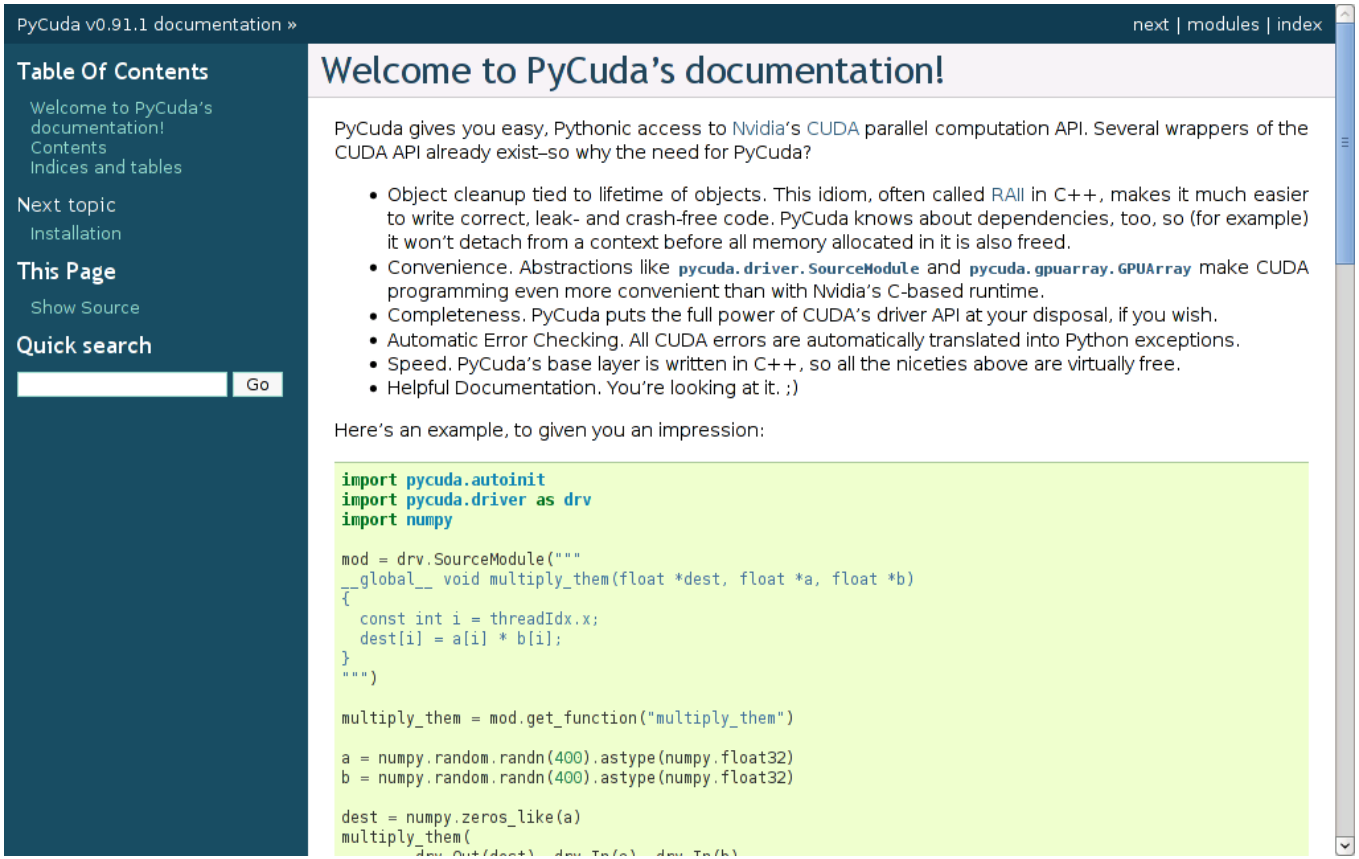
PyCuda: Completeness

PyCuda supports every OS that CUDA supports.

- Linux
- Windows
- OS X

PyCuda: Documentation



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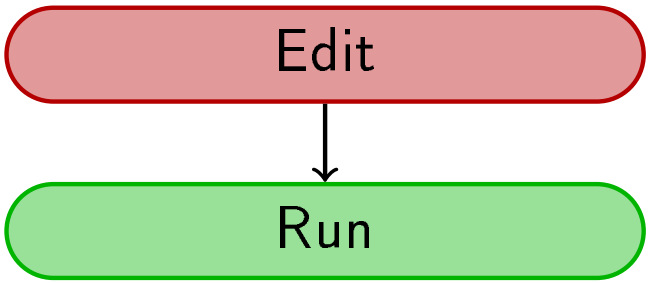

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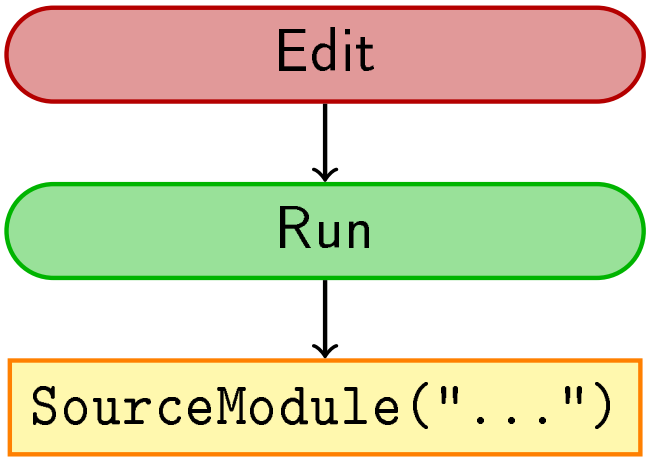

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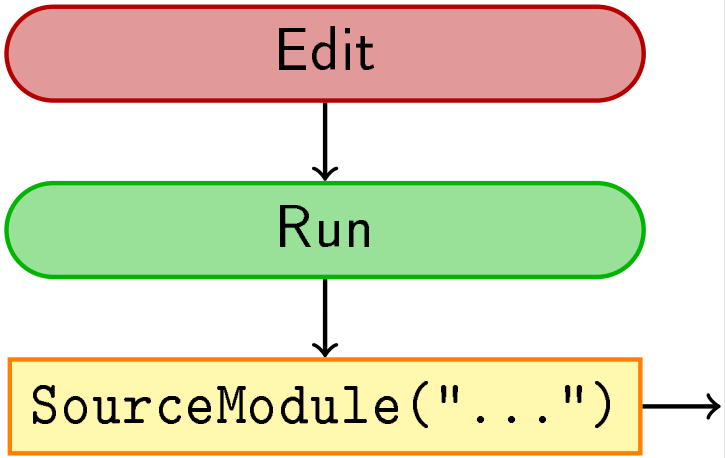

PyCuda

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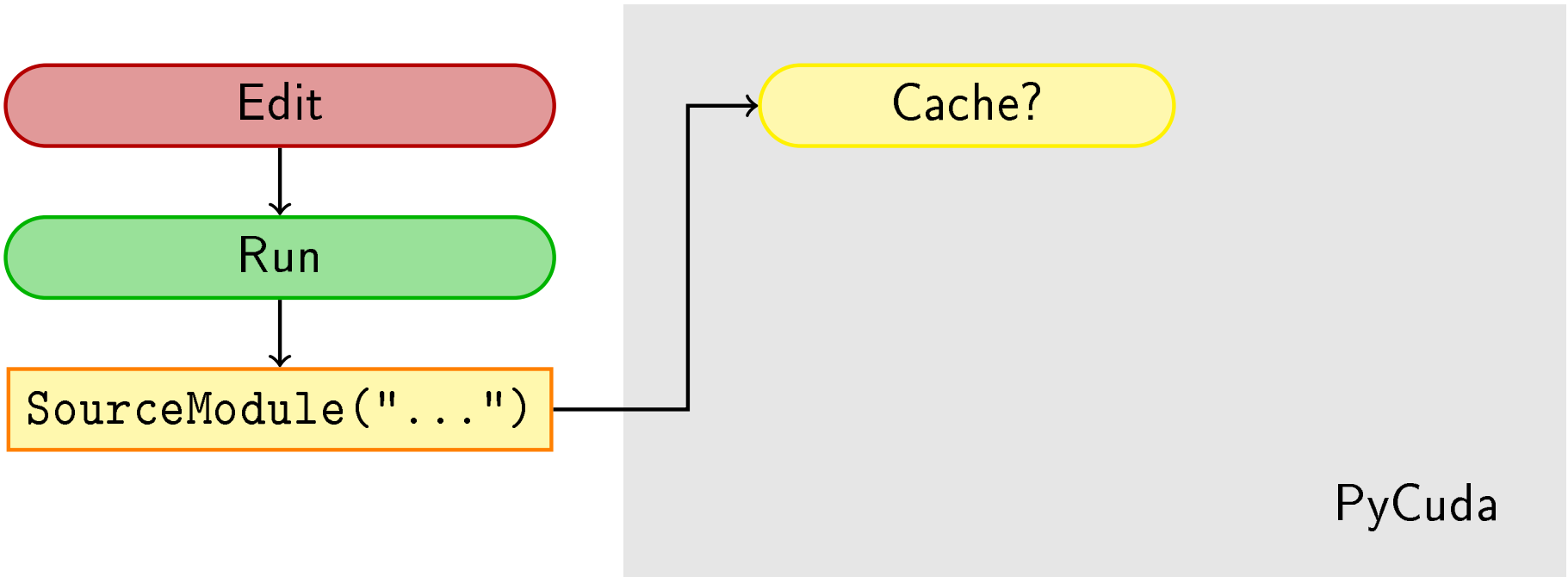

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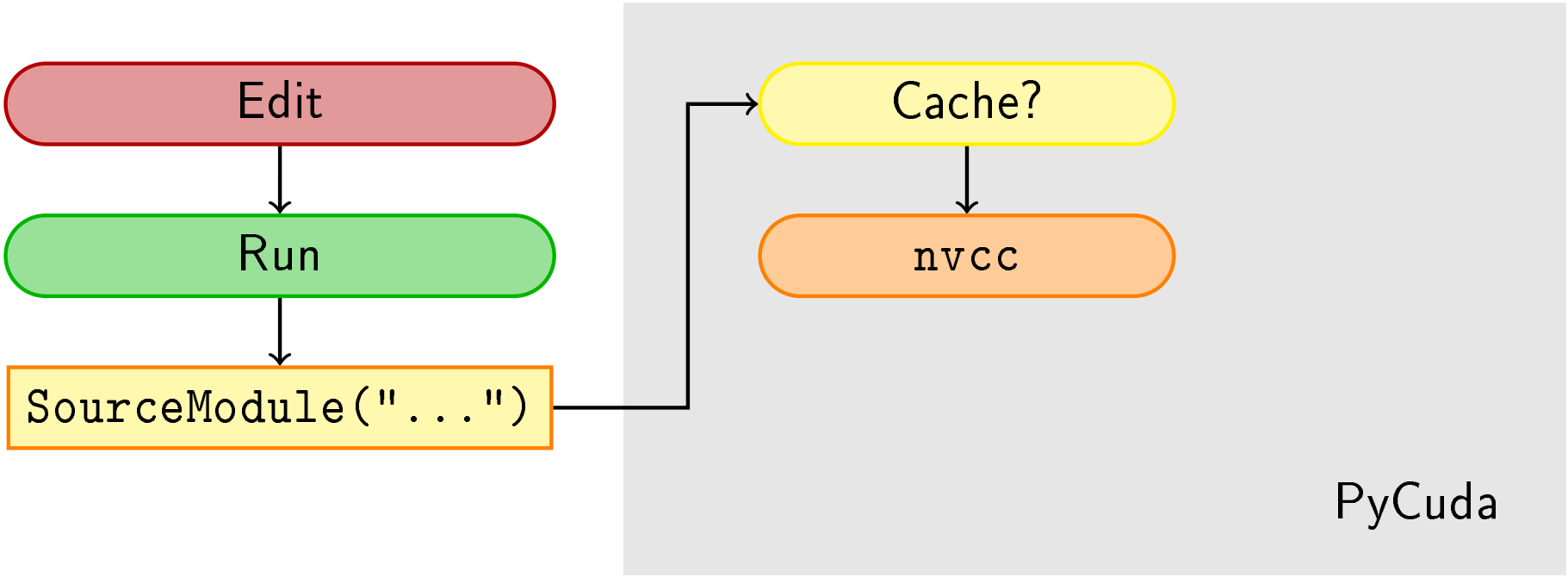

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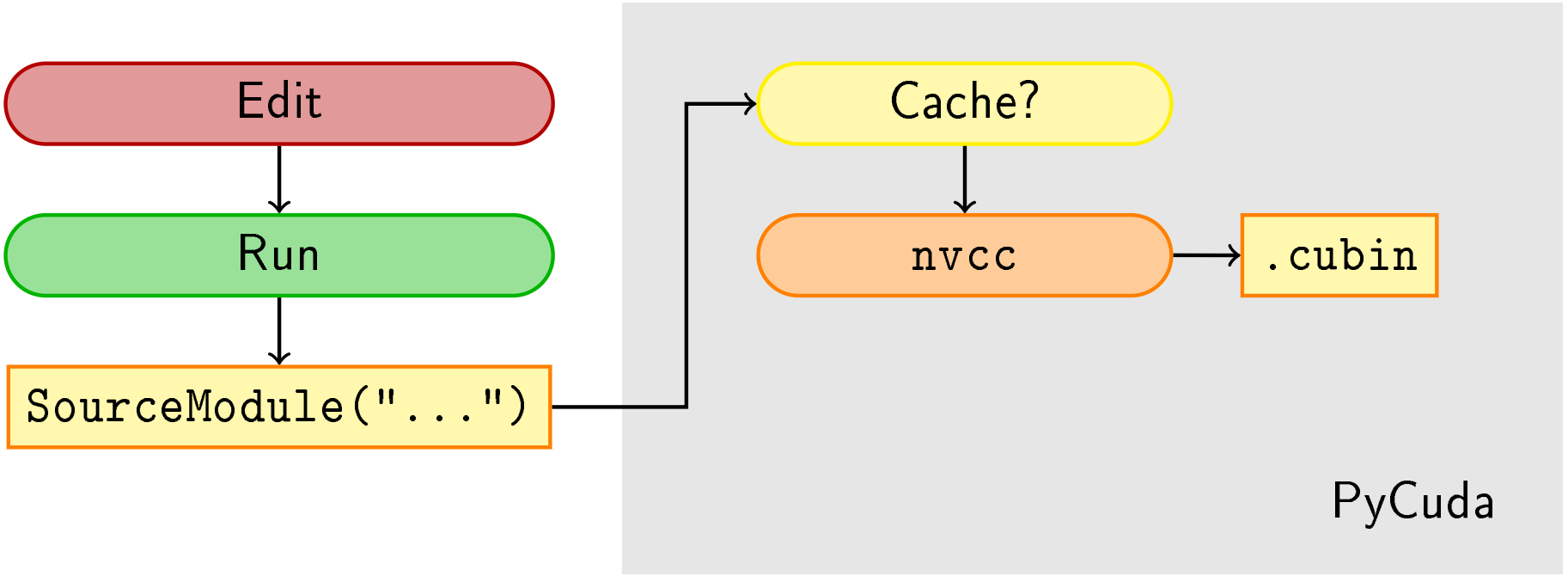

