Easy, Effective, Efficient: GPU Programming in Python with PyOpenCL and PyCUDA

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Outline

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The OpenCL Ecosystem: One Language, Many Devices

OpenCL generalizes over many types of devices:

- Multicore CPUs
- Various GPU architectures
- Accelerator boards

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Devices differ by

- Memory Types, Latencies, Bandwidths
- Vector Widths
- Units of Scheduling

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Devices differ by

- Memory Types, Latencies, Bandwidths
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Optimally tuned code will (often) be different for each device

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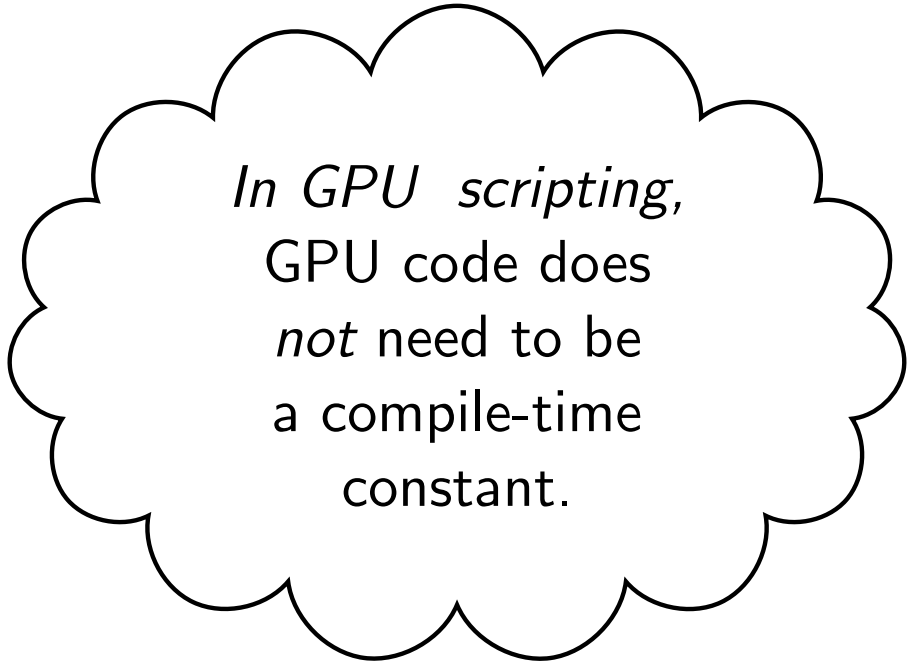
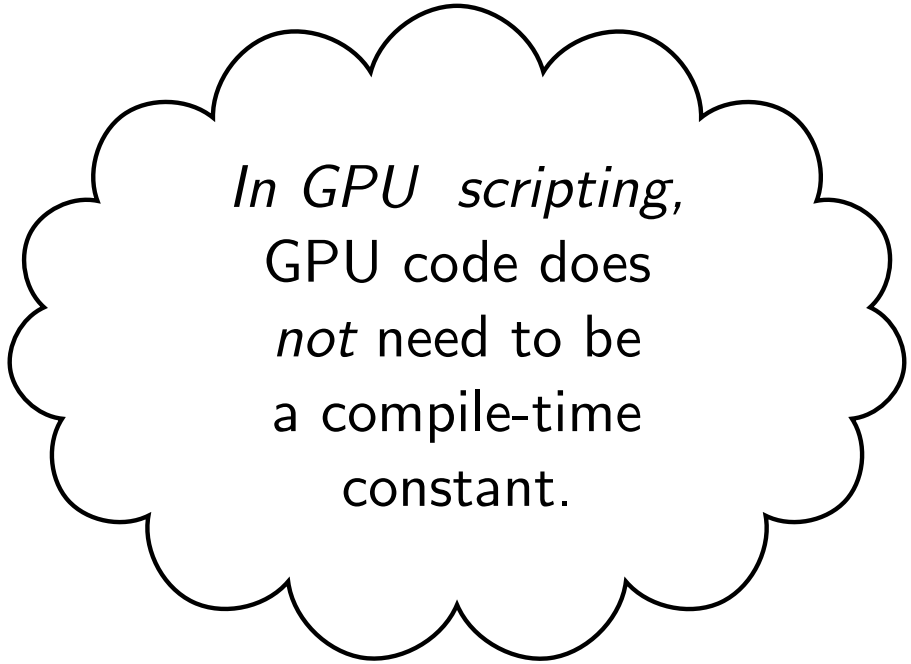
Metaprogramming



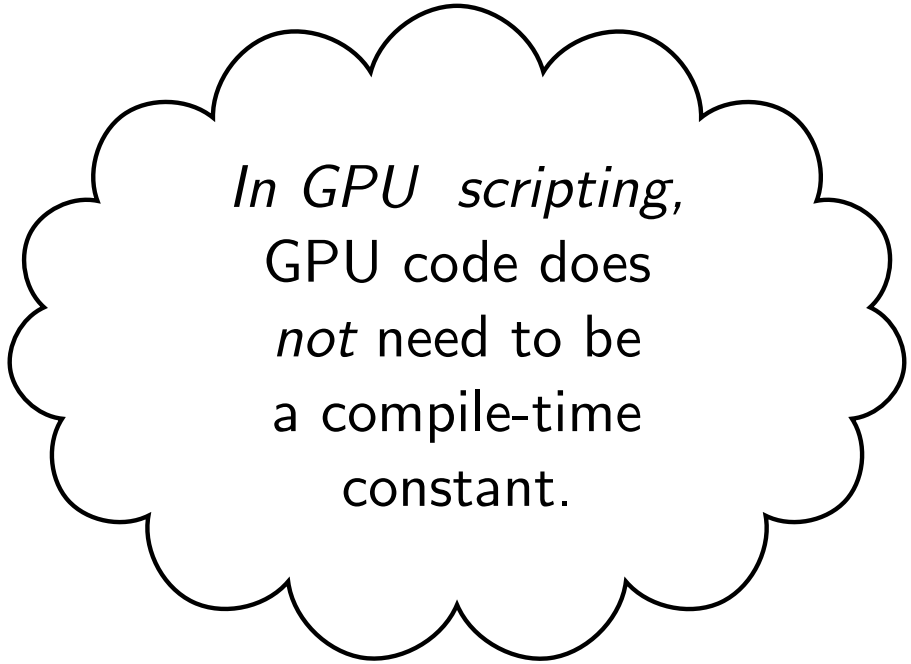
Metaprogramming



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

Metaprogramming

Idea



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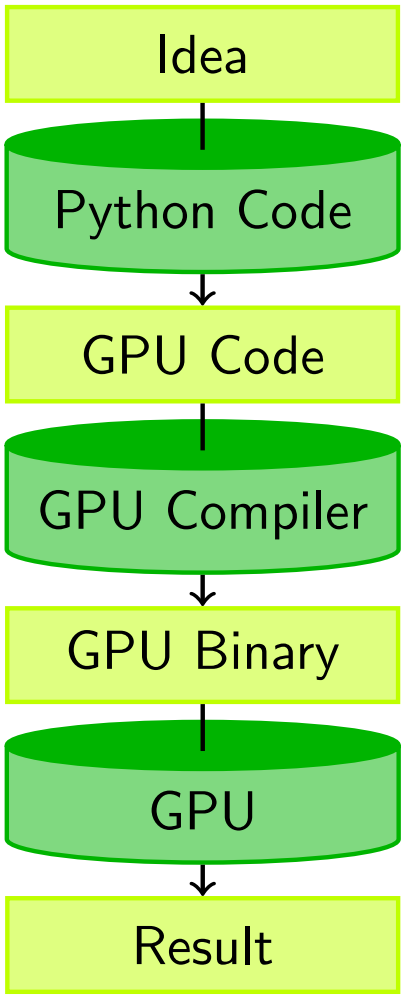

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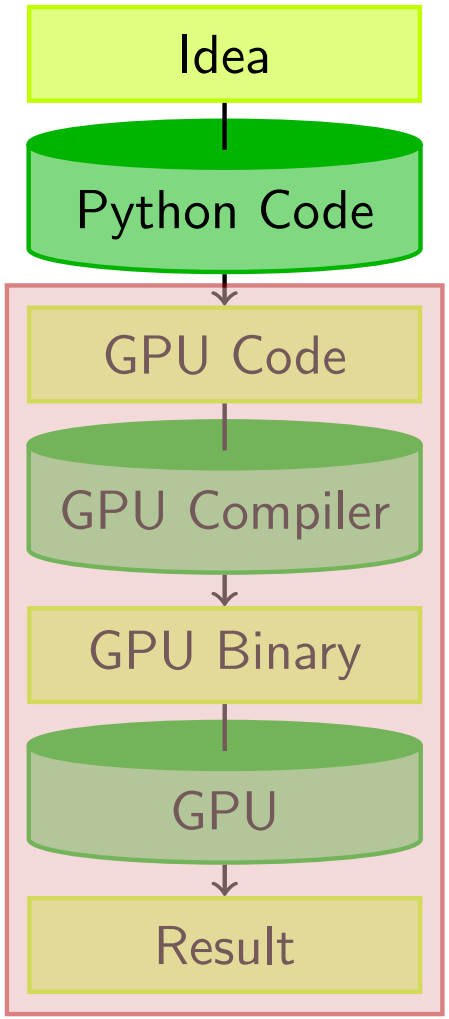

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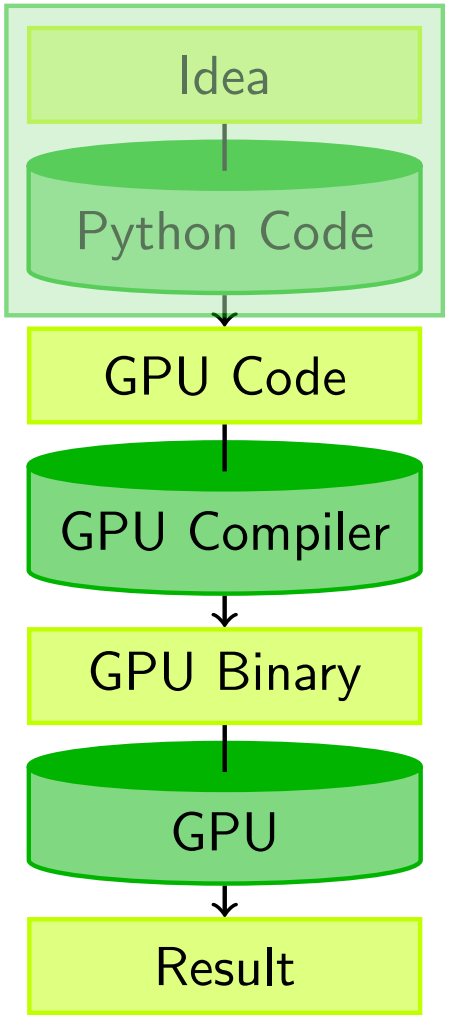

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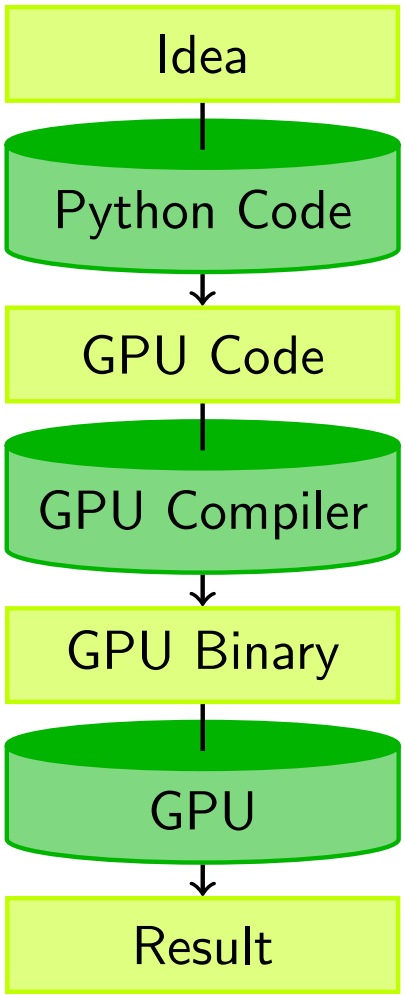