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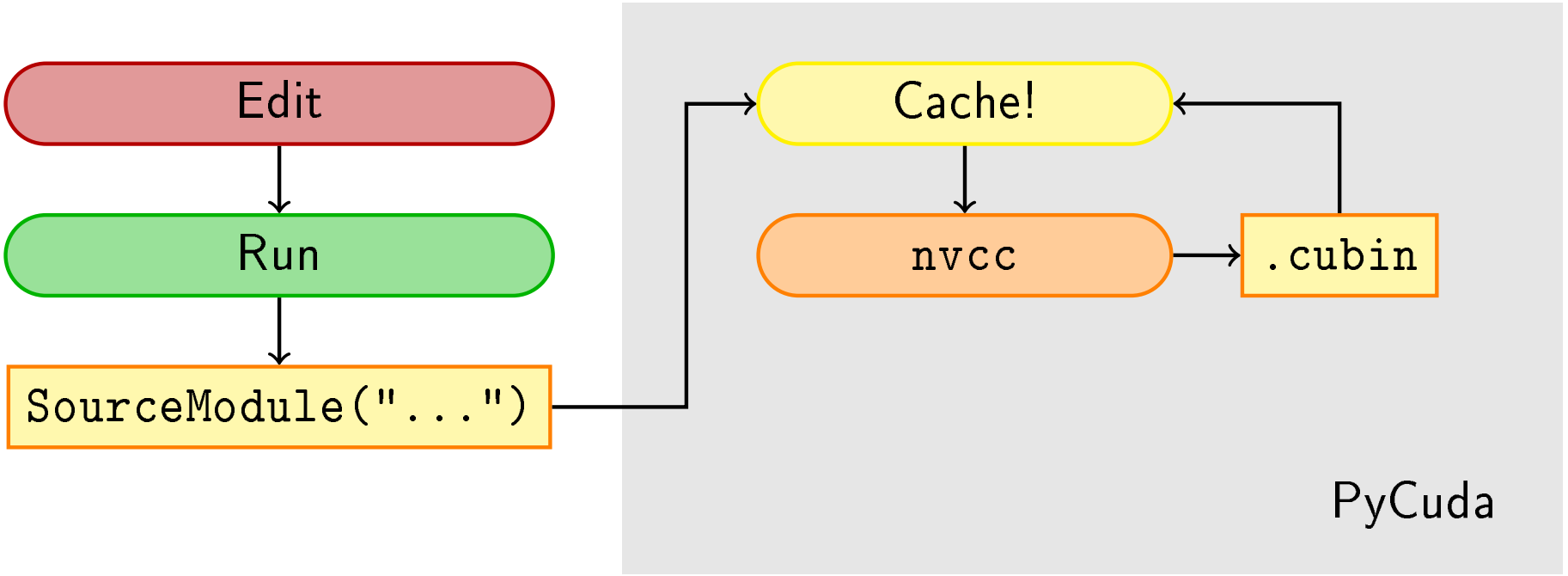

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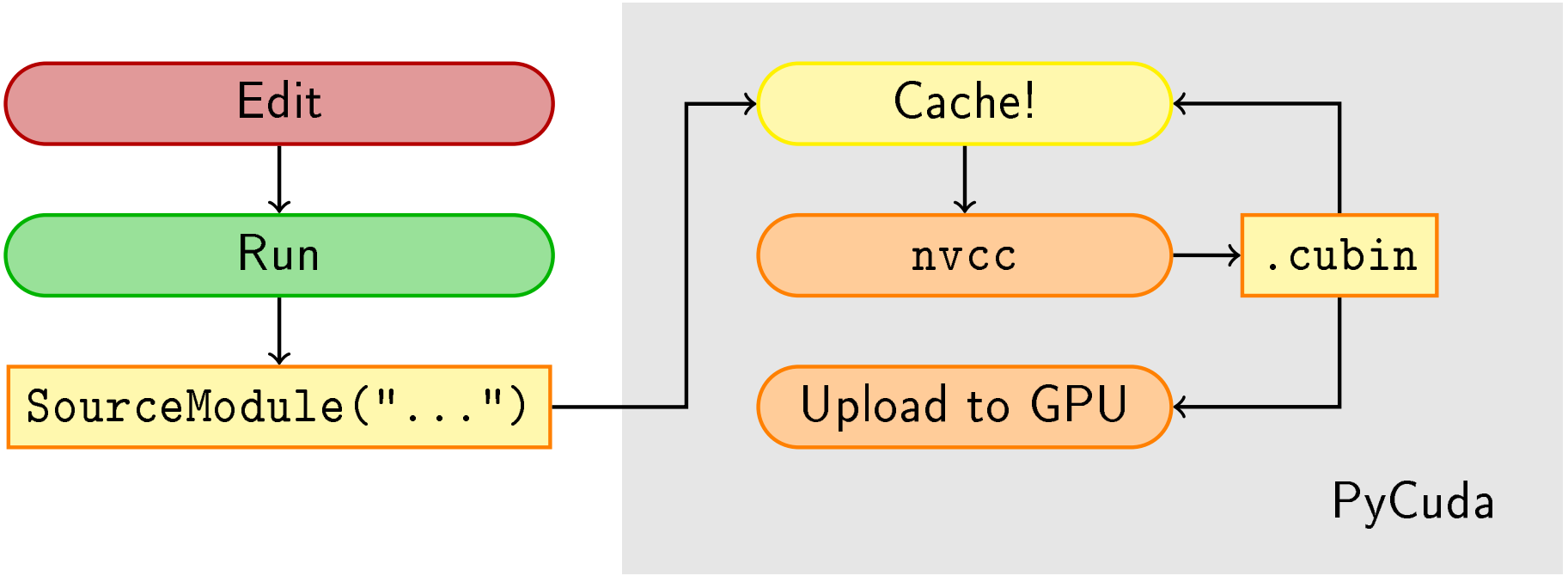

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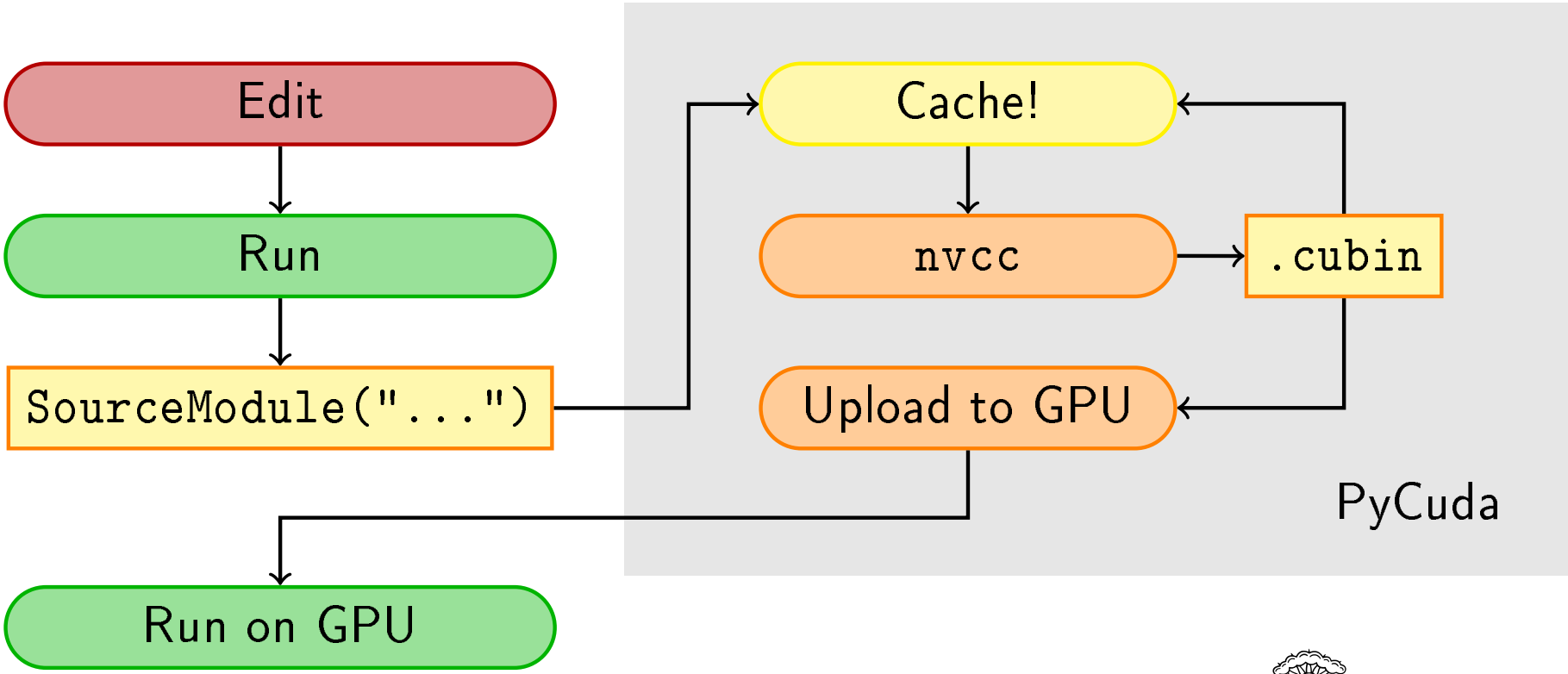

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func(numpy.int32(17), mem, block=(tx,ty,tz), grid=(bx,by))
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func.prepared_call((bx,by), 17, mem)
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- Prepared: Fast, Safe

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Two ways:

- Immediate: Convenient :-)

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Kernel Invocation: Automatic Copies

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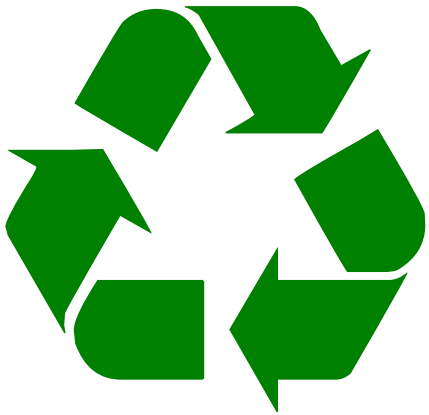
```

- "InOut" exists, too.
- Only for immediate invocation style.

Automatic Cleanup

- Reachable objects (memory, streams, ...) are never destroyed.



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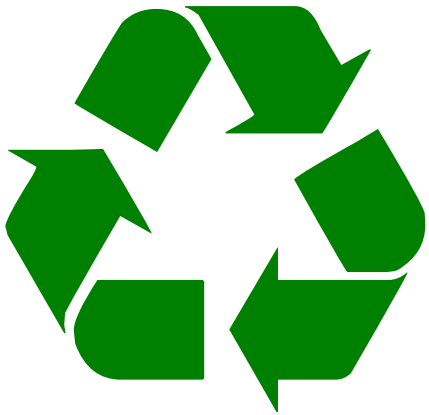
- Once unreachable, released at an unspecified future time.



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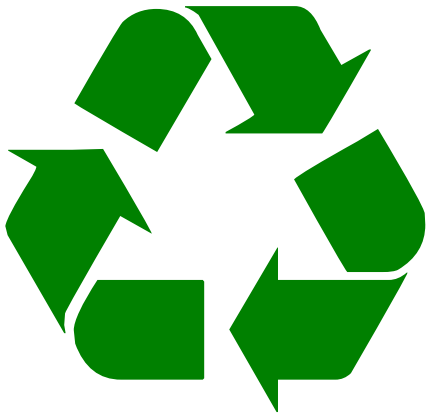

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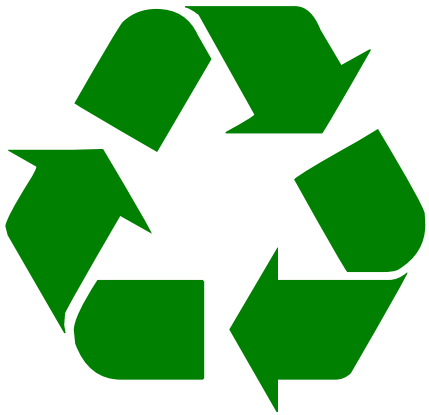
Automatic Cleanup

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



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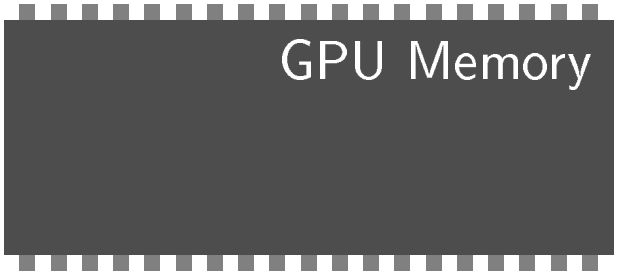
Working with Textures

```
mem = cuda.mem_alloc(size)
```



Working with Textures

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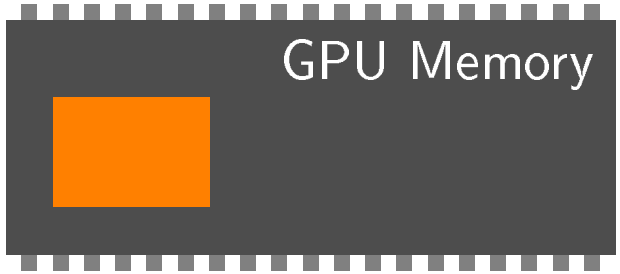

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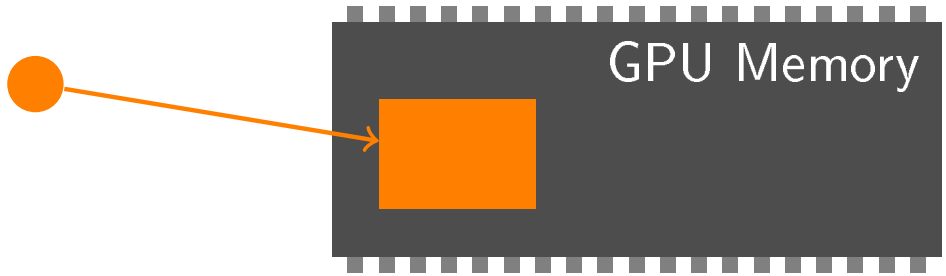

Working with Textures

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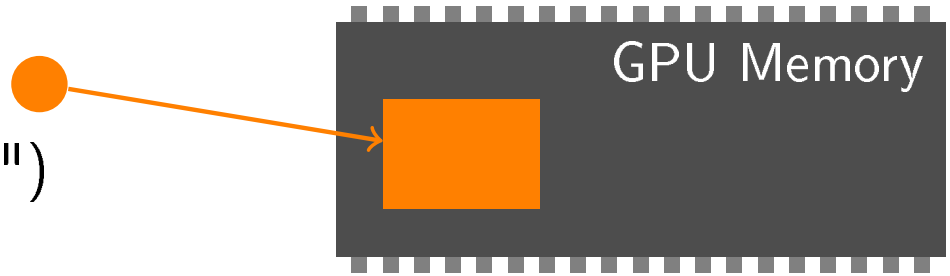
mem = cuda.mem_alloc(size)
mod = cuda.SourceModule("...")
```



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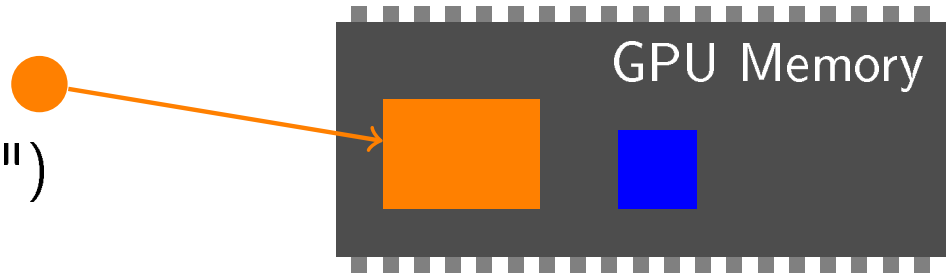