Good for code generation

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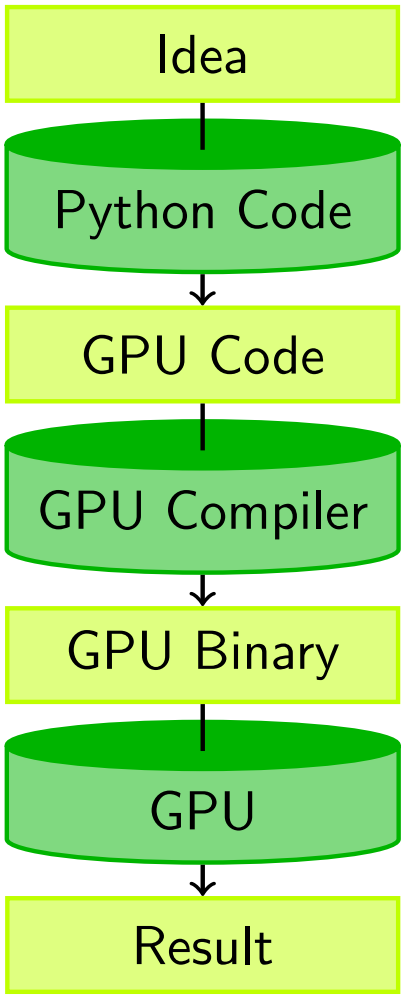

Good for code generation

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

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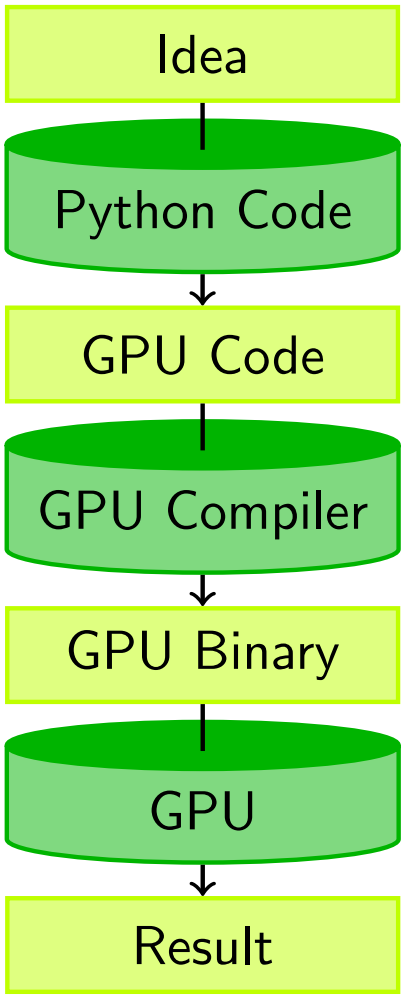

Good for code generation

In PyOpenCL 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

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PyOpenCL: Support for Metaprogramming

Three (main) ways of generating code:

- Simple %-operator substitution
  - Combine with C preprocessor: simple, often sufficient
- Use a templating engine (Mako works very well)
- `codepy`:
  - Build C syntax trees from Python
  - Generates readable, indented C

Many ways of evaluating code–most important one:

- Exact device timing via events

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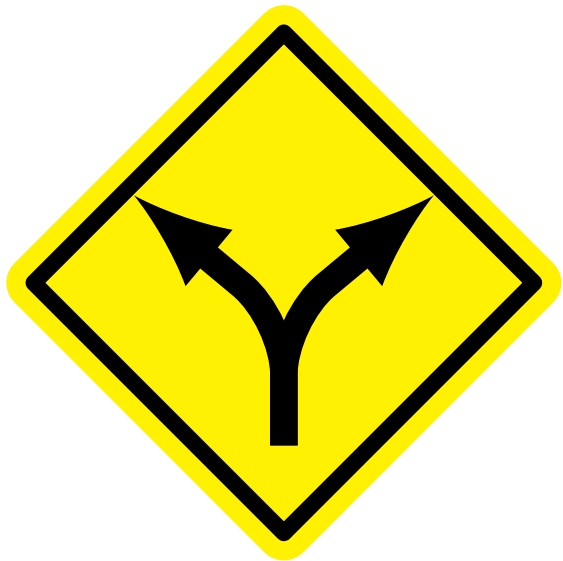
How are High-Performance Codes constructed?

- "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.



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pyopencl.elementwise: Elementwise expressions

Avoiding extra store-fetch cycles for elementwise math:

```
n = 10000
a_gpu = cl_array.to_device(
        ctx, queue, numpy.random.randn(n).astype(numpy.float32))
b_gpu = cl_array.to_device(
        ctx, queue, numpy.random.randn(n).astype(numpy.float32))

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

c_gpu = cl_array.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
```

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RTCG via Substitution

```
source = ("""
    __kernel void %(name)s(%(arguments)s)
    {
      unsigned lid = get_local_id (0);
      unsigned gsize = get_global_size (0);
      unsigned work_item_start = get_local_size (0)*get_group_id (0);

      for (unsigned i = work_item_start + lid; i < n; i += gsize)
      {
        %(operation)s;
      }
    }
    """ % {
      "arguments": ", ".join(arg.declarator() for arg in arguments),
      "operation": operation,
      "name": name,
      "loop_prep": loop_prep,
      })

prg = cl.Program(ctx, source).build()
```

RTCG via Templates

```
from mako.template import Template

tpl = Template("""
    __kernel void add(
            __global ${ type_name } *tgt,
            __global const ${ type_name } *op1,
            __global const ${ type_name } *op2)
    {
      int idx = get_local_id(0)
        + ${ local_size } * ${ thread_strides }
        * get_group_id(0);

      % for i in range( thread_strides ):
          <% offset = i* local_size %>
          tgt[idx + ${ offset }] =
            op1[idx + ${ offset }]
            + op2[idx + ${ offset } ];
      % endfor
    }""")

rendered_tpl = tpl.render(type_name="float",
    local_size=local_size, thread_strides=thread_strides)
```

RTCG via AST Generation

```
from cgen import *
from cgen.opencl import \
        CLKernel, CLGlobal, CLRequiredWorkGroupSize

mod = Module([
    FunctionBody(
        CLKernel(CLRequiredWorkGroupSize((local_size,),
            FunctionDeclaration(Value("void", "twice"),
            arg_decls=[CLGlobal(Pointer(Const(POD(dtype, "tgt"))))])),
        Block([
            Initializer (POD(numpy.int32, "idx"),
                " get_local_id (0) + %d * get_group_id(0)"
                % ( local_size * thread_strides ))
            ]+[
            Statement("tgt[idx+%d] *= 2" % (o*local_size))
            for o in range( thread_strides )]
            ))])

knl = cl.Program(ctx, str(mod)).build(). twice
```

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Reduction

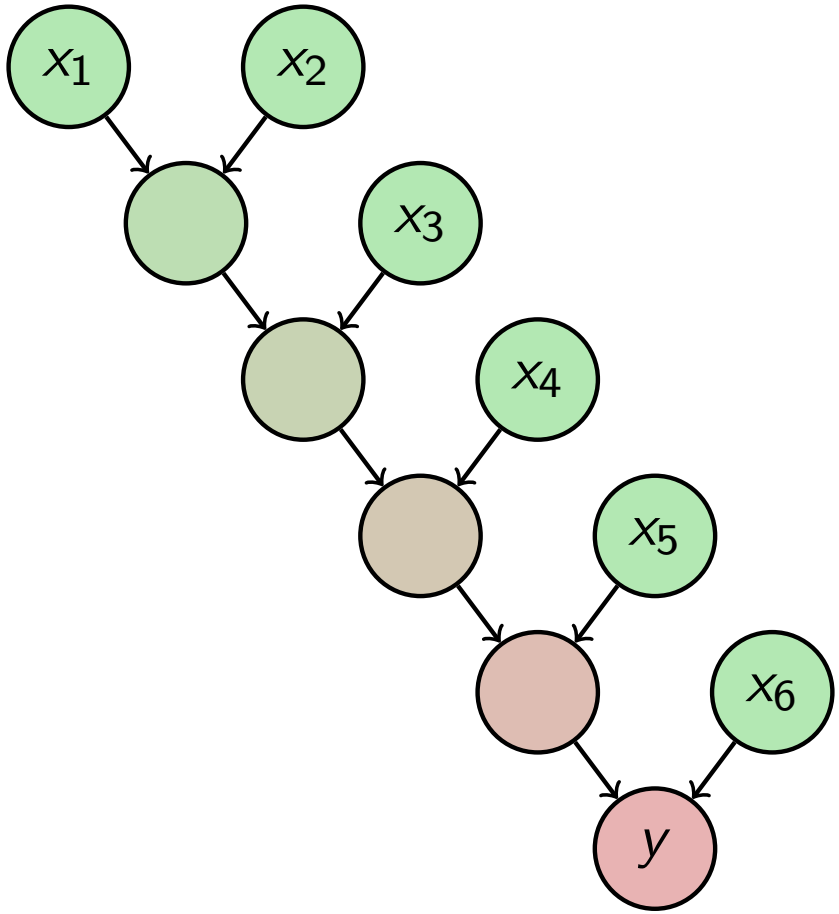
$$y = f(\cdots f(f(x_1, x_2), x_3), \ldots, x_N)$$

where N is the input size.

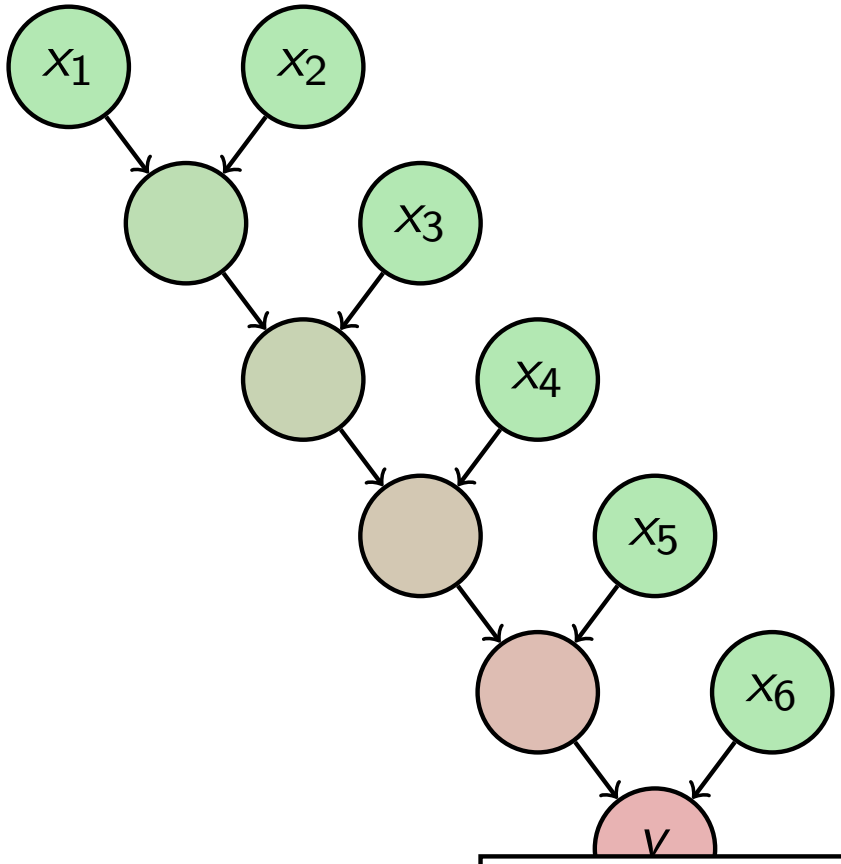
Also known as...