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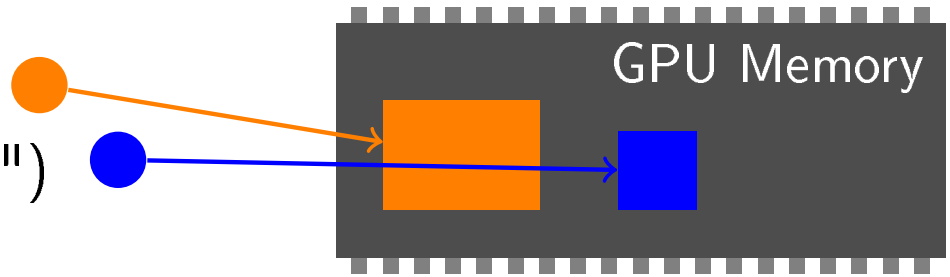

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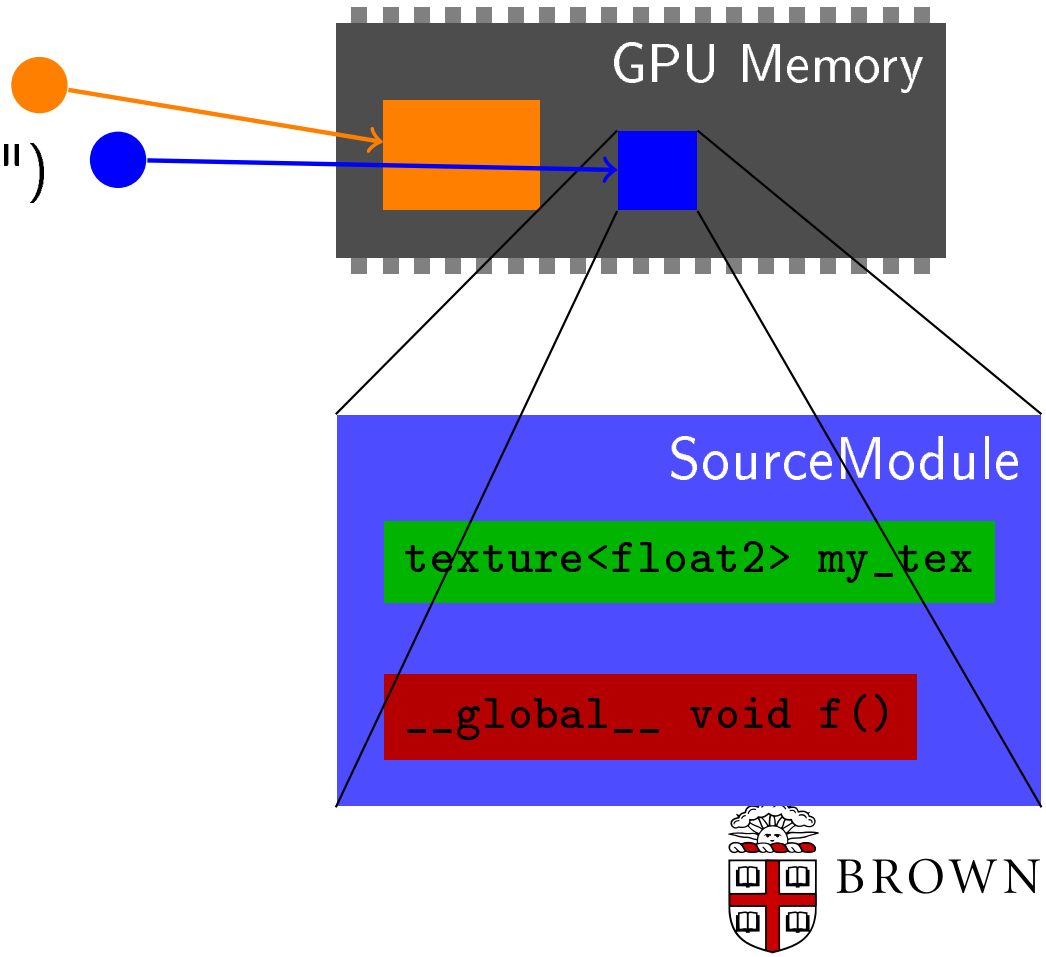

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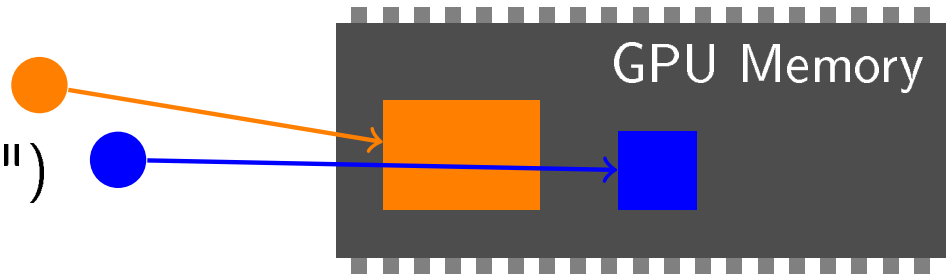

SourceModule

```
texture<float2> my_tex
```

```
__global__ void f()
```

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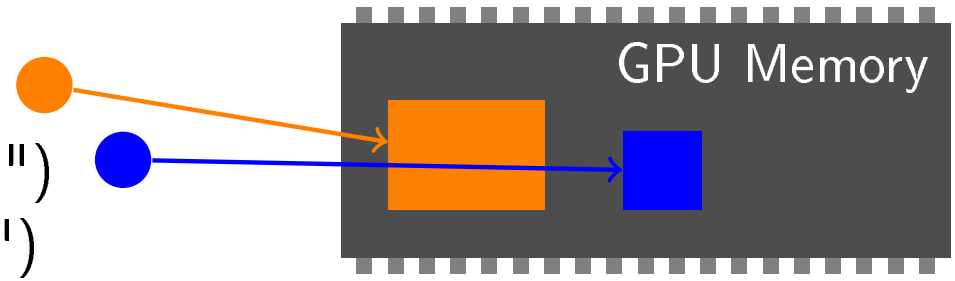
Working with Textures

```
mem = cuda.mem_alloc(size)
mod = cuda.SourceModule("...")
tr = mod.get_texref("my_tex")
```



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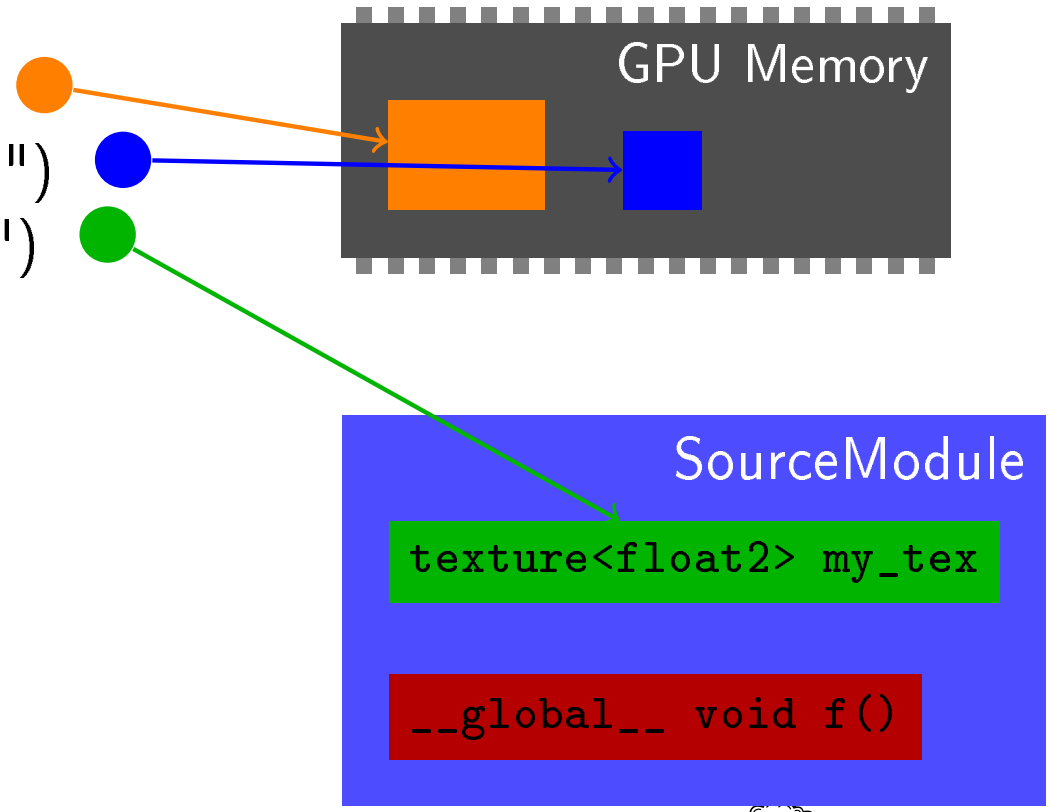

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Working with Textures

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mem = cuda.mem_alloc(size)
mod = cuda.SourceModule("...")
tr = mod.get_texref("my_tex")
tr.set_address(mem, size)
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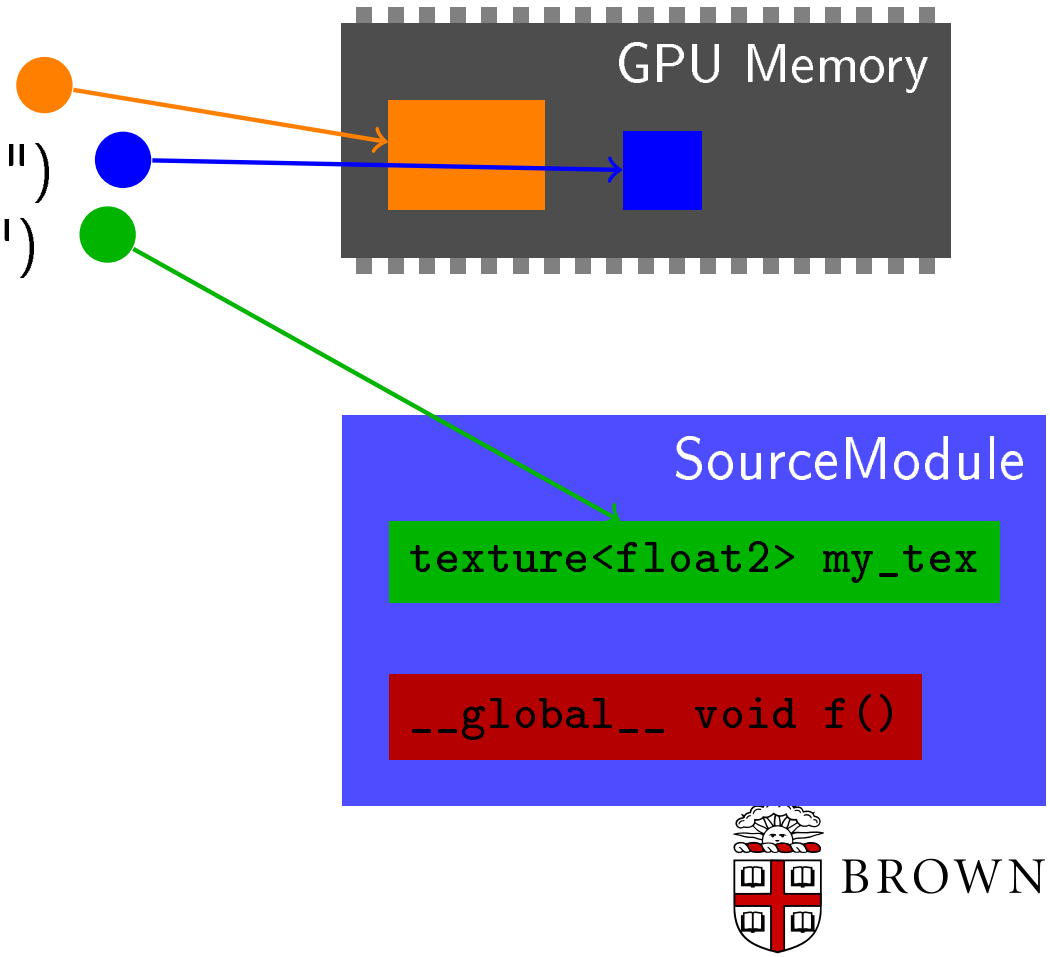

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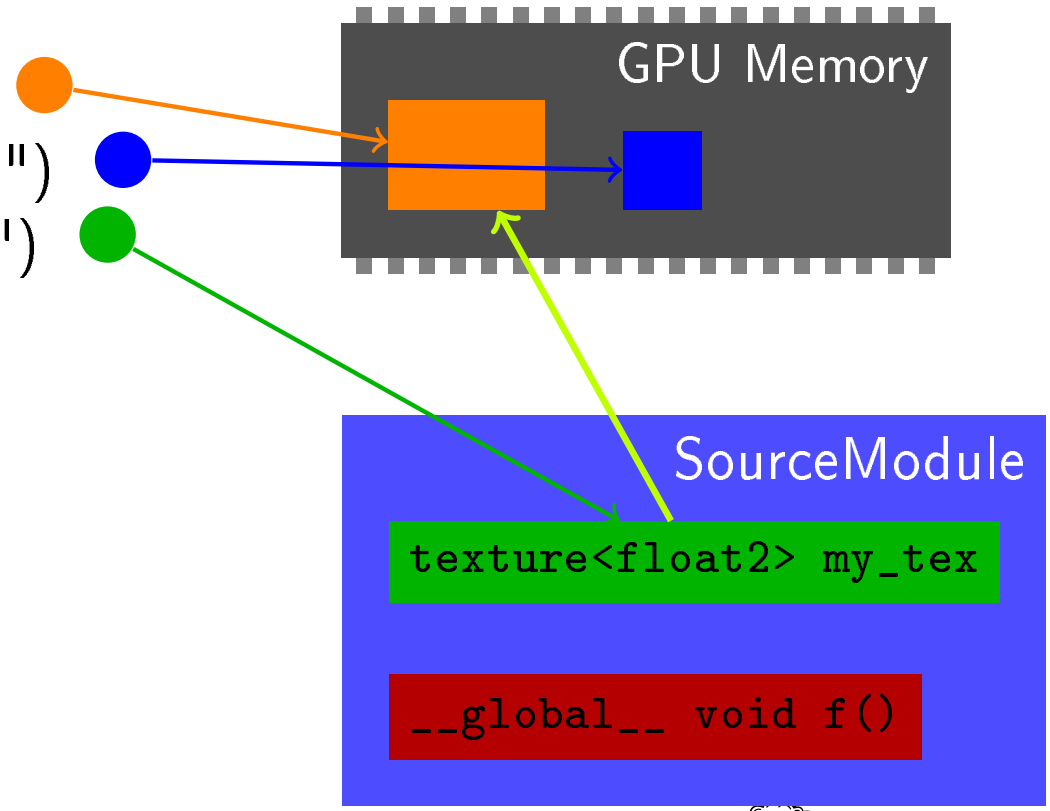