- Lisp/Python function `reduce` (Scheme: `fold`)
- C++ STL `std::accumulate`

Reduction: Graph

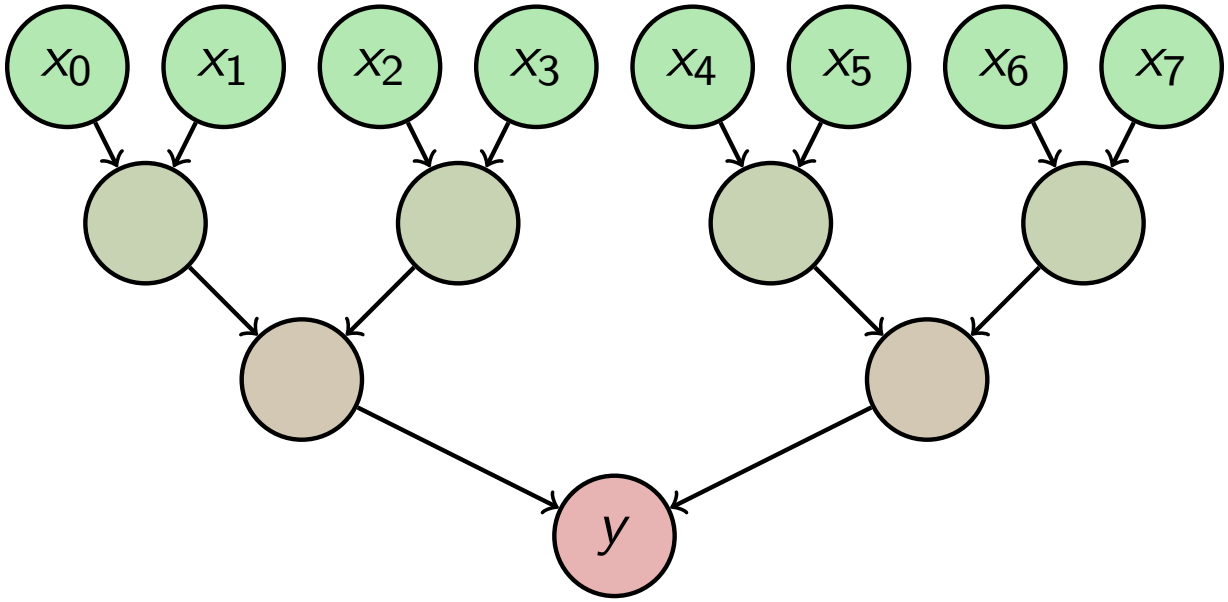


Reduction: Graph



Painful! Not parallelizable.

Reduction: A Better Graph



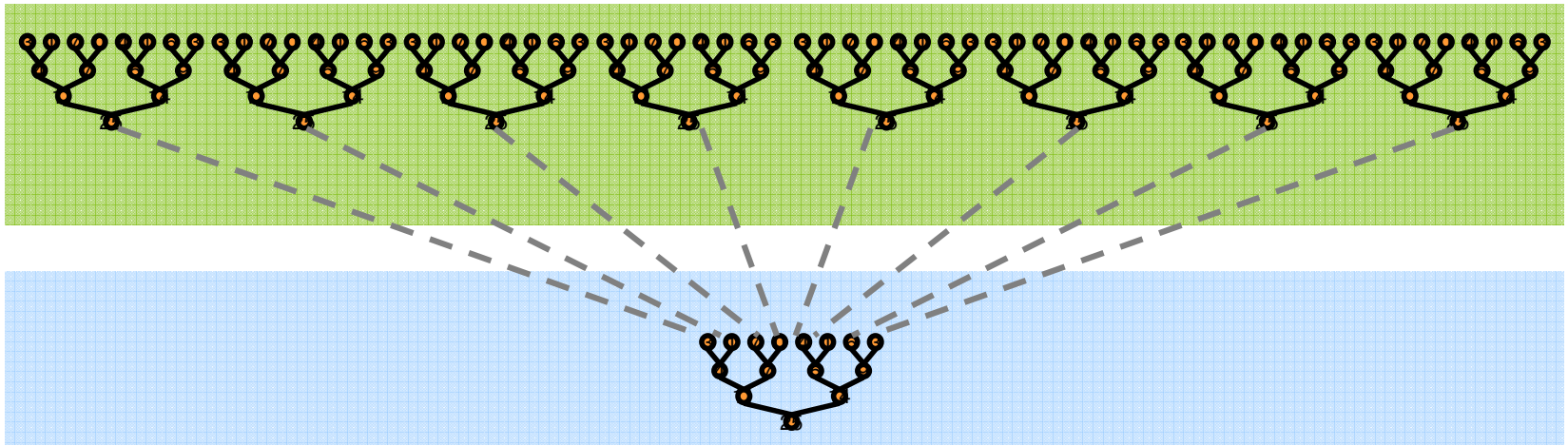
Mapping Reduction to the GPU

- Obvious: Want to use tree-based approach.
- Problem: Two scales, Work group and Grid
  - Need to occupy both to make good use of the machine.
- In particular, need synchronization after each tree stage.

With material by M. Harris (Nvidia Corp.)

Mapping Reduction to the GPU

- Obvious: Want to use tree-based approach.
- Problem: Two scales, Work group and Grid
  - Need to occupy both to make good use of the machine.
- In particular, need synchronization after each tree stage.
- Solution: Use a two-scale algorithm.



In particular: Use multiple grid invocations to achieve inter-group synchronization.

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Kernel V1

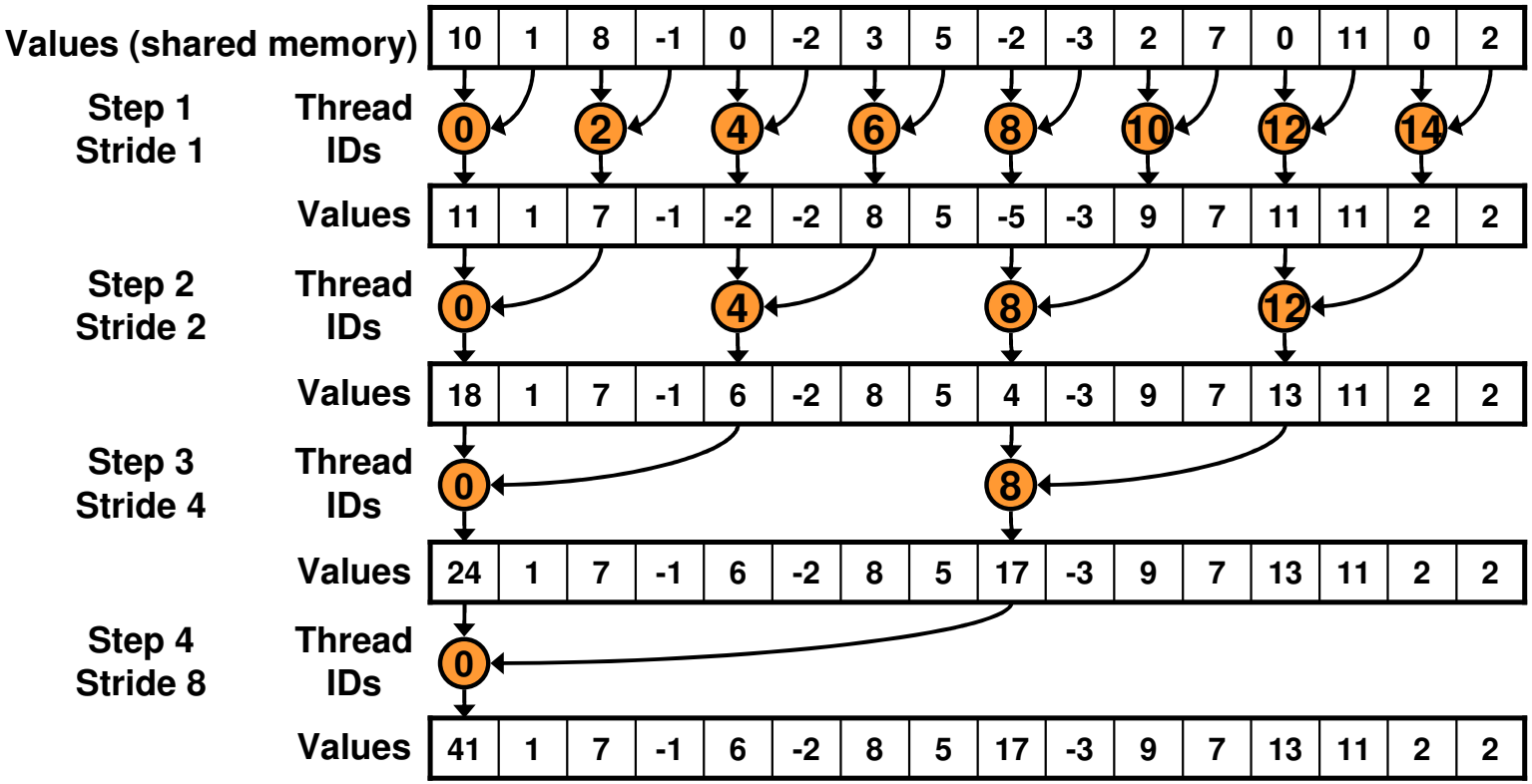
```
__kernel void reduce0(__global T *g_idata, __global T *g_odata,
    unsigned int n, __local T* ldata)
{
    unsigned int lid = get_local_id(0);
    unsigned int i = get_global_id(0);

    ldata[lid] = (i < n) ? g_idata[i] : 0;
    barrier(CLK_LOCAL_MEM_FENCE);

    for(unsigned int s=1; s < get_local_size(0); s *= 2)
    {
        if ((lid % (2*s)) == 0)
            ldata[lid] += ldata[lid + s];
        barrier(CLK_LOCAL_MEM_FENCE);
    }

    if (lid == 0) g_odata[get_group_id(0)] = ldata[0];
}
```

Interleaved Addressing



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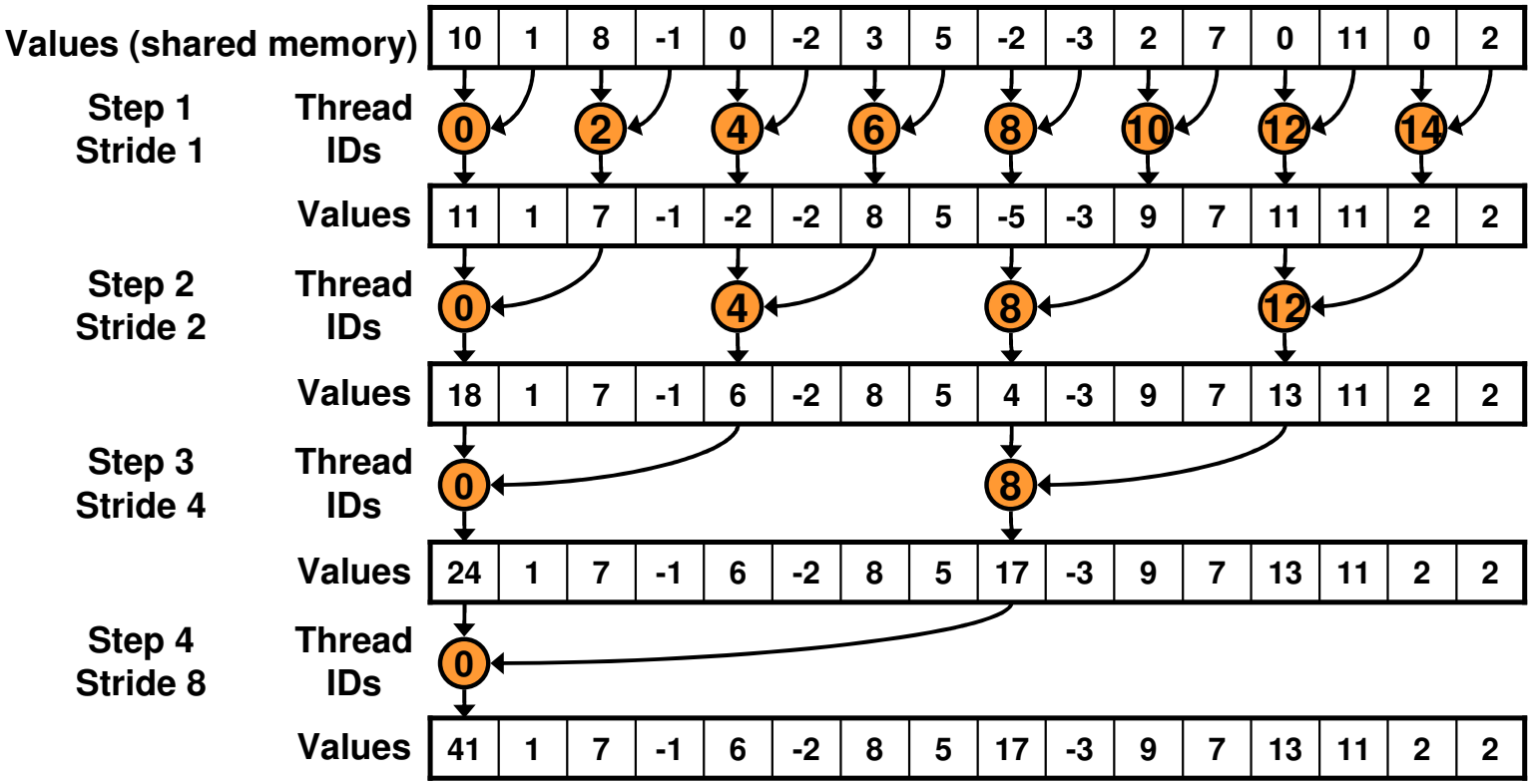