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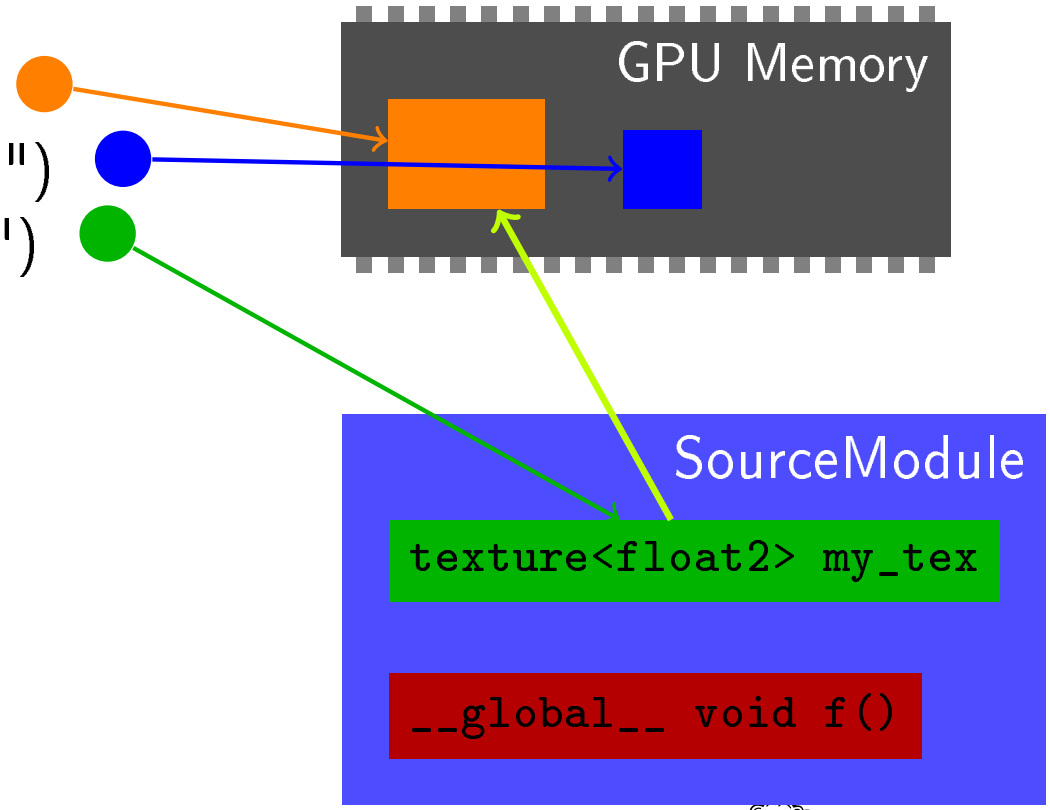

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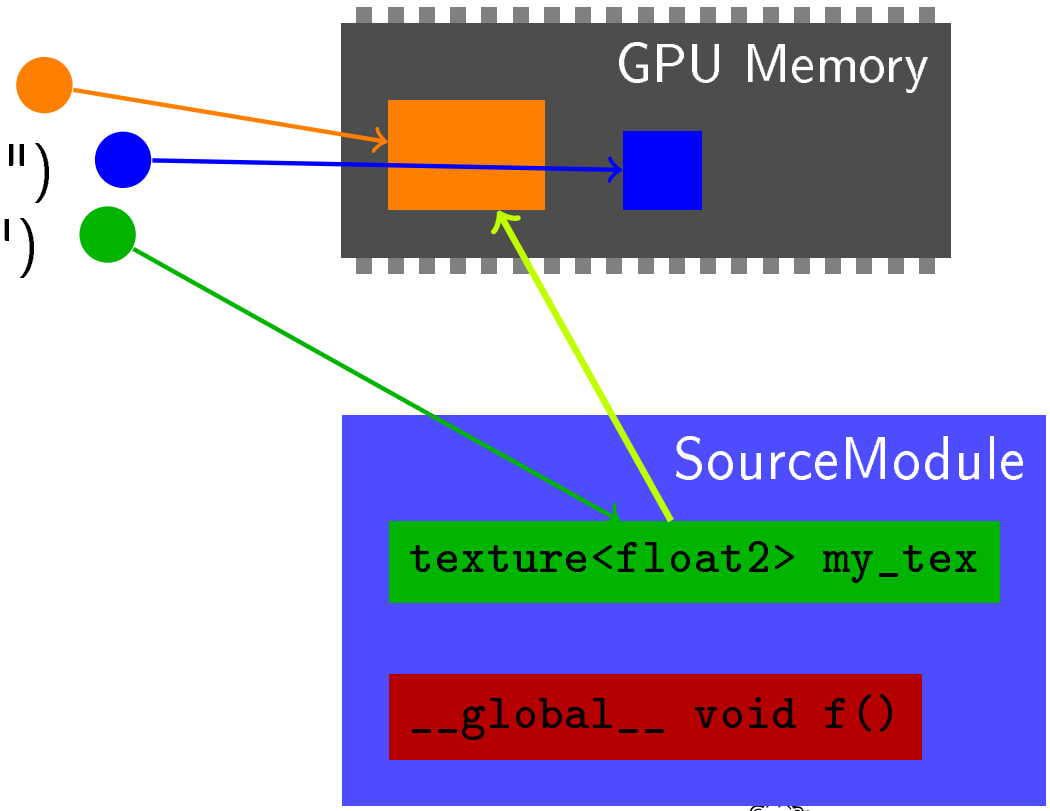

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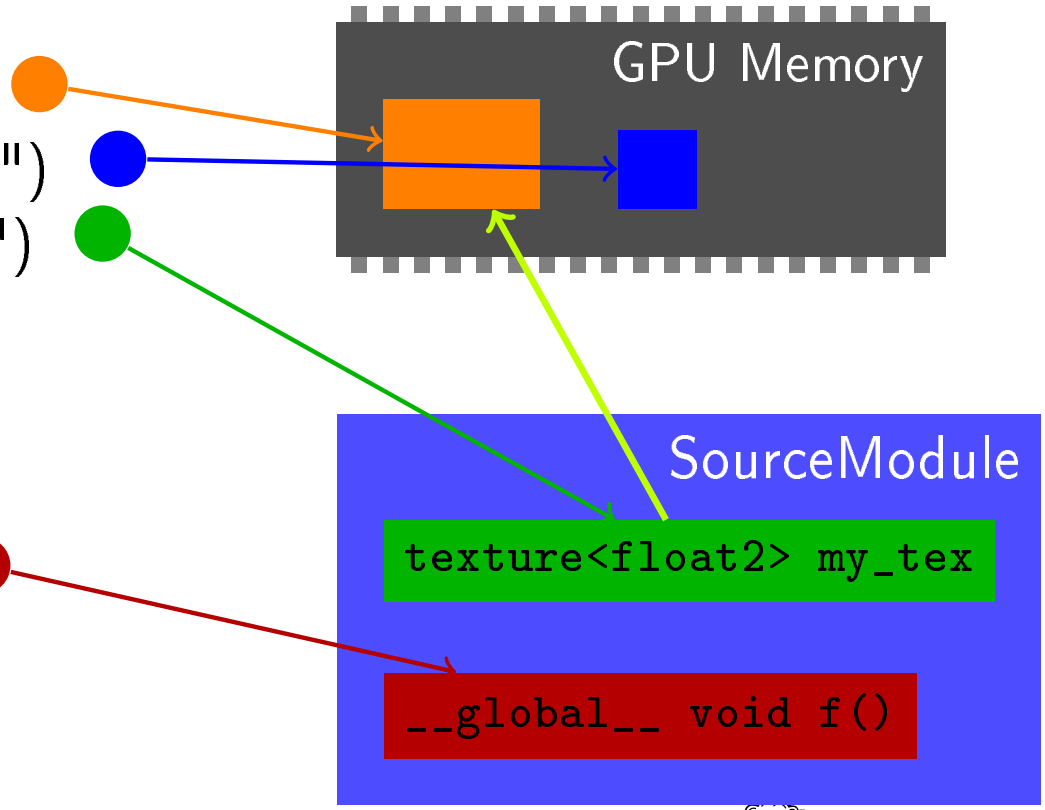

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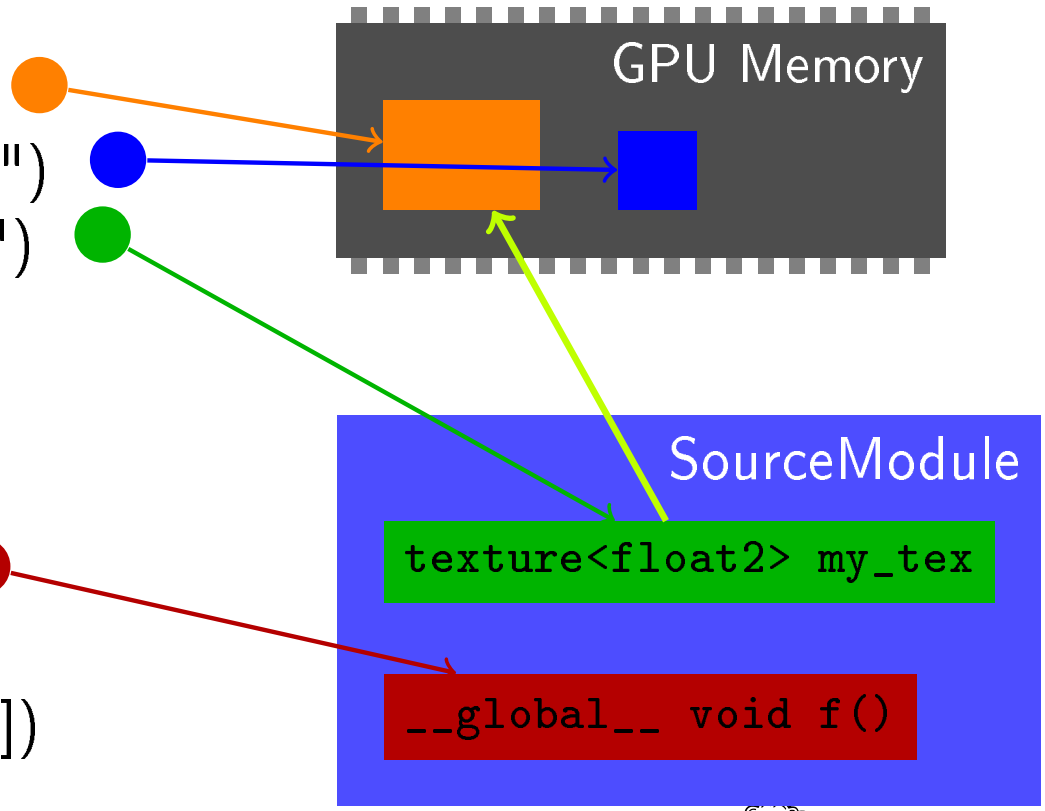

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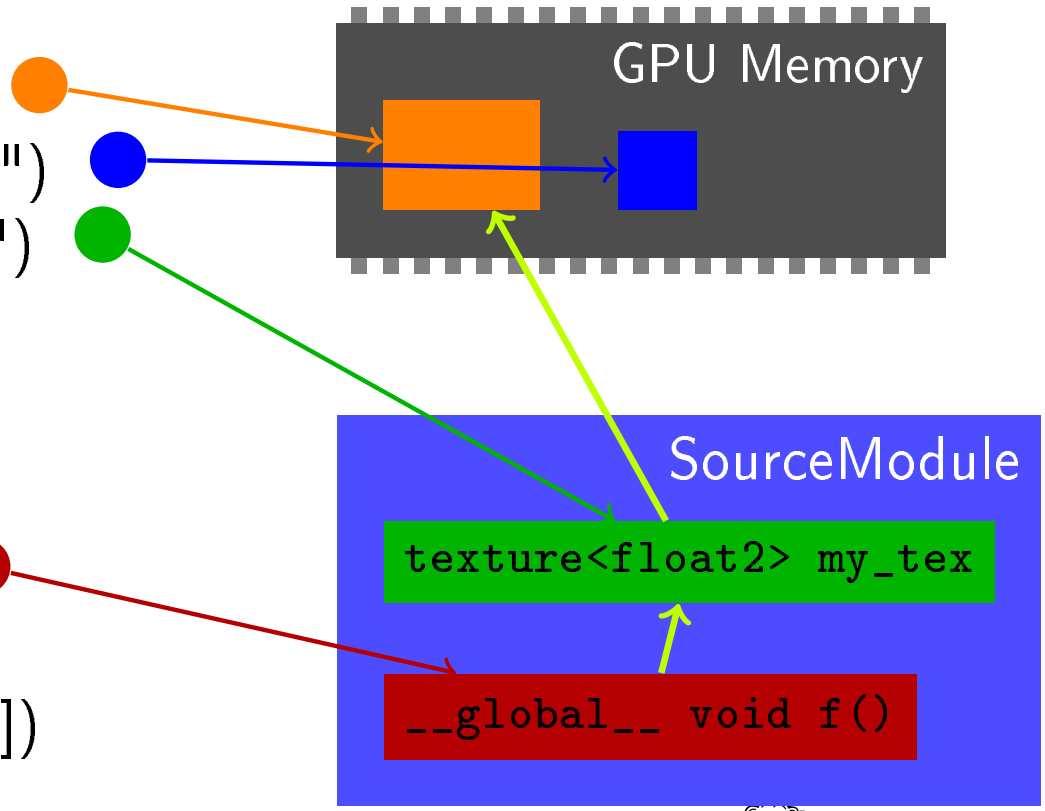

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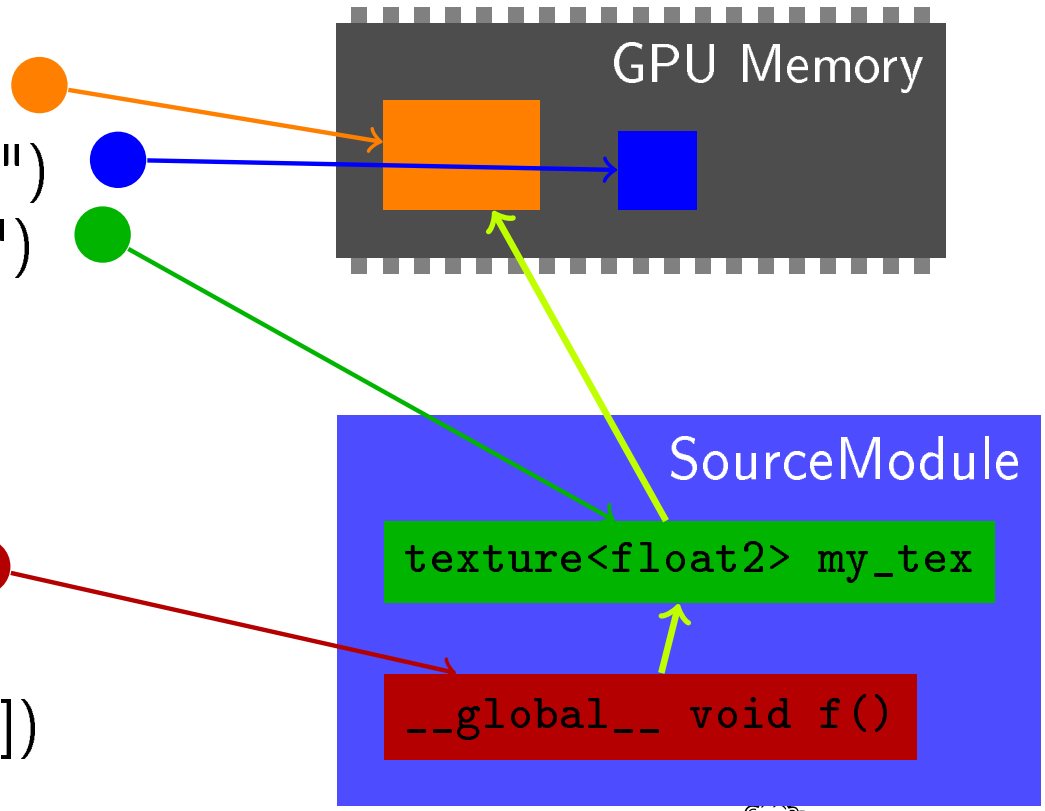