Issue: Slow modulo, Divergence

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Kernel V2

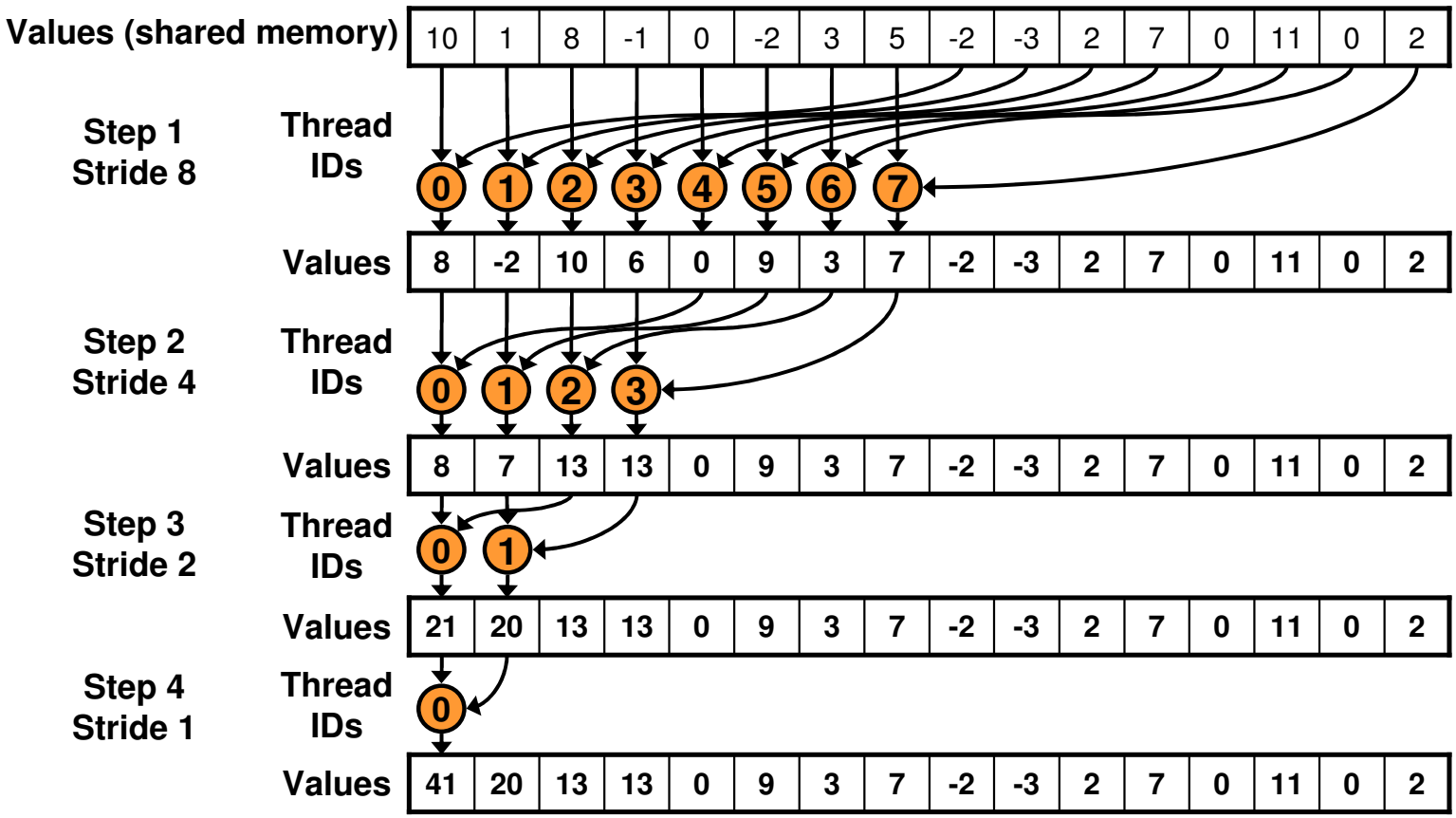
```
__kernel void reduce2(__global T *g_idata, __global T *g_odata,
    unsigned int n, __local T* ldata)
{
    unsigned int lid = get_local_id (0);
    unsigned int i = get_global_id (0);

    ldata[lid] = (i < n) ? g_idata[i] : 0;
    barrier (CLK_LOCAL_MEM_FENCE);

    for(unsigned int s= get_local_size (0)/2; s>0; s>>=1)
    {
        if (lid < s)
            ldata[lid] += ldata[lid + s];
        barrier (CLK_LOCAL_MEM_FENCE);
    }

    if (lid == 0) g_odata[get_local_size (0)] = ldata[0];
}
```

Sequential Addressing



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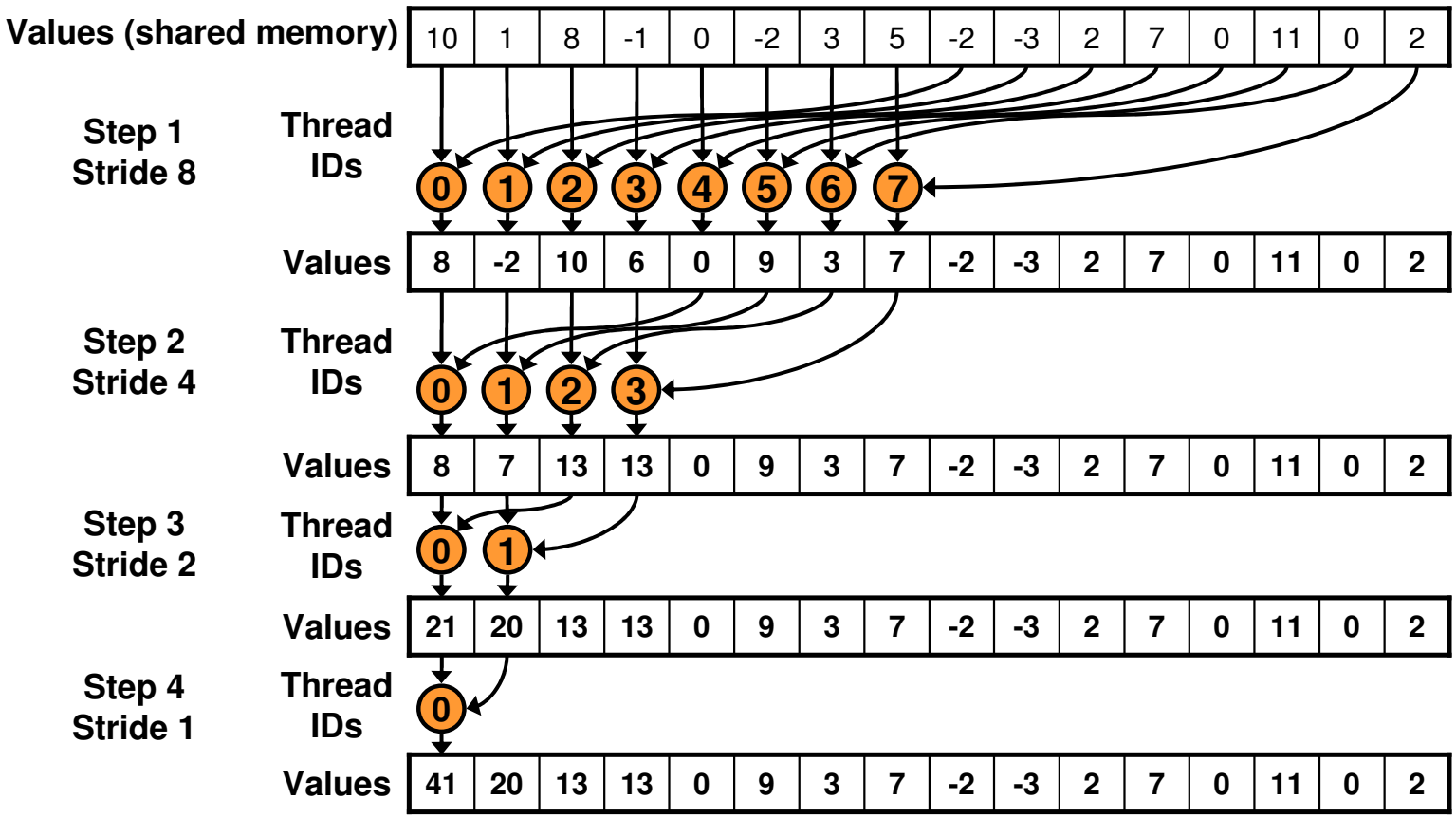
Sequential Addressing



Better! But still not "efficient".

Only half of all work items after first round, then a quarter, ...

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Thinking about Parallel Complexity

Distinguish:

- Time on T processors: T_P
- **Step Complexity/Span** T_∞: Minimum number of steps taken if an infinite number of processors are available
- Work per step S_t
- **Work Complexity/Work** $T_1 = \sum_{t=1}^{T_\infty} S_t$: Total number of operations performed
- **Parallelism** T_1/T_∞: average amount of work along span
  - $P > T_1/T_\infty$ doesn't make sense.

Algorithm-specific!

Thinking about Parallel Complexity

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  - $P > T_1/T_\infty$ c

Algorithm-specific!

- How parallel is our current version?
- Can we improve it?

Kernel V3 Part 1

```
__kernel void reduce6(__global T *g_idata, __global T *g_odata,
    unsigned int n, volatile __local T* ldata)
{
    unsigned int lid = get_local_id (0);
    unsigned int i = get_group_id(0)*(
        get_local_size (0)*2) + get_local_id (0);
    unsigned int gridSize = GROUP_SIZE*2*get_num_groups(0);
    ldata[lid] = 0;

    while (i < n)
    {
        ldata[lid] += g_idata[i];
        if (i + GROUP_SIZE < n)
            ldata[lid] += g_idata[i+GROUP_SIZE];
        i += gridSize;
    }
    barrier (CLK_LOCAL_MEM_FENCE);
```

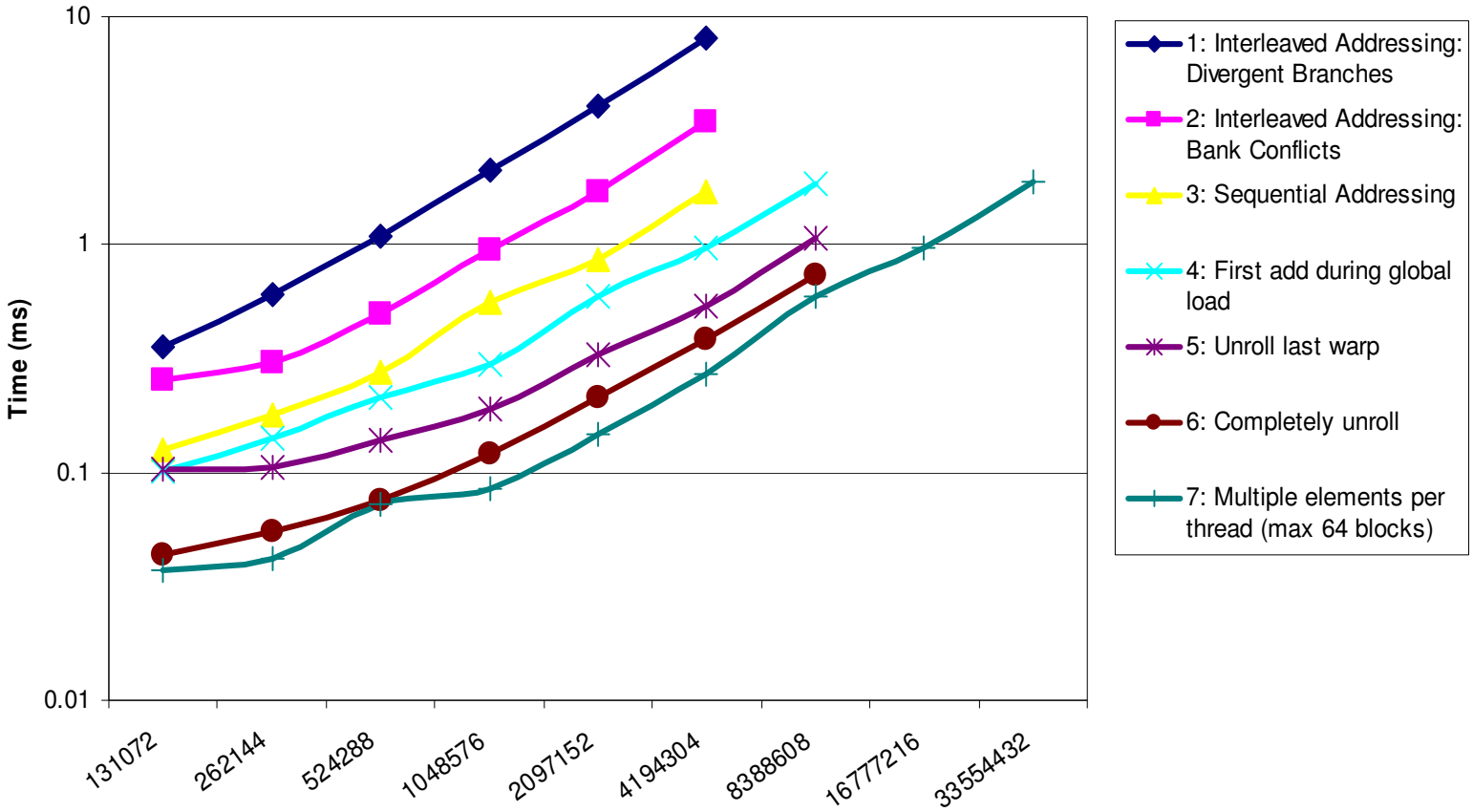
Kernel V3 Part 2

```
    if (GROUP_SIZE >= 512)
    {
      if (lid < 256) { ldata[lid] += ldata[lid + 256]; }
      barrier(CLK_LOCAL_MEM_FENCE);
    }
    // ...
    if (GROUP_SIZE >= 128)
    { /* ... */ }

    if (lid < 32)
    {
      if (GROUP_SIZE >= 64) { ldata[lid] += ldata[lid + 32]; }
      if (GROUP_SIZE >= 32) { ldata[lid] += ldata[lid + 16]; }
      // ...
      if (GROUP_SIZE >= 2) { ldata[lid] += ldata[lid + 1]; }
    }

    if (lid == 0) g_odata[get_group_id(0)] = ldata[0];
}
```

Performance Comparison



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Generic CL Reduction: Preparation

```
#define GROUP_SIZE ${group_size}
#define READ_AND_MAP(i) (${map_expr})
#define REDUCE(a, b) (${reduce_expr})

% if double_support:
    #pragma OPENCL EXTENSION cl_khr_fp64: enable
% endif

typedef ${out_type} out_type;

${preamble}
```

CL Reduction: Sequential Part

```
__kernel void ${name}(
  __global out_type *out, ${arguments},
  unsigned int seq_count, unsigned int n)
{
  __local out_type ldata[GROUP_SIZE];
  unsigned int lid = get_local_id(0);
  unsigned int i = get_group_id(0)*GROUP_SIZE*seq_count + lid;

  out_type acc = ${neutral};
  for (unsigned s = 0; s < seq_count; ++s)
  {
    if (i >= n) break;
    acc = REDUCE(acc, READ_AND_MAP(i));
    i += GROUP_SIZE;
  }
```

CL Reduction: Explicitly Synchronized Part

```
ldata[lid] = acc;

<% cur_size = group_size %>

% while cur_size > no_sync_size:
    barrier(CLK_LOCAL_MEM_FENCE);

    <%
    new_size = cur_size // 2
    assert new_size * 2 == cur_size
    %>

    if (lid < ${new_size})
    {
      ldata[lid] = REDUCE(
        ldata[lid],
        ldata[lid + ${new_size}]);
    }

    <% cur_size = new_size %>

% endwhile
```

CL Reduction: Implicitly Synchronized Part

```
        % if cur_size > 1:
            barrier(CLK_LOCAL_MEM_FENCE);

            if (lid < ${no_sync_size})
            {
                __local volatile out_type *lvdata = ldata;
                % while cur_size > 1:
                    <%
                    new_size = cur_size // 2
                    assert new_size * 2 == cur_size
                    %>
                    lvdata[lid] = REDUCE(
                      lvdata[lid],
                      lvdata[lid + ${new_size}]);
                    <% cur_size = new_size %>
                % endwhile
            }
        % endif

        if (lid == 0) out[get_group_id(0)] = ldata[0];
    }
```

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Judging Code Quality

Possible information sources for judging code quality/desirability:

- Heuristics (e.g. Occupancy, Flops/Byte, ...?)
- OpenCL Event profiling
  - Makes comp. synchronous on Nvidia!
- Wall time (!)
- Compiler build log
- Vendor Profiler

Search Strategies

Possible search strategies:

- Exhaustive
- Exhaustive + Heuristics
- Grouped Orthogonal Search
- Genetic Algorithms
- (your invention here)

Compiler cache makes repeated searches fast.

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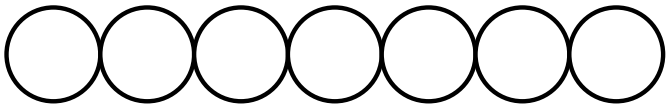
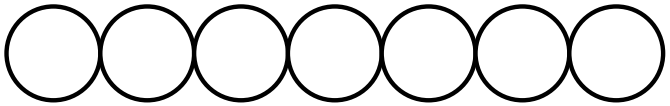
Grouped Orthogonal Search

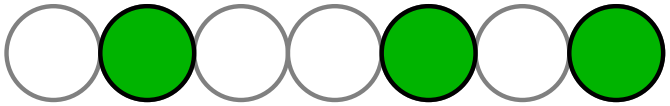


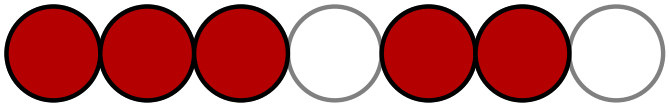
GAOS: Adrian Tate, Cray, Inc.

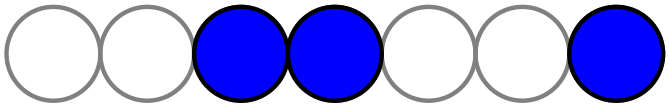
Grouped Orthogonal Search

Define groups









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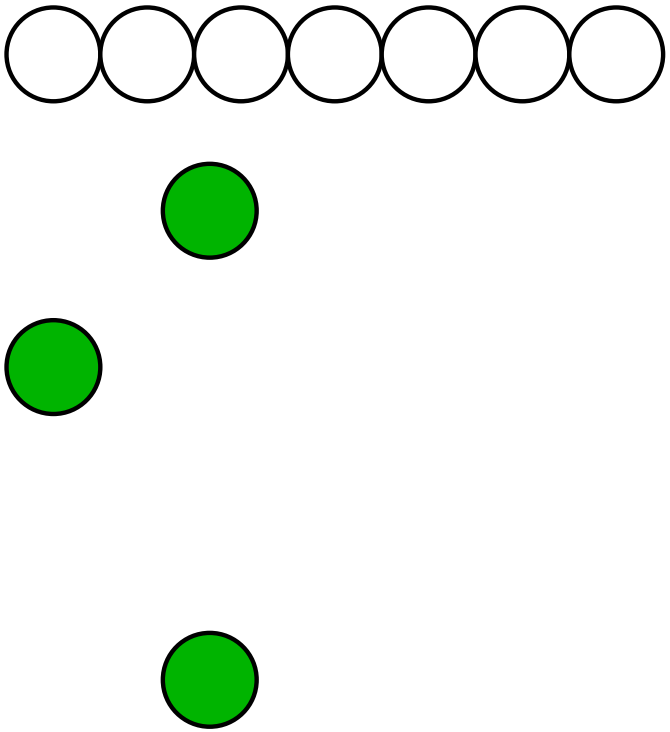
Grouped Orthogonal Search

Choose group



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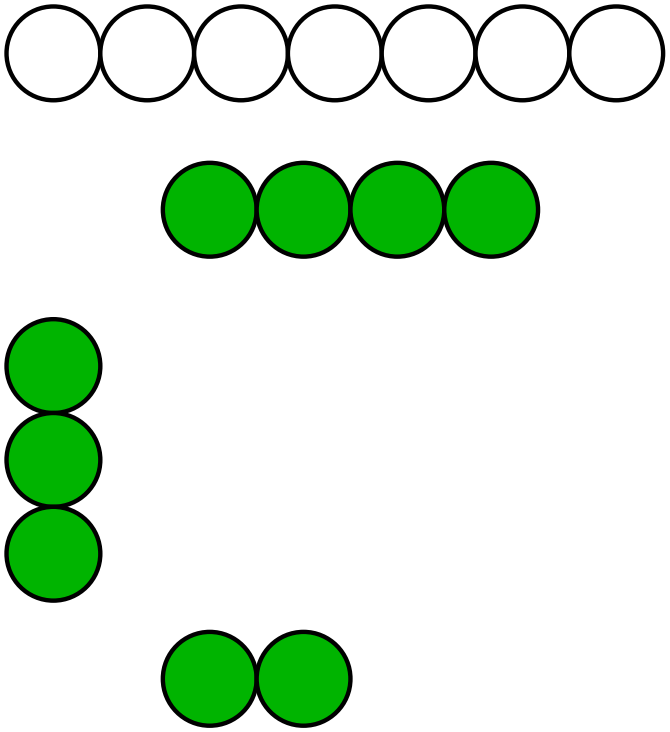
Grouped Orthogonal Search

Map admissible options



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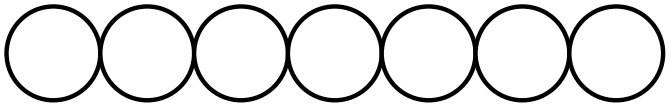
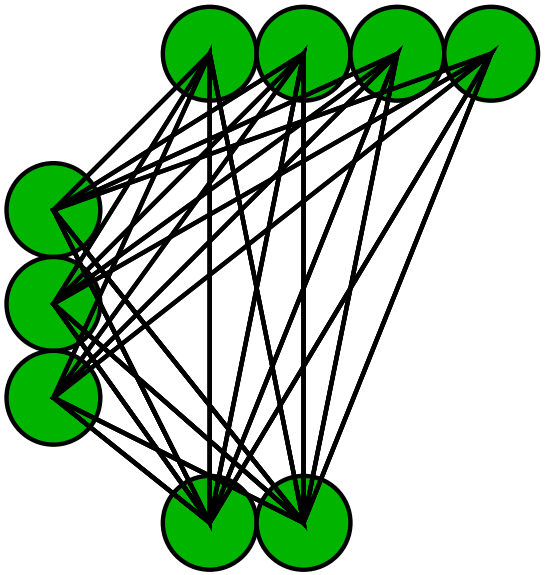
Grouped Orthogonal Search

Group-wide exhaustive search





GAOS: Adrian Tate, Cray, Inc.