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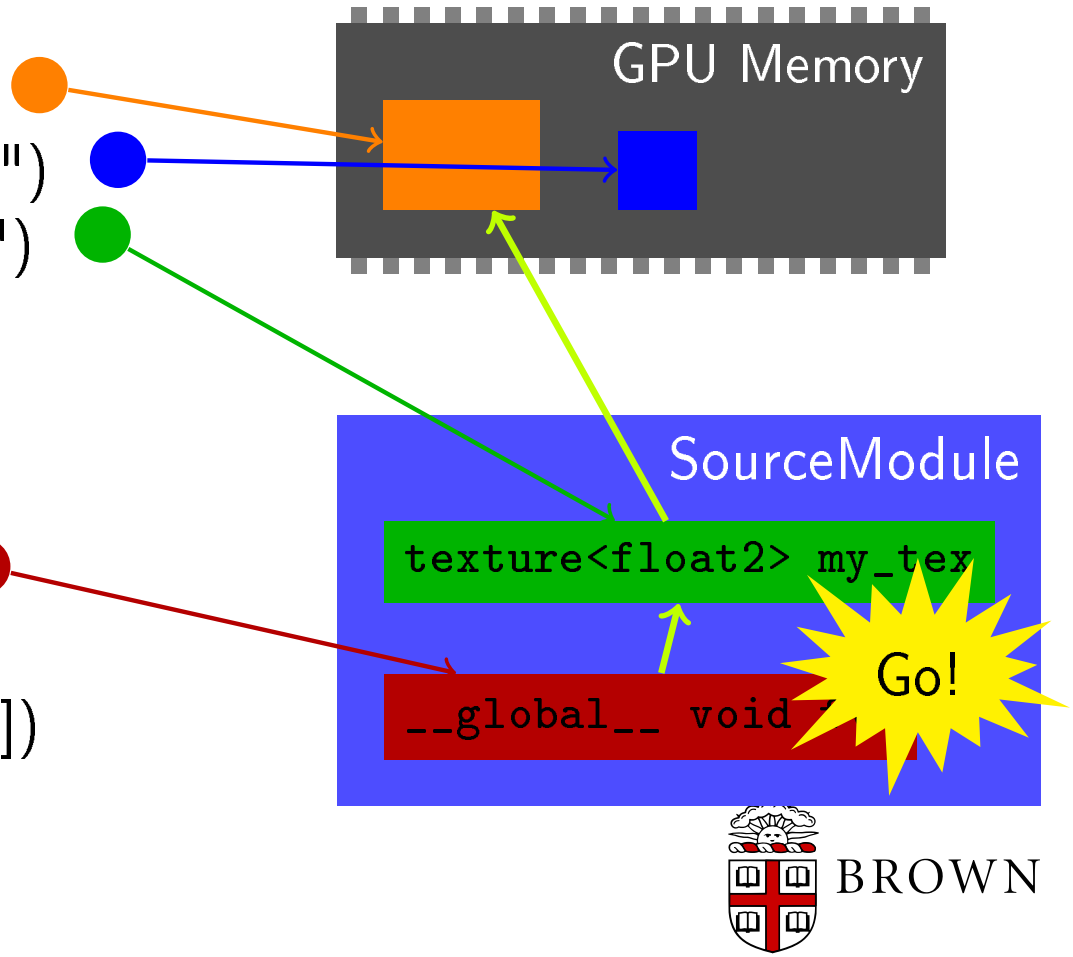

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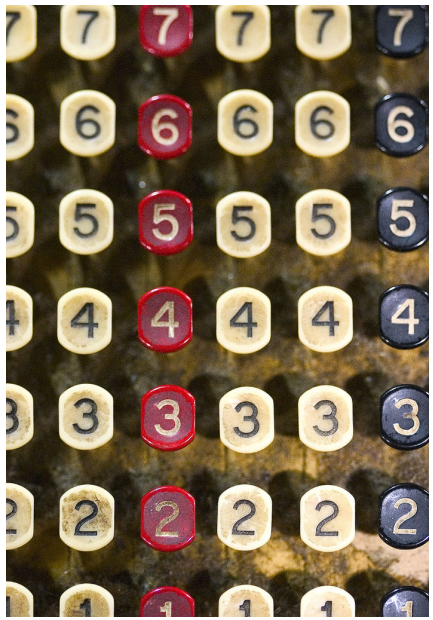
gpuarray: Simple Linear Algebra

`pycuda.gpuarray`:

- Meant to look and feel just like `numpy`.



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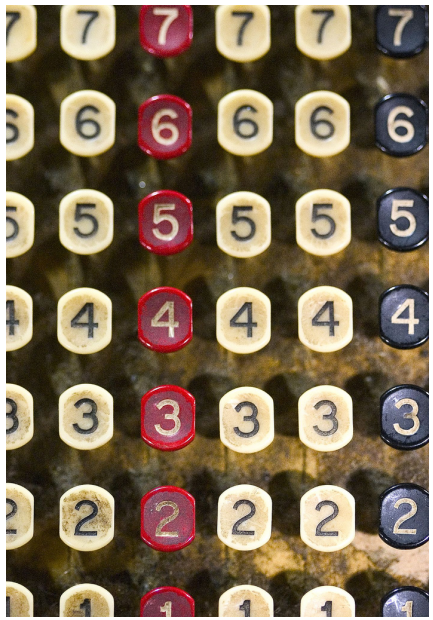

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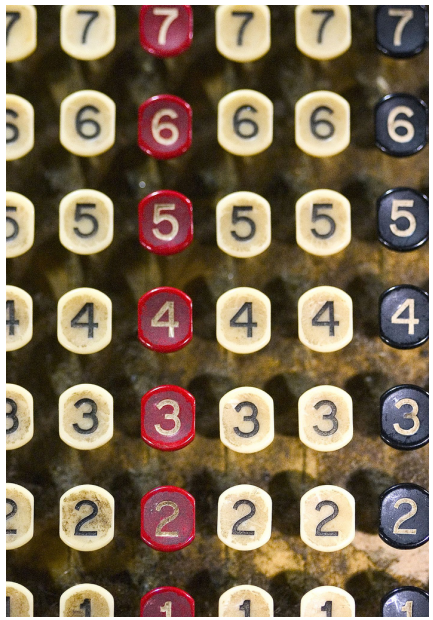

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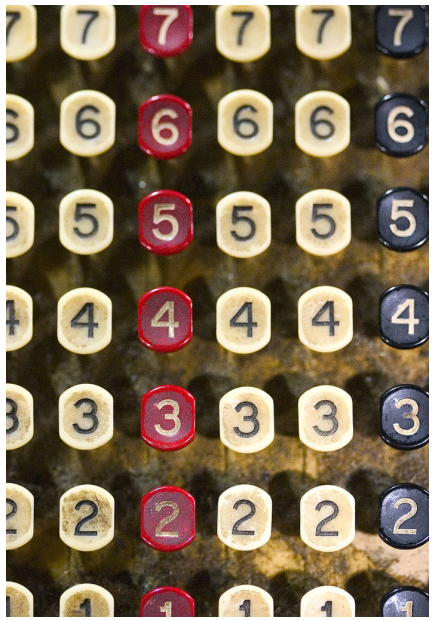

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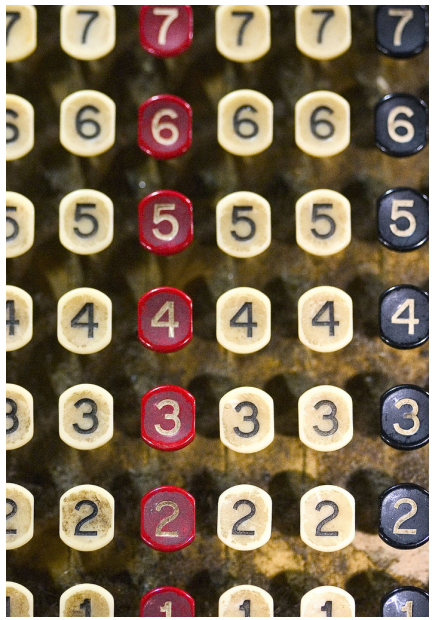

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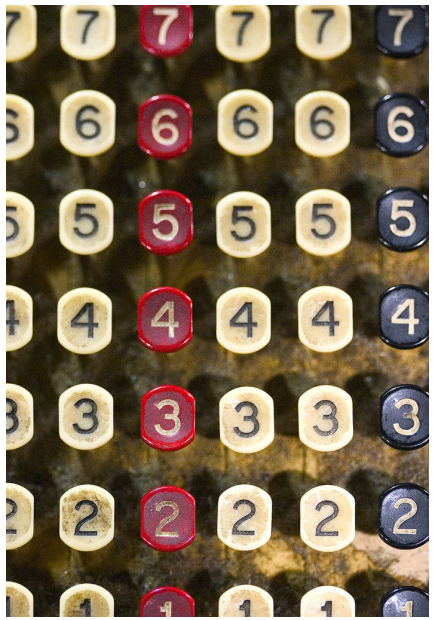

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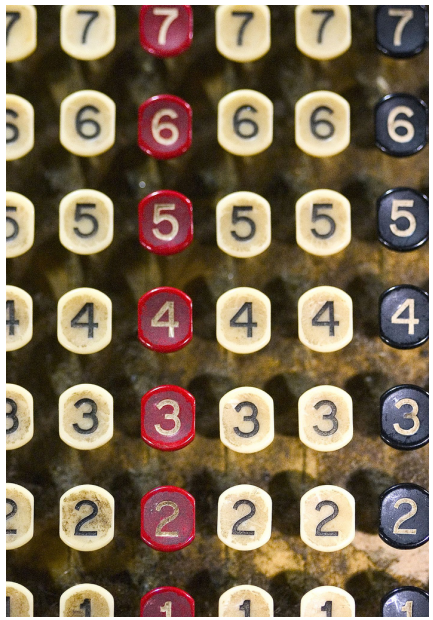

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PyCuda: Vital Information

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

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Outline

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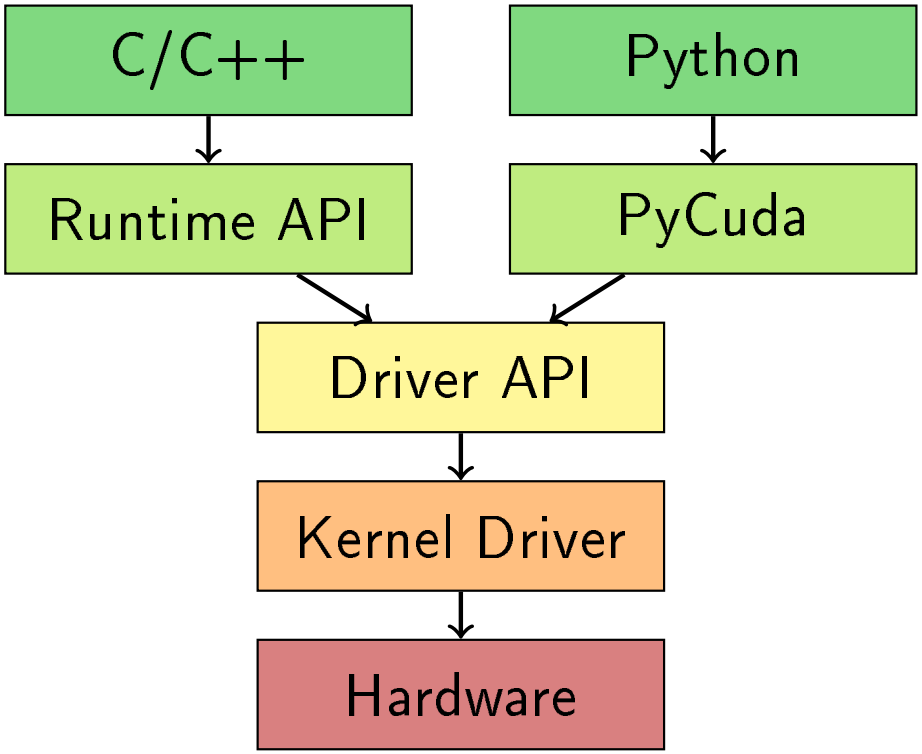
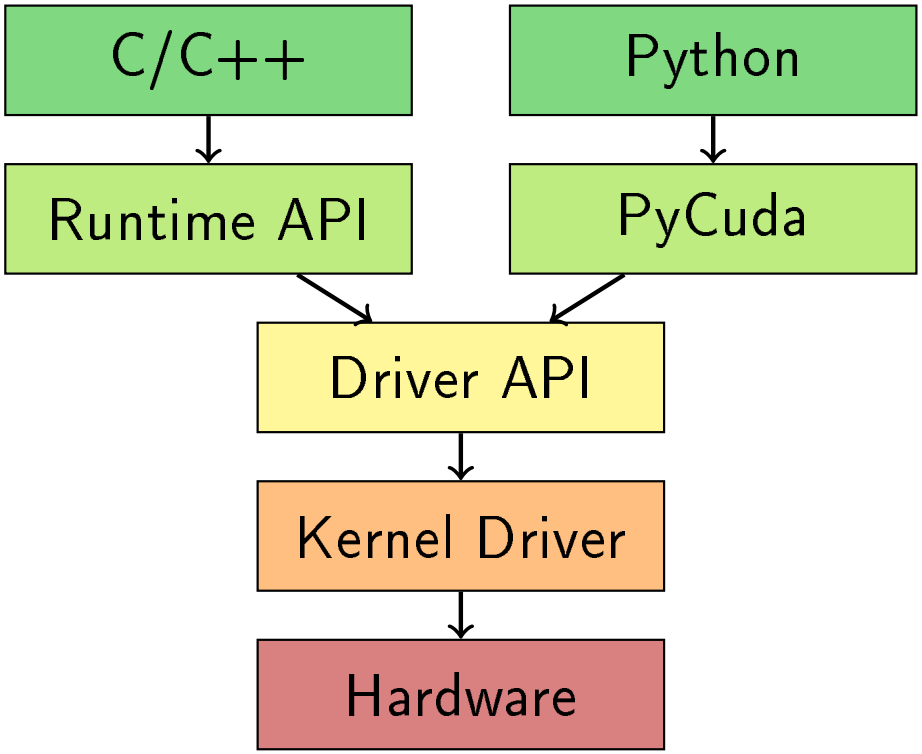
CUDA APIs


C/C++
Python
Runtime API
PyCuda
Driver API
Kernel Driver
Hardware

CUDA APIs



CUDA has two Programming Interfaces:

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- "Driver"


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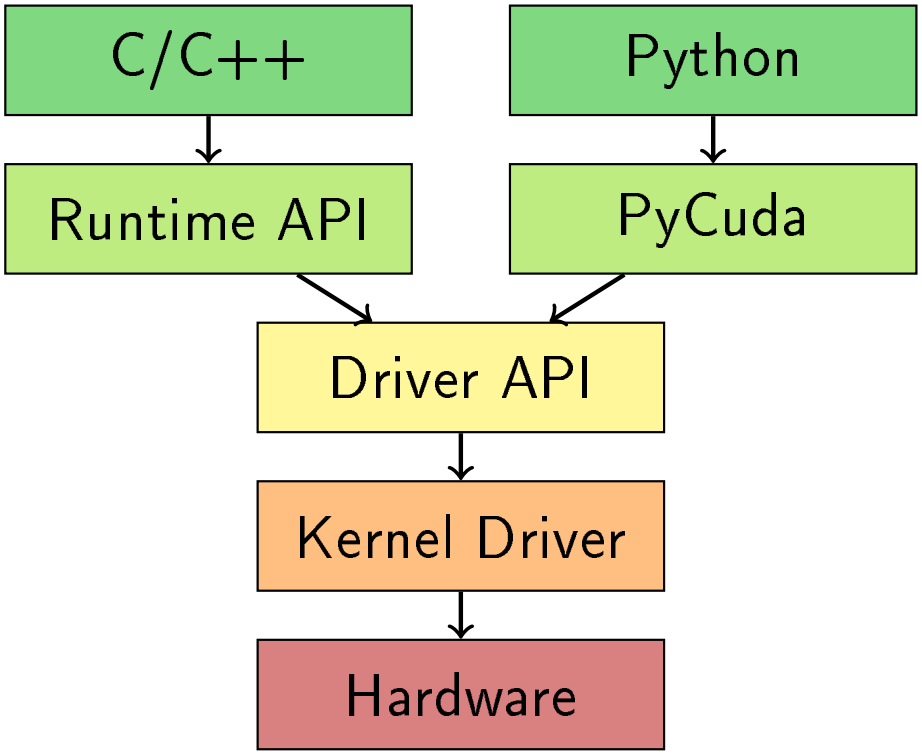
CUDA APIs