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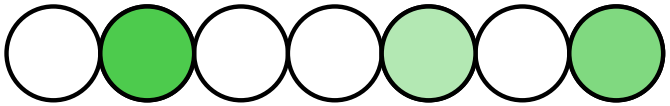
Grouped Orthogonal Search

Start over with best result $\rightarrow$ pick new group...



GAOS: Adrian Tate, Cray, Inc.

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Using the Nvidia profiler in-process

```
# enable profiler
import os
os.environ["COMPUTE_PROFILE"] = "1"
with open("/tmp/myprg-prof-config", "w") as prof_config:
    prof_config.write("\n".join(events))
os.environ["COMPUTE_PROFILE_CONFIG"] = "/tmp/myprg-prof-config"

# obtain timing data
prof_f = open("opencl_profile_0.log", "r")
gain_count = 0

while gain_count < 2:
    # run kernel here
    prof_output = prof_f.readlines()
    if prof_output:
        print "gained %d lines" % len(prof_output)
        gain_count += 1
        if gain_count == 2:
            print "".join(l for l in prof_output[1:-1]
                          if kernel_name in l)
```

Using the Nvidia profiler in-process

```
1  # enable profiler
2  import os
3  os.environ["COMPUTE_PROFILE"] = "1"
4  with open("/tmp/myprg-prof-config", "w") as prof_config:
5      prof_config.write("\n".join(events))
6  os.environ["COMPUTE_PROFILE_CONFIG"] = "/tmp/myprg-prof-config"
7
8  # obtain timing data
9  prof_f = open("opencl_profile_0.log", "r")
10 gain_count = 0
11
12 while gain_count < 2:
13     # run
14     prof_ou
15     if prof
16         pri
17         gai
18         if
19
20
```

Sample output:

```
method=[ matvec ] gputime=[ 7218.048 ] cputime=[ 12.000 ] occupancy=[ 1.000 ]
method=[ matvec ] gputime=[ 7267.456 ] cputime=[ 14.000 ] occupancy=[ 1.000 ]
method=[ matvec ] gputime=[ 7264.640 ] cputime=[ 12.000 ] occupancy=[ 1.000 ]
method=[ matvec ] gputime=[ 7270.048 ] cputime=[ 15.000 ] occupancy=[ 1.000 ]
method=[ matvec ] gputime=[ 7262.976 ] cputime=[ 12.000 ] occupancy=[ 1.000 ]
method=[ matvec ] gputime=[ 7237.152 ] cputime=[ 23.000 ] occupancy=[ 1.000 ]
```

Nvidia GPU Profiler: Events

gld_request : Number of executed global load instructions per warp in a SM

gst_request : Number of executed global store instructions per warp in a SM

divergent_branch : Number of unique branches that diverge

instructions : Instructions executed

warp_serialized : Number of SIMD groups that serialize on address conflicts to local memory

And many more: see (root of CUDA toolkit)/(doc/Compute_Profiler_VERSION.txt
(Careful: CUDA terminology)

Outline

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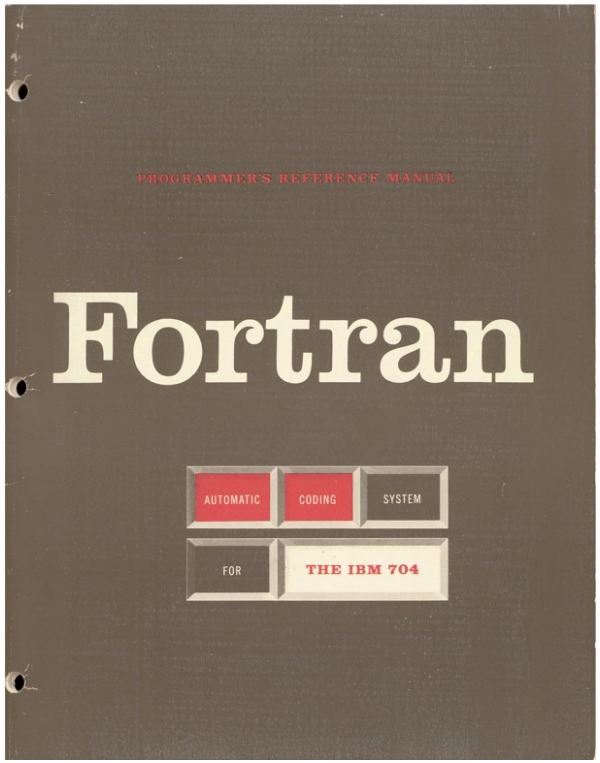
Outline

F2Py



f2py...

- very easily exposes Fortran routines
  - just add `intent(in/out)`
- supports F77 and much of F90 (not data types)
- Allows call-back into Python
- Much easier than C
  - No issues with pointer ownership
- PyOpenCL+F2Py: Good way of bringing Fortran codes into the "GPU age"

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Simple f2py example

```
subroutine fib(a,n)
  integer, intent(in) :: n
  real*8, intent(out) :: a(n)

  do i=1,n
     if (i.eq.1) then
        a(i) = 0.0d0
     elseif (i.eq.2) then
        a(i) = 1.0d0
     else
        a(i) = a(i-1) + a(i-2)
     endif
  enddo
end
```

Code Credit: Pearu Peterson

Simple f2py example

```
subroutine fib(a,n)
  integer, intent(in) :: n
  real*8, intent(out) :: a(n)

  do i=1,n
     if (i.eq.1)
        a(i) = (
     elseif (i.e
        a(i) = 
     else
        a(i) = a
     endif
  enddo
end
```

```
$ f2py -m f2pyex -c f2pyex.f90
$ python
>>>import f2pyex
>>>print f2pyex.fib.__doc__
fib - Function signature:
  a = fib(n)
Required arguments:
  n : input int
Return objects:
  a : rank-1 array('d') with bounds (n)
```

Code Credit: Pearu Peterson

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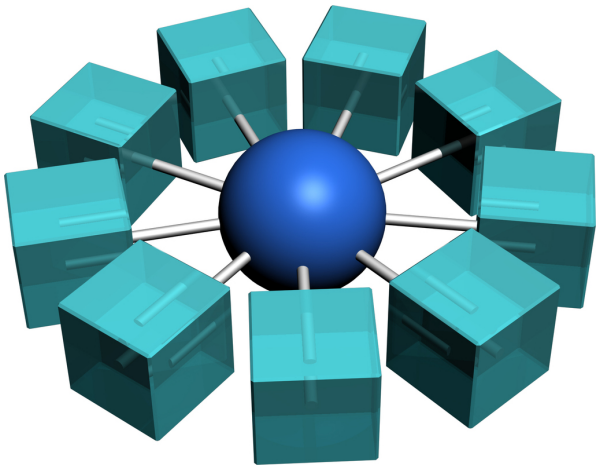
mpi4py: Using MPI from Python



mpi4py...

- wraps MPI 2 into Python
- aimed at numpy arrays and general data
- interfaces with Fortran/F2Py, SWIG, Cython

`https://code.google.com/p/mpi4py/`

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Simple MPI with Python objects

```
from mpi4py import MPI

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

if rank == 0:
    data = {'a': 7, 'b': 3.14}
    comm.send(data, dest=1, tag=11)
elif rank == 1:
    data = comm.recv(source=0, tag=11)
```

- Can communicate arbitrary Python objects
- Versatile, potentially slow
  - CPU needs to pack data into buffer

Code Credit: Lisandro Dalcin (CIMEC, Argentina)

MPI with numpy objects

```
from mpi4py import MPI
import numpy

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

if rank == 0:
    data = numpy.arange(100, dtype=numpy.float64)
    comm.Send(data, dest=1, tag=13)
elif rank == 1:
    data = numpy.empty(100, dtype=numpy.float64)
    comm.Recv(data, source=0, tag=13)
```

- Can communicate "POD" numpy arrays
- Fast: No Copying
- Note difference: `Send` vs. `send`

Code Credit: Lisandro Dalcin (CIMEC, Argentina)

MPI with numpy objects

```
from mpi4py import MPI
import numpy

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

if rank == 0:
    data = numpy.arange(100, dtype=numpy.float64)
    comm.Send(data, dest=1, tag=13)
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    data = numpy.empty(100, dtype=numpy.float64)
    comm.Recv(data, source=0, tag=13)
```

- Can communicate "POD" numpy arrays
- Fast: No Copying
- Note difference: `Send` vs

If non-blocking, same issue with buffer lifetime as PyOpenCL.

Code Credit: Lisandro Dalcin (CIME

MPI collectives

```
from mpi4py import MPI

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

if rank == 0:
    data = [(i+1)**2 for i in range(size)]
else:
    data = None
data = comm.scatter(data, root=0)
assert data == (rank+1)**2
```

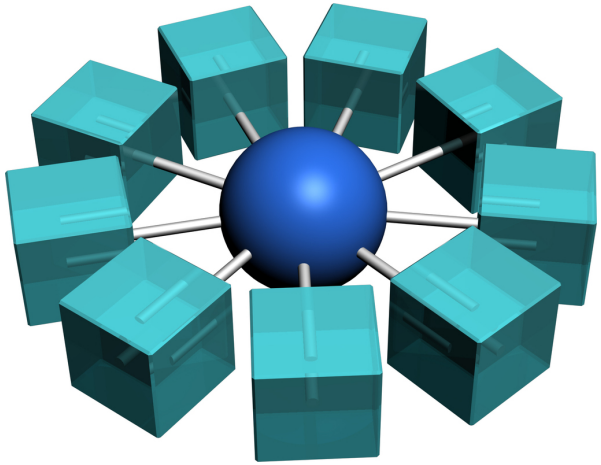
Also available:

- One-sided, non-blocking, synchronous, ...
- Dynamic process creation
- MPI I/O

Code Credit: Lisandro Dalcin (CIMEC, Argentina)

mpi4py: Final Observations

- Common theme with PyOpenCL: numpy arrays work well as a vehicle for bulk data
  - Side Corollary: Avoid touching bulk data in Python
- Nvidia GPUDirect:
  - Use host-mapped GPU arrays for MPI communication
  - Avoid GPU $\rightarrow$ ~~Host~~ $\rightarrow$ IB copies
  - ```
    b = cl.Buffer(...,
      cl.mem_flags.ALLOC_HOST_PTR)
    cl.enqueue_map_buffer(
      queue, b, ...)
    ```



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    ```

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Boost.Python: Connecting C/C++ and Python

Boost.Python (BPL)...

- uses `template` "magic" to introspect C++
- provides enough tools to write 'idiomatic' wrappers
- wraps the Python/C API to make it 'idiot-proof'
- deals well with complicated pointer ownership
- is used by PyOpenCL, PyCUDA, ...

`http://boost.org/`

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Simple BPL example

```
#include <boost/python.hpp>

static char const *greet()
{
  return "hello world";
}

BOOST_PYTHON_MODULE(module)
{
  boost::python::def("greet", &greet);
}
```

- Wrapper generation happens in pure C++
  - Good if wrapping complicated types
  - Wrapper generator exists
- Compile with 'Distutils' (see PyOpenCL build system for example)

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Whetting your appetite

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

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

Whetting your appetite

```
1  mod = pycuda.compiler.SourceModule("""
2        __global__ void twice( float *a)
3       {
4         int idx = threadIdx.x + threadIdx.y*4;
5         a[idx] *= 2;
6       }
7       """)
8
9  func = mod.get_function("twice")
10 func(a_gpu, block=(4,4,1))
11
12 a_doubled = numpy.empty_like(a)
13 cuda.memcpy_dtoh(a_doubled, a_gpu)
14 print a_doubled
15 print a
```

Whetting your appetite

```
1  mod = pycuda.compiler.SourceModule("""
2      __global__ void twice( float *a)
3      {
4        int idx = threadIdx.x + threadIdx.y*4;
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11
12 a_doubled = numpy.empty_like(a)
13 cuda.memcpy_dtoh(a_doubled, a_gpu)
14 print a_doubled
15 print a
```

Compute kernel

Whetting your appetite, Part II

Did somebody say "Abstraction is good"?

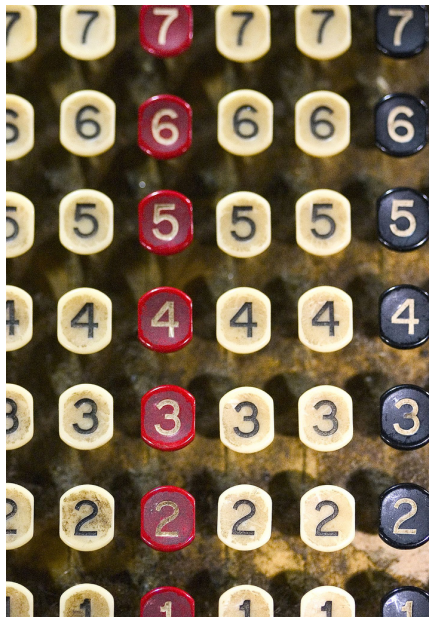
Whetting your appetite, Part II

```
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
```

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.



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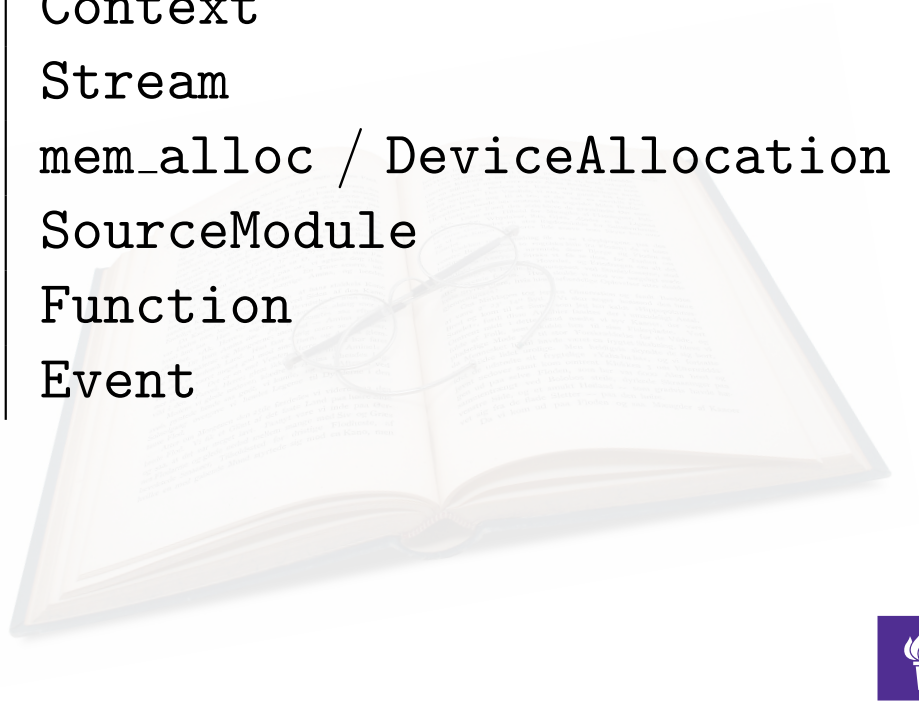
PyOpenCL ↔ PyCUDA: A (rough) dictionary

PyOpenCL	PyCUDA
`Context`	`Context`
`CommandQueue`	`Stream`
`Buffer`	`mem_alloc` / `DeviceAllocation`
`Program`	`SourceModule`
`Kernel`	`Function`
`Event` (eg. `enqueue_marker`)	`Event`



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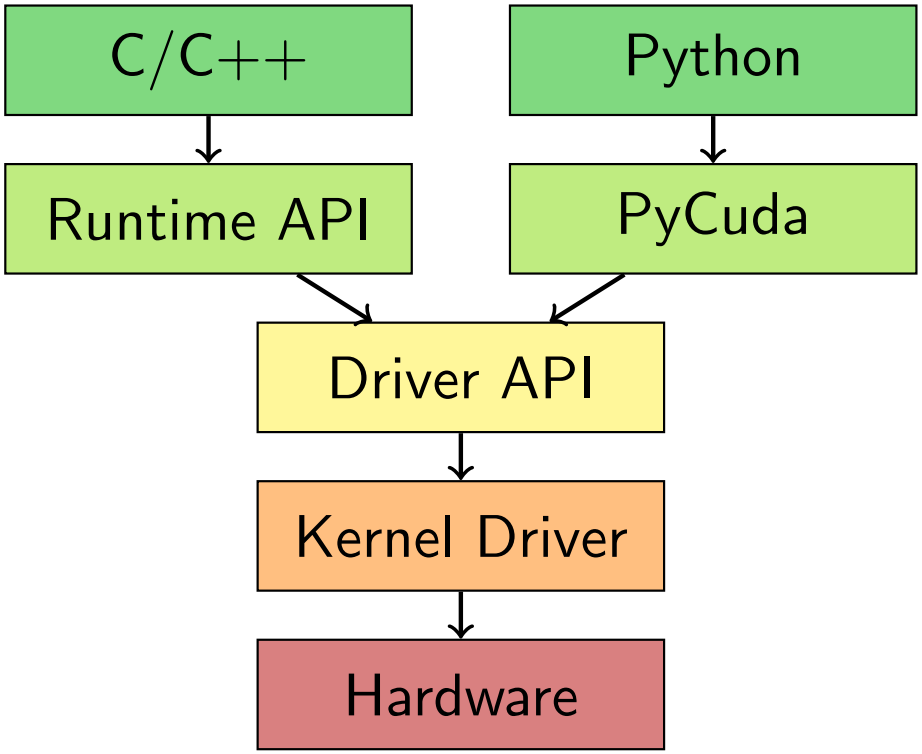
PyCUDA in the CUDA ecosystem



CUDA has two Programming Interfaces:

- "Runtime" high-level (separate install)
- "Driver" low-level (`libcuda.so`, comes with GPU driver)

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PyCUDA: Vital Information

- `http://mathema.tician.de/software/pycuda`
- Complete documentation
- X Consortium License
  (no warranty, free for all use)
- Convenient abstractions
  Array, Fast Vector Math, Reductions
- Requires: numpy, Python 2.4+
  (Win/OS X/Linux)

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Automating GPU Programming

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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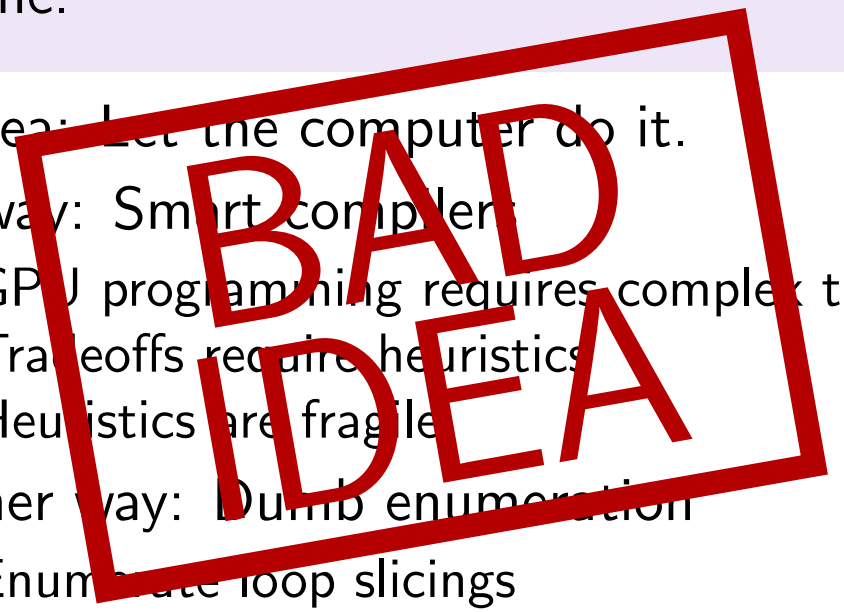

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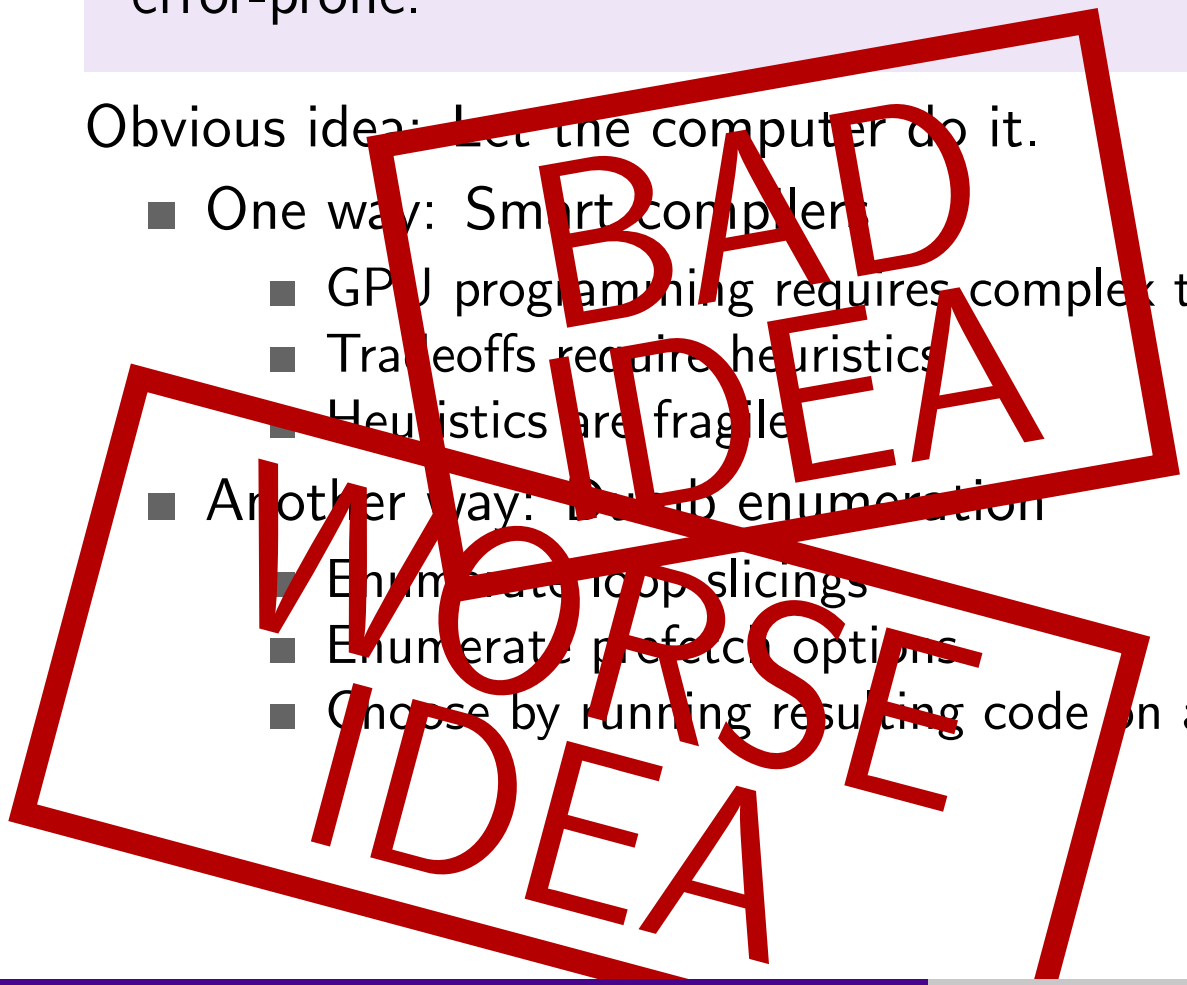
Automating GPU Programming

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: Brute-force enumeration
  - Enumerate loop slicings
  - Enumerate prefetch options
  - Choose by running resulting code on actual hardware



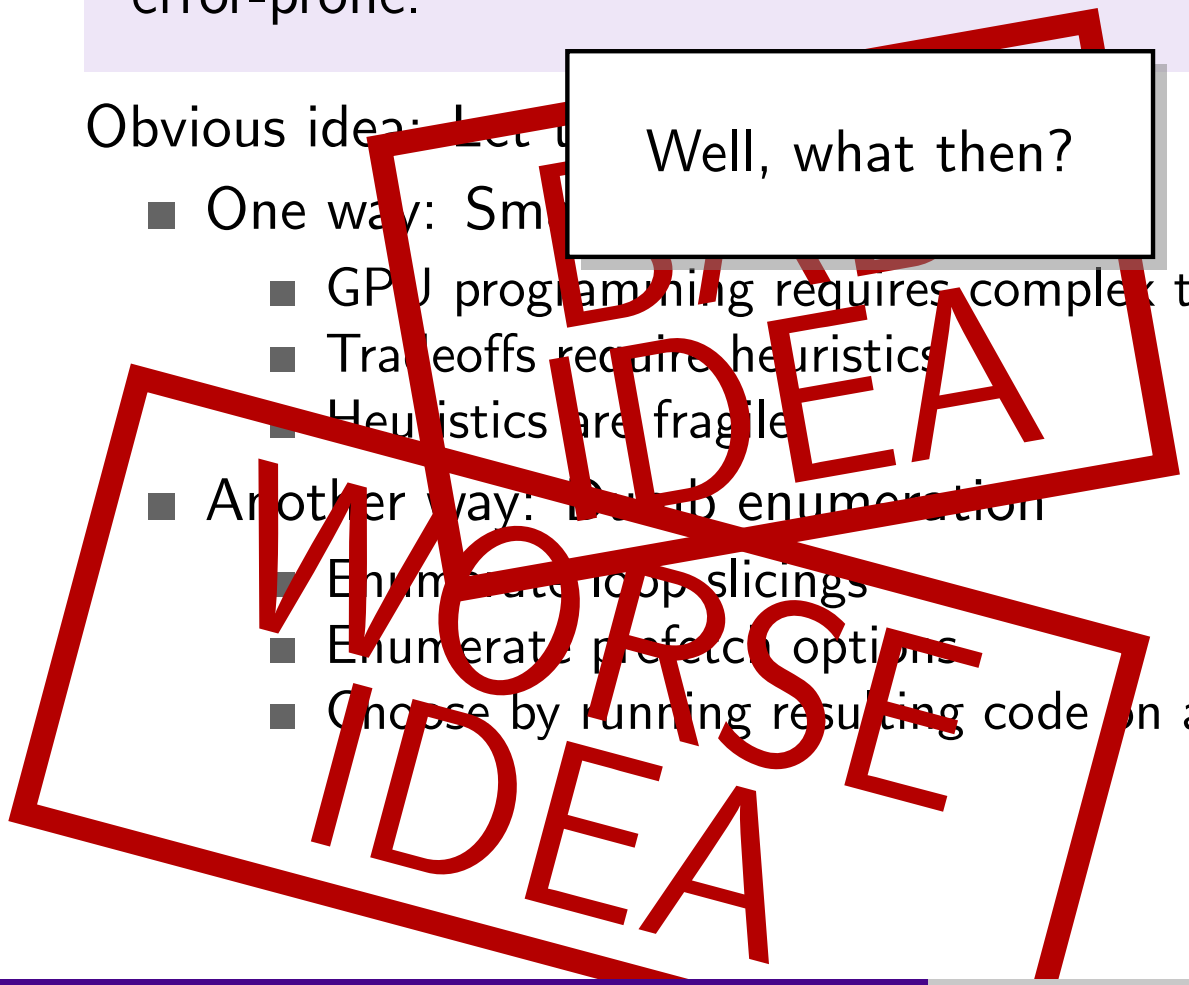
Automating GPU Programming

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

Well, what then?

Obvious idea: Let t

- One way: Sm
  - GPU programming requires complex tradeoffs
  - Tradeoffs require heuristics
  - Heuristics are fragile
- Another way: Brute enumeration
  - Enumerate loop slicings
  - Enumerate prefetch options
  - Choose by running resulting code on actual hardware



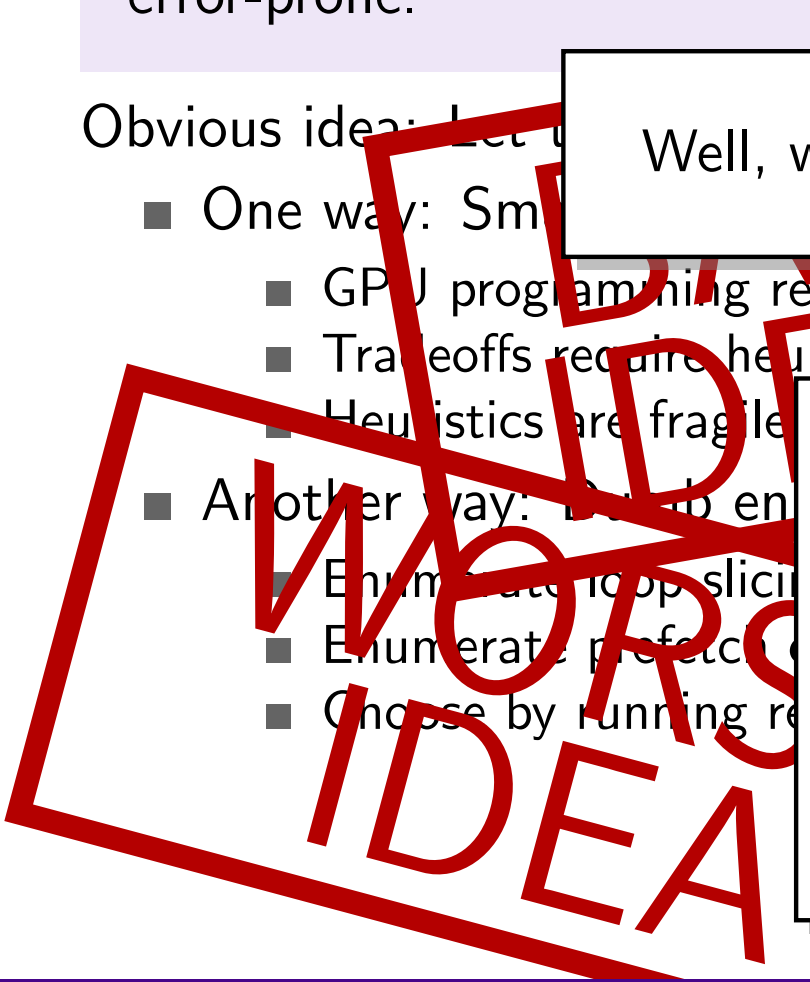
Automating GPU Programming

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

Obvious idea: Let t

- One way: Sm
  - GPU programming requires complex tradeoffs
  - Tradeoffs require heuristics
  - Heuristics are fragile
- Another way: Build en
  - Enumerate loop slici
  - Enumerate prefetch
  - Choose by running re

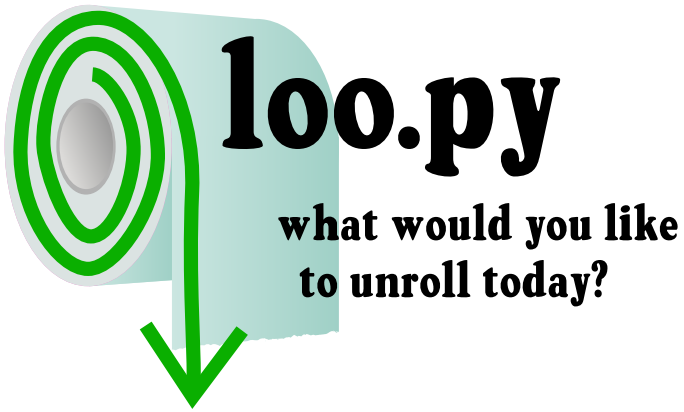
Well, what then?



My experience:
Users know what they're doing, but they're lazy and in a hurry.

So give them tools and get out of the way.

Enter: Loo.py



Idea: Expose loop transformations that compilers can do *to the user*.

- Somewhat similar to directive-based model
- But not really: Loop kernel is a Python object
  - Can query it for its properties
  - Can control transformation according to target device
  - Can easily integrate into other software
- Use polyhedral model to represent loop bounds
  - And knowledge about divisibility, parameters, etc.

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Loo.py Example