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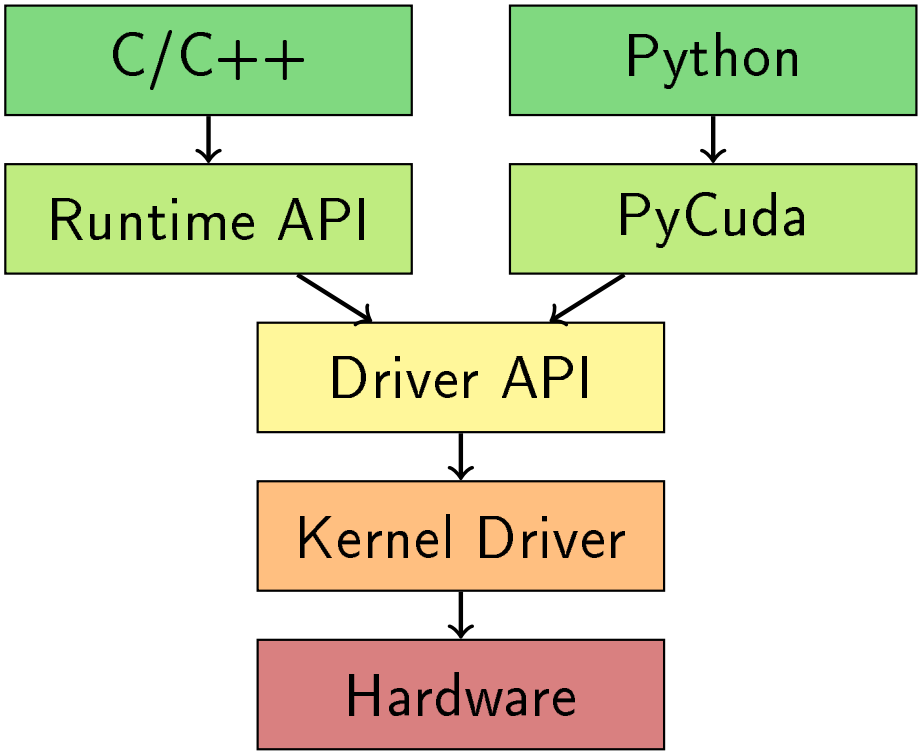
CUDA APIs



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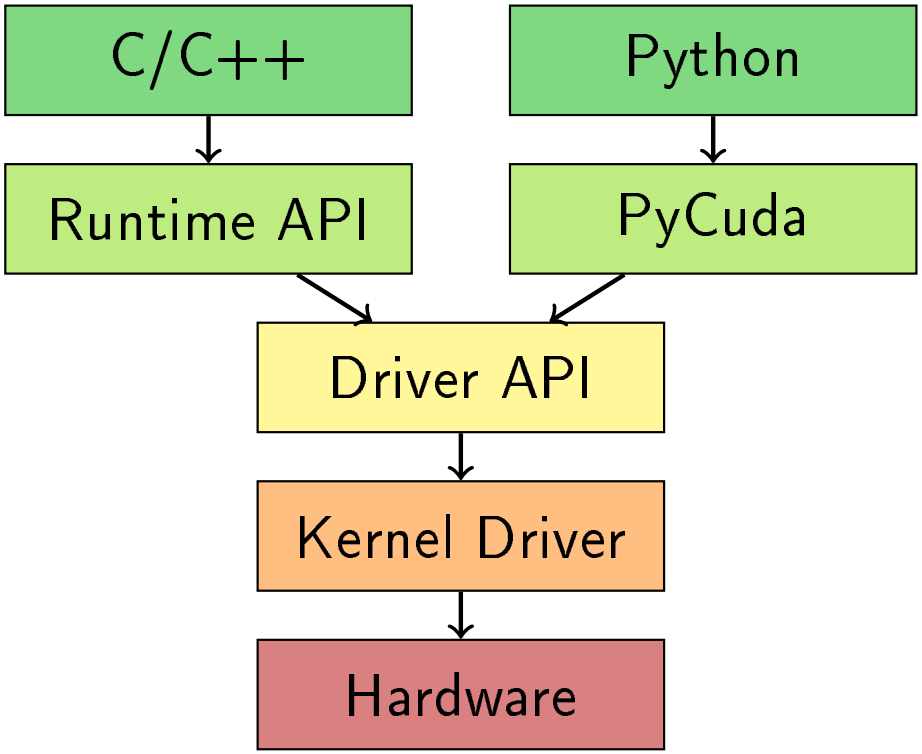
CUDA APIs



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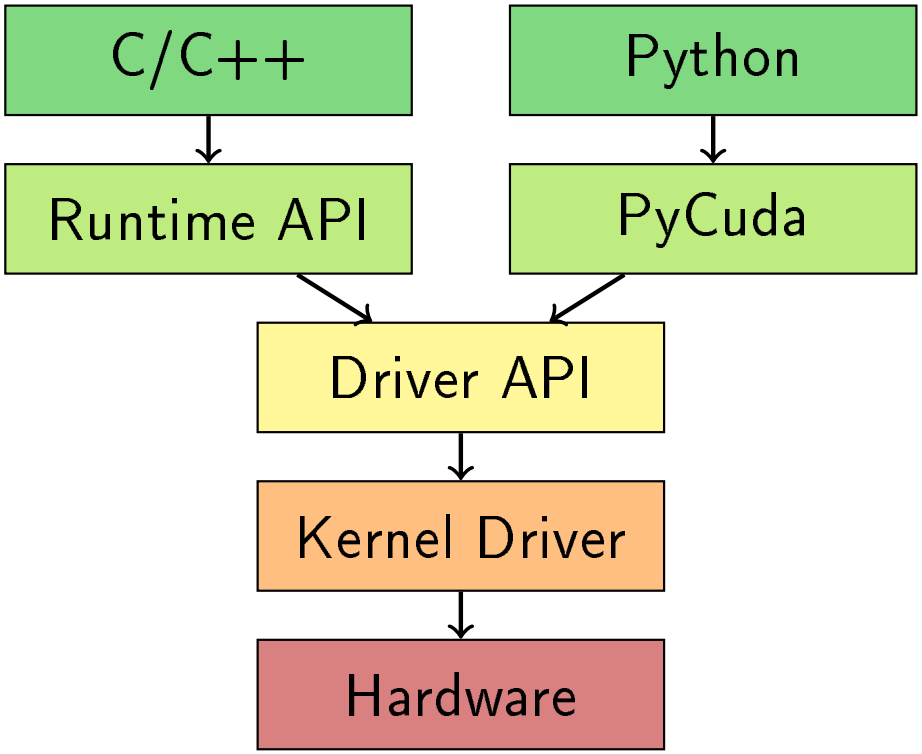

CUDA has two Programming Interfaces:

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(mutually exclusive)

Runtime vs. Driver API

Runtime $\leftrightarrow$ Driver differences:

- Explicit initialization.

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- Only needs `nvcc` for compiling GPU code.

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Runtime vs. Driver API

Runtime $\leftrightarrow$ Driver differences:

- Explicit initialization.
- Code objects ("Modules") become programming language objects.
- Texture handling requires slightly more work.
- Only needs `nvcc` for compiling GPU code.

Driver API:

- Conceptually cleaner
- Less sugar-coating (provide in Python)
- Not very different otherwise

PyCuda: API Tracing

With `./configure --cuda-trace=1`:

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With `./configure --cuda-trace=1`:

```
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.size * a.dtype.itemsize)
cuda.memcpy_htod(a_gpu, a)

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

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

```
cuInit
cuDeviceGetCount
cuDeviceGet
cuCtxCreate
cuMemAlloc
cuMemcpyHtoD
cuCtxGetDevice
cuDeviceComputeCapability
cuModuleLoadData
cuModuleGetFunction
cuFuncSetBlockShape
cuParamSetv
cuParamSetSize
cuLaunchGrid
cuMemcpyDtoH
cuCtxPopCurrent
cuCtxPushCurrent
cuMemFree
cuCtxPopCurrent
cuCtxPushCurrent
cuModuleUnload
cuCtxPopCurrent
cuCtxDestroy
```

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Questions?

?

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Outline

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CUDA C code
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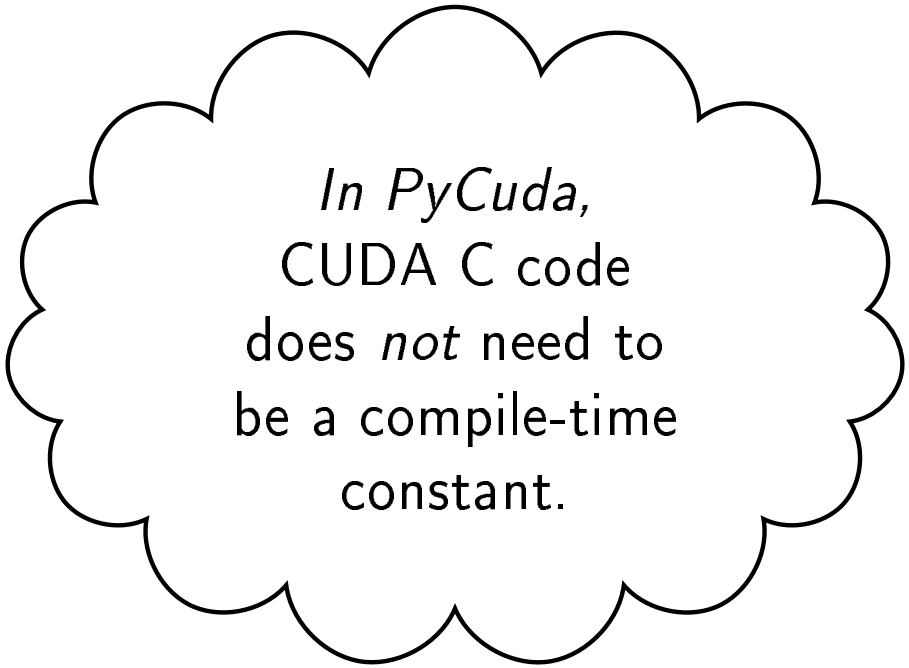
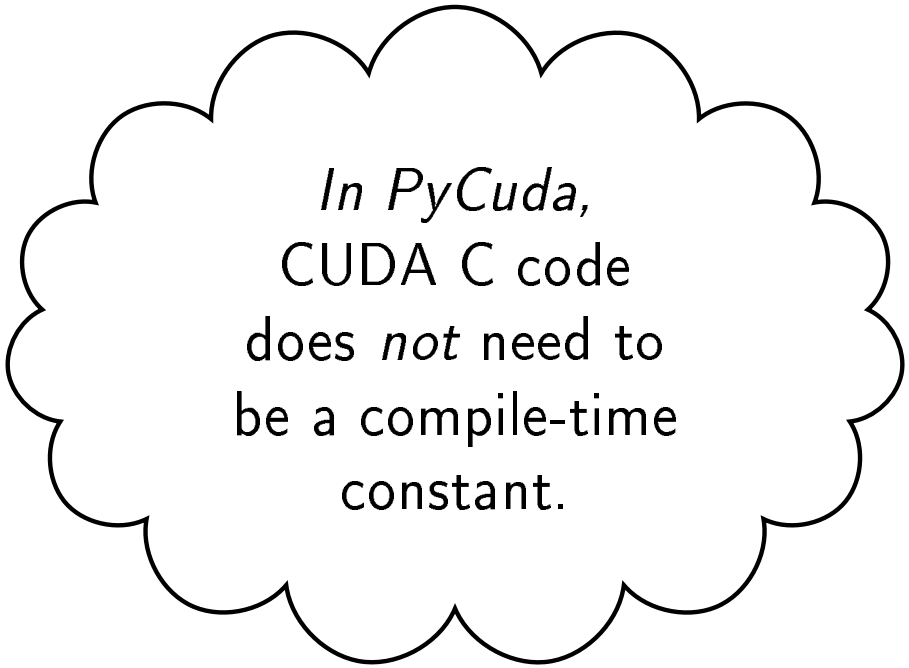
Metaprogramming



(unlike the CUDA Runtime API)

Metaprogramming

Idea



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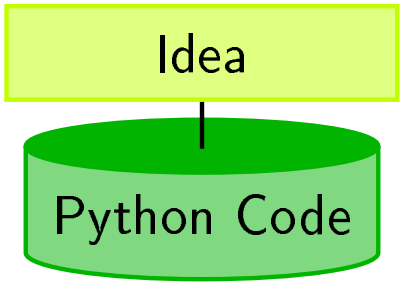
Metaprogramming



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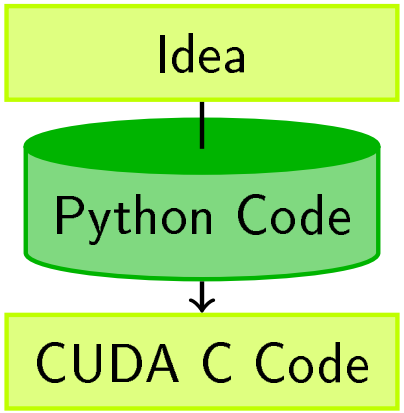

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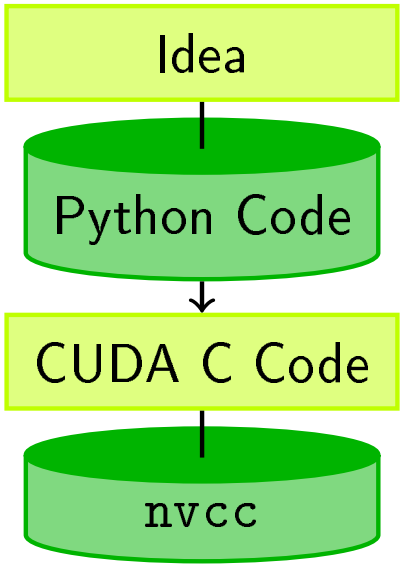

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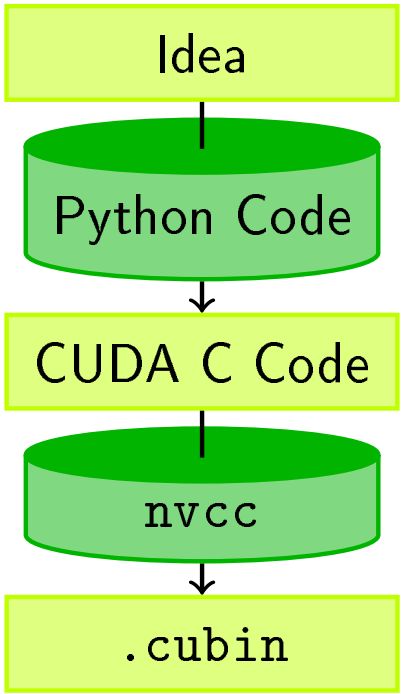

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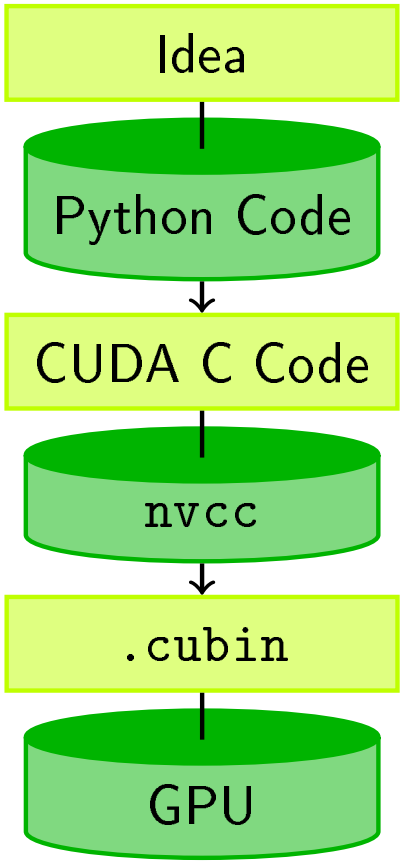

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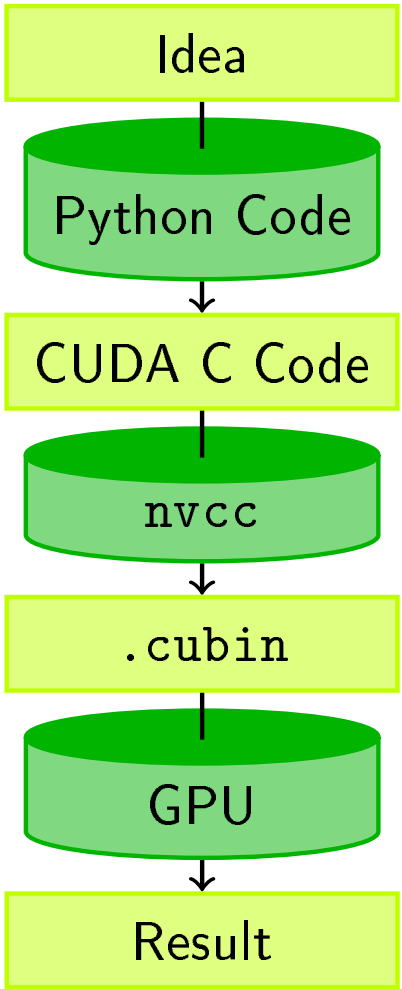

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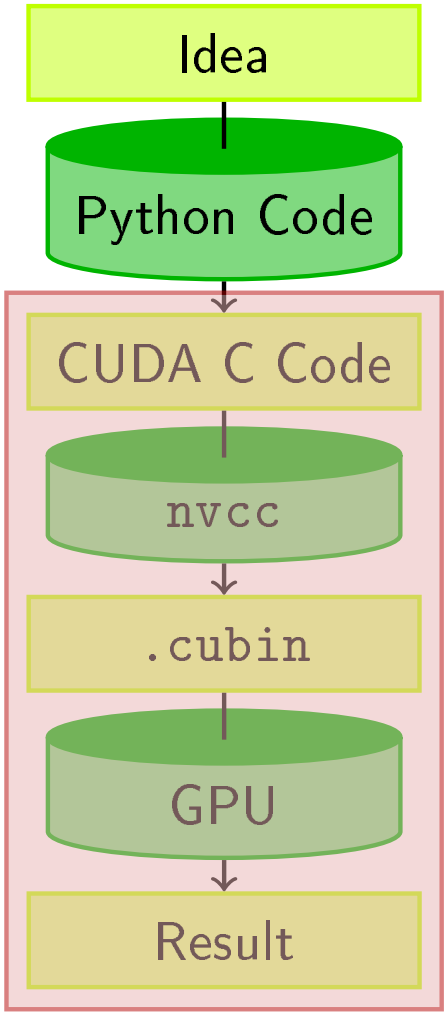

Machine

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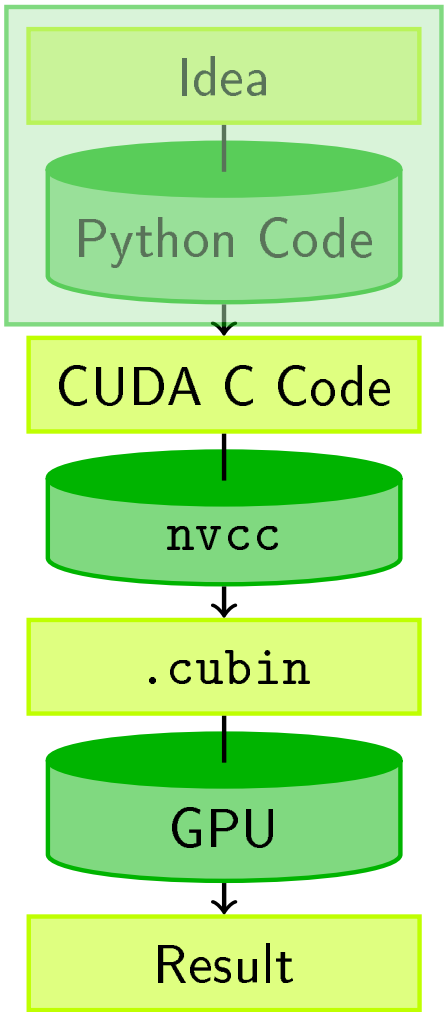

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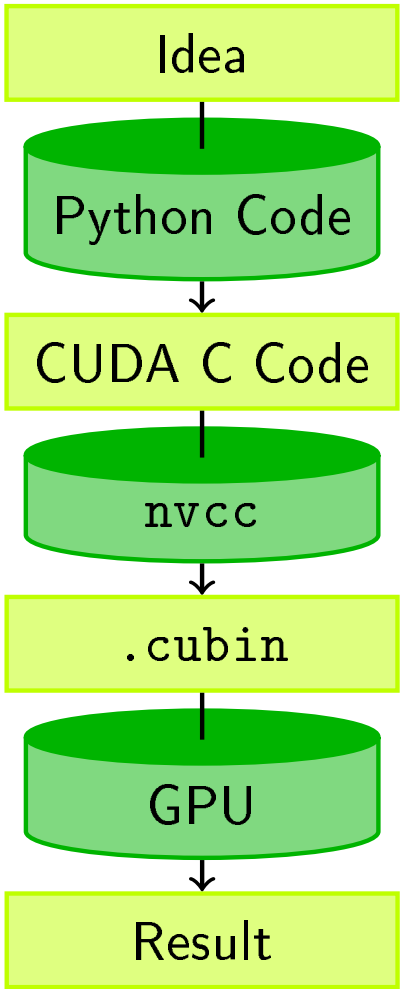

Easy to write

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Machine-generated Code

Why machine-generate code?

- Automated Tuning
  (cf. ATLAS, FFTW)

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  - Unreleased (but in public VC–ask me)

Questions?

?

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Outline

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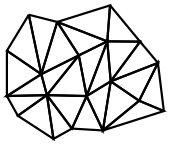
Discontinuous Galerkin Method

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



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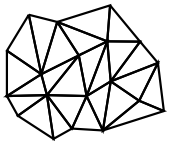

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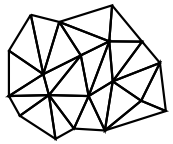

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Example

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:

$$0 = \int_{D_k} u_t \varphi + [\nabla \cdot F(u)] \varphi \, dx$$

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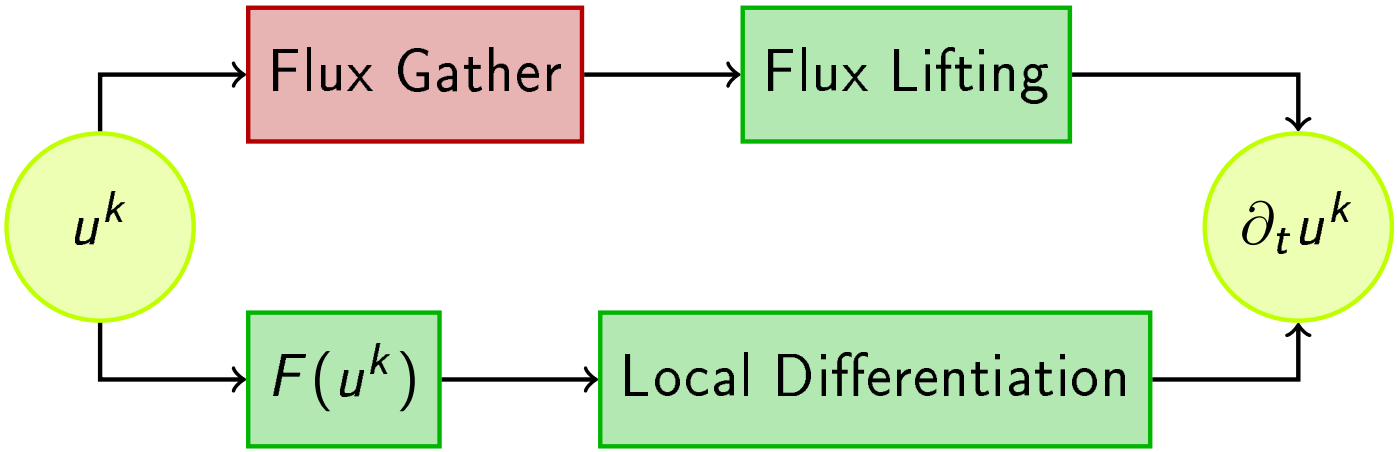
For straight-sided simplicial elements:
Reduce D^{∂_ν} and L to reference matrices.

Decomposition of a DG operator into Subtasks

DG's execution decomposes into two (mostly) separate branches:



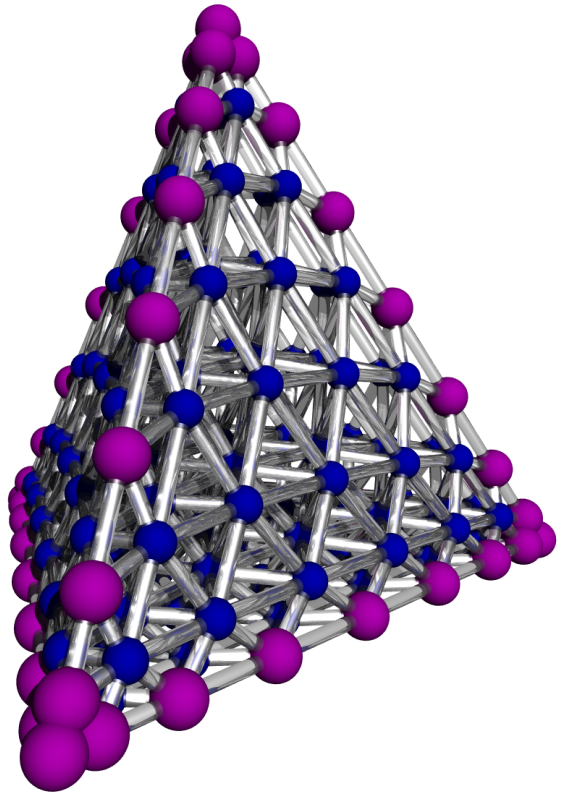
Green: Element-local parts of the DG operator.

Note: Explicit timestepping.

DG: Properties

Flexible:

- Variable order of accuracy



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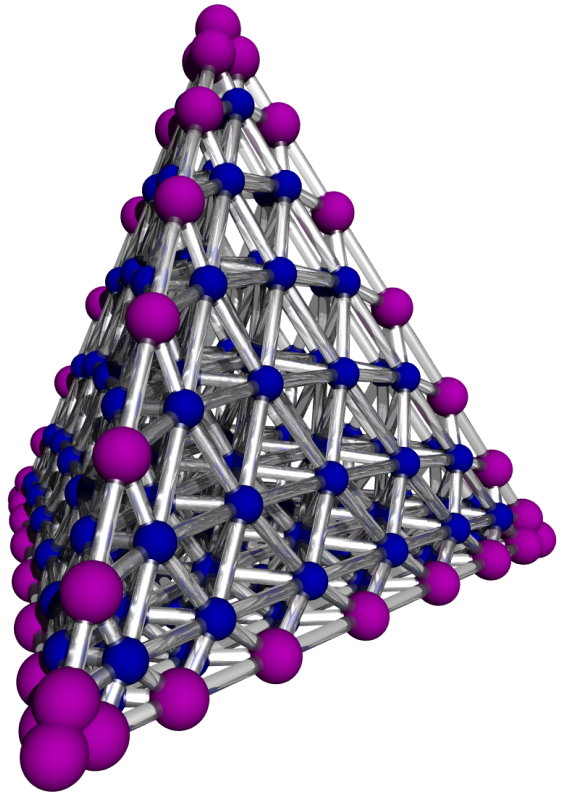

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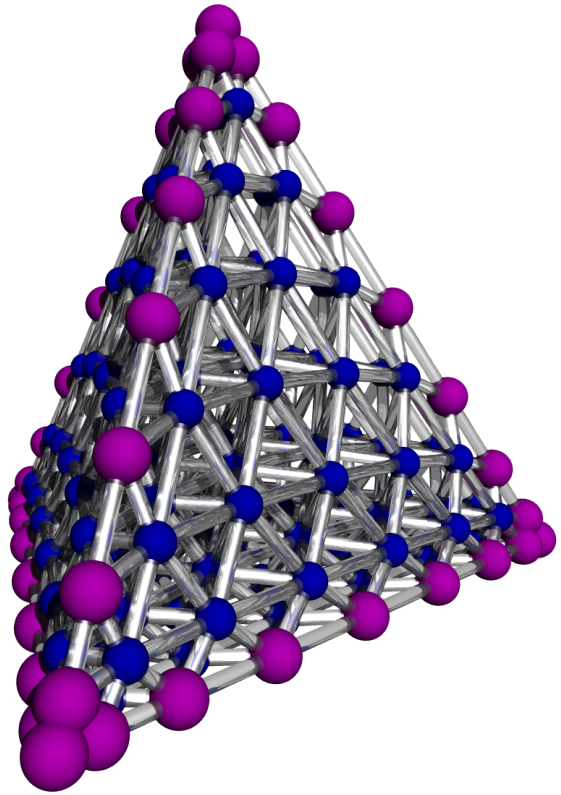

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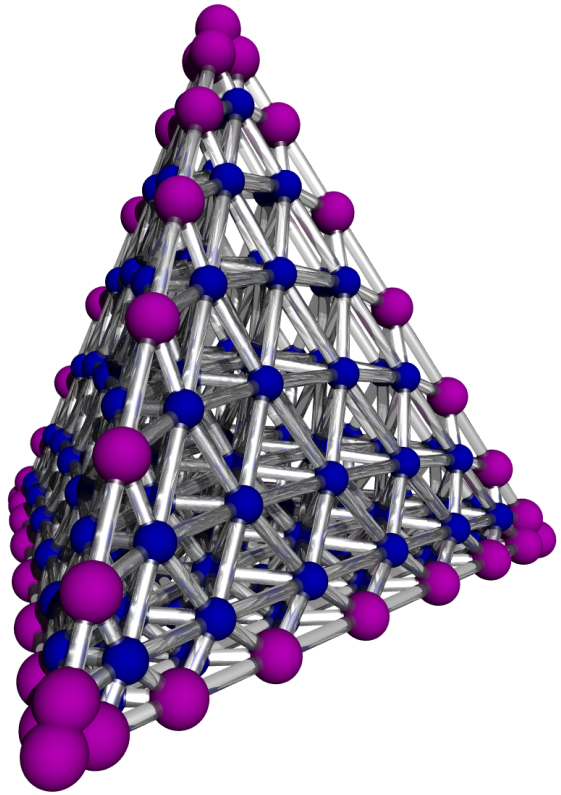

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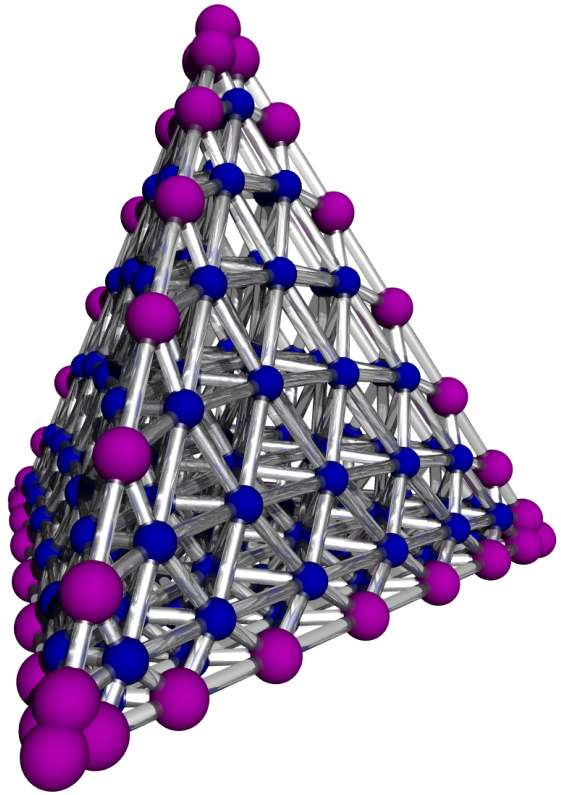

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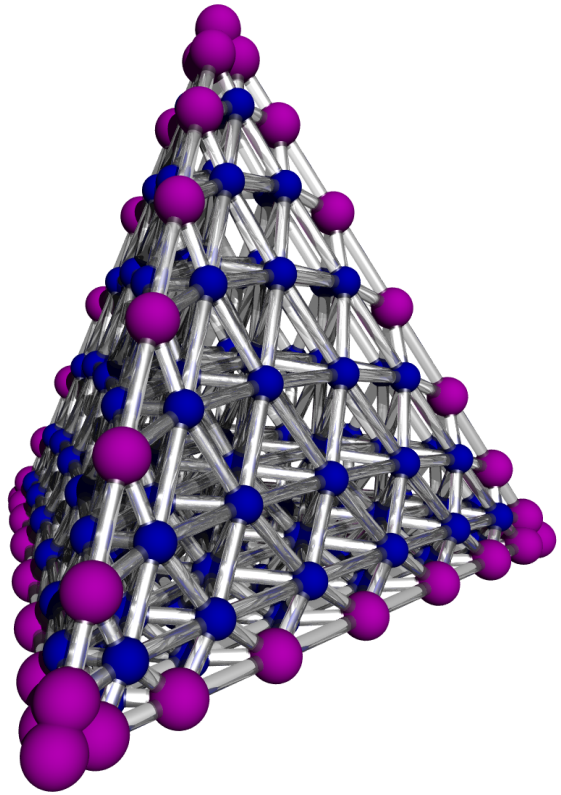

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DG: Properties

Flexible:

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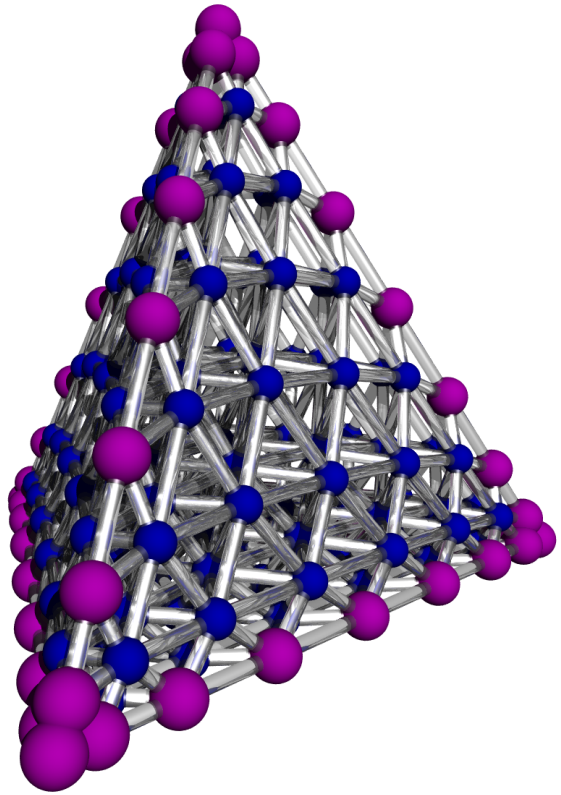
Implementation-friendly:

- Good stability properties
- Parallelizes well
- Simple (compared to other high-order unstructured methods)



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Why do DG on Graphics Cards?

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"A match made in heaven?"

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Outline

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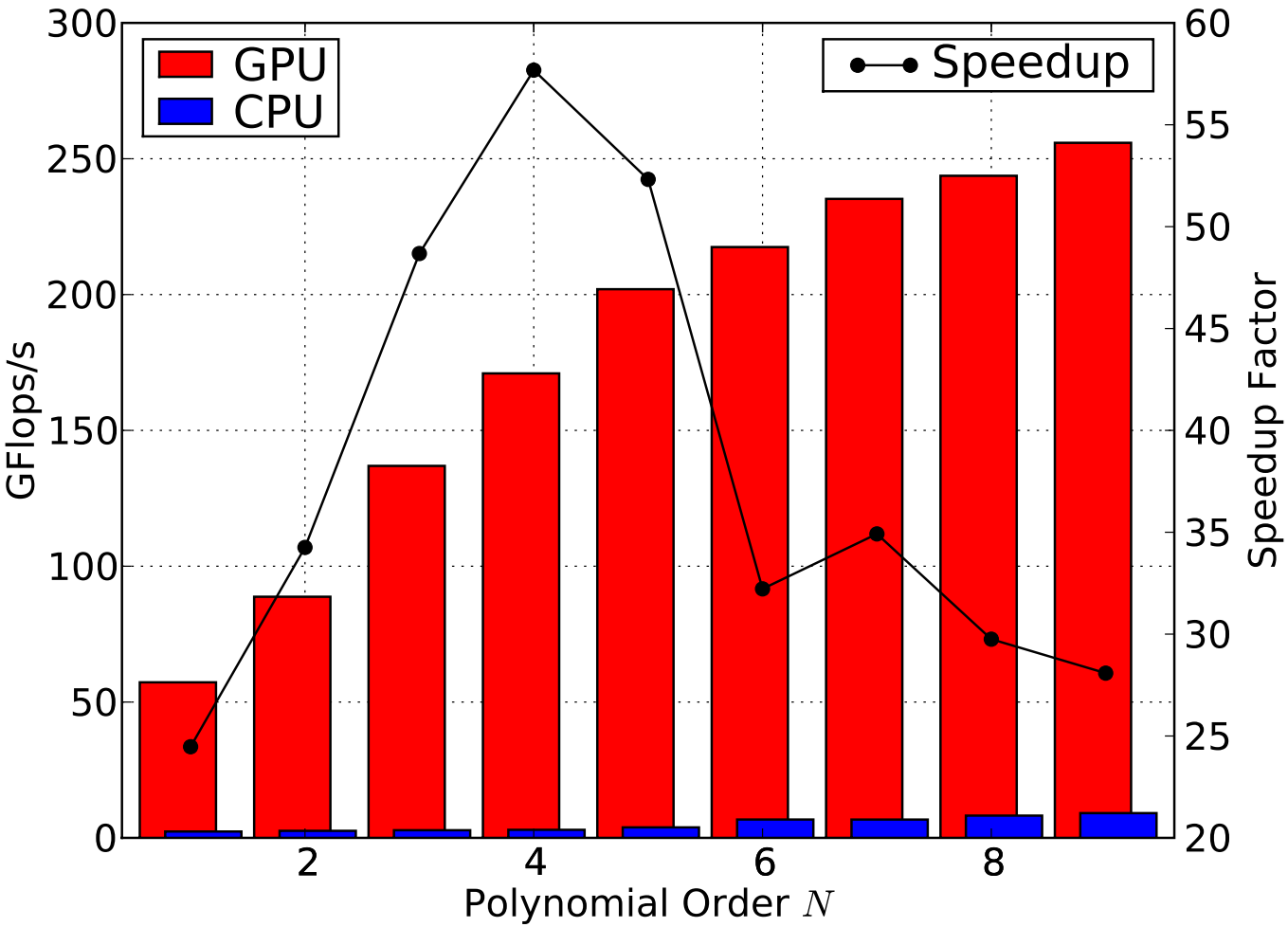
GTX280 vs. single core of Intel Core 2 Duo E8400



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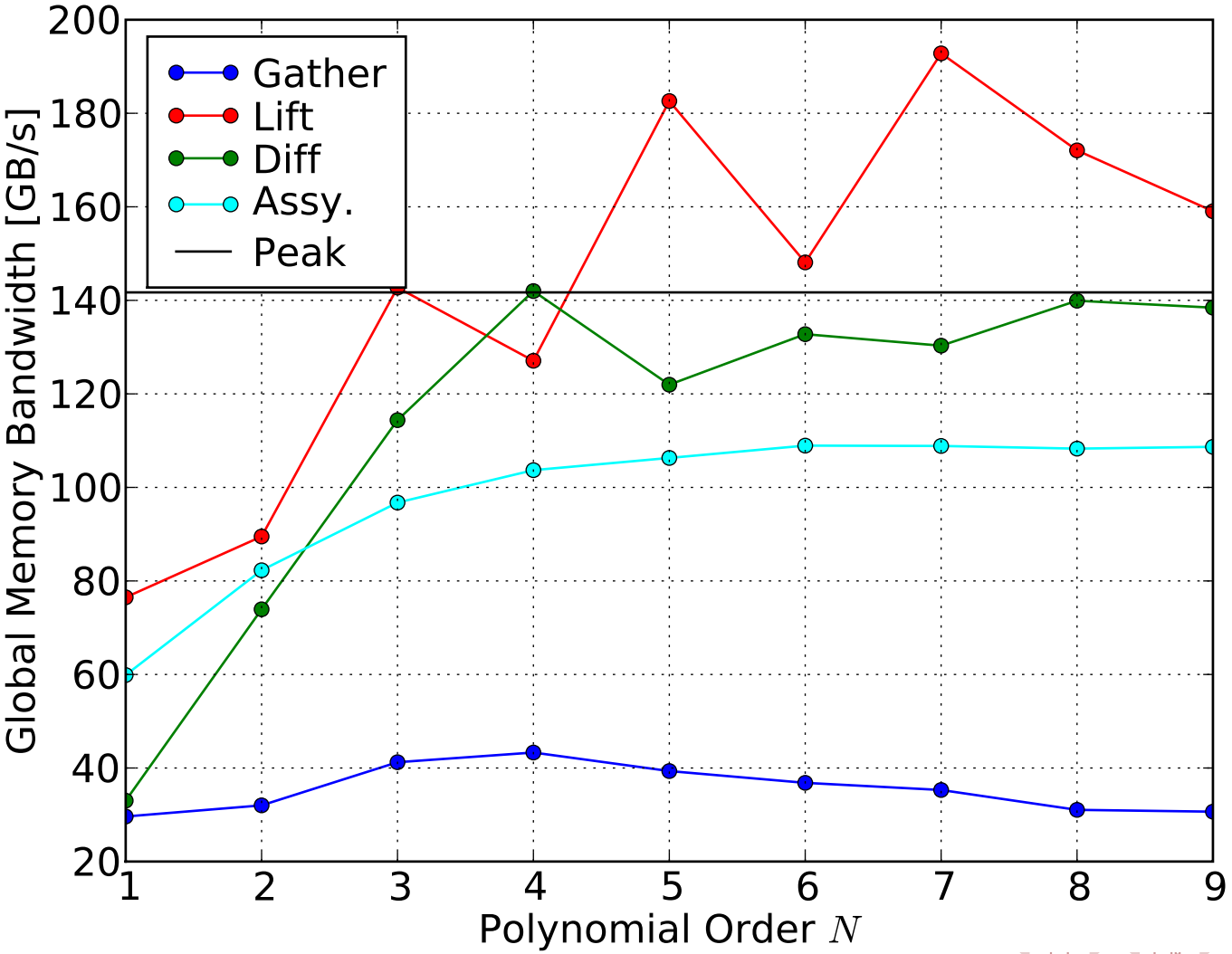
Memory Bandwidth on a GTX 280



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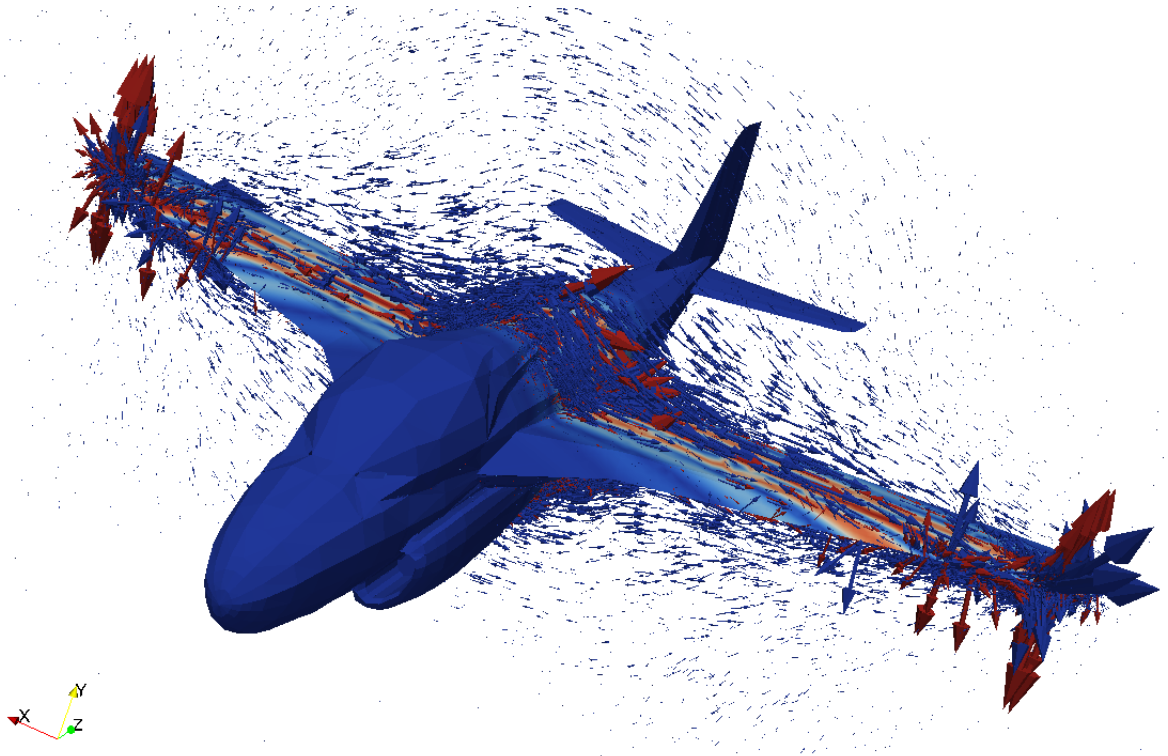
"Real-World" Scattering Calculation



Order $N = 4$,
78745 elements,
$2.7M \cdot 6$ DOFs,
single Tesla C1060.

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Outline

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- Fun time to be in computational science

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- Use Python and PyCuda to have even more fun :-)
  - With no compromise in performance
- CUDA tuning too tedious? Need more speed?
  - Automate it: Metaprogramming
- Further work in CUDA-DG:
  - Multi-GPU
  - Other equations (Euler, Poisson, possibly Navier-Stokes?)
  - Double Precision

Where to from here?

PyCuda Homepage

(also these slides, tonight)

→ `http://mathema.tician.de/software/pycuda`

CUDA-DG Preprint

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

→ `http://arxiv.org/abs/0901.1024`

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Questions?

?

Thank you for your attention!

http://mathema.tician.de/software/pycuda

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