```
knl = lp.LoopKernel(ctx.devices[0],
        "{[i,j,k]: 0<=i,j,k<1600}",
        [
            (c[i, j], a[i, k]*b[k, j])
            ],
        [
            lp.ArrayArg("a", dtype, shape=(1600, 1600), order="C"),
            lp.ArrayArg("b", dtype, shape=(1600, 1600), order="C"),
            lp.ArrayArg("c", dtype, shape=(1600, 1600), order="C"),
            ],
        name="matmul")

knl = lp.split_dimension(knl, "i", 16, outer_tag="g.0", inner_tag="l.1")
knl = lp.split_dimension(knl, "j", 16, outer_tag="g.1", inner_tag="l.0")
knl = lp.split_dimension(knl, "k", 16)
knl = lp.add_prefetch(knl, 'a', ["k_inner", "i_inner"])
knl = lp.add_prefetch(knl, 'b', ["j_inner", "k_inner", ])
```

Lo

```
#define i_outer (0 + (int) get_group_id(0)) /* [0, 10) */
#define j_outer (0 + (int) get_group_id(1)) /* [0, 10) */
#define j_inner (0 + (int) get_local_id(0)) /* [0, 16) */
#define i_inner (0 + (int) get_local_id(1)) /* [0, 16) */

__kernel void __attribute__ ((reqd_work_group_size(16, 16, 1)))
matmul(__global float const *restrict a, __global float const *restrict b, __global float *restrict c)
{ __local float prefetch_a_0[16][16]; __local float prefetch_b_1[16][16];
  float tmp_c_0 = 0;
  for (int k_outer = 0; 9 - k_outer >= 0; ++k_outer)
  { barrier(CLK_LOCAL_MEM_FENCE);
    {
      int const loopy_prefetch_dim_idx_0 = (int) get_local_id(0);
      int const loopy_prefetch_dim_idx_1 = (int) get_local_id(1);
      prefetch_b_1[loopy_prefetch_dim_idx_0][loopy_prefetch_dim_idx_1] =
        b[loopy_prefetch_dim_idx_0 + j_outer*16 + 160*(loopy_prefetch_dim_idx_1 + k_outer*16)];
    }
    { {
        int const loopy_prefetch_dim_idx_0 = (int) get_local_id(0);
        int const loopy_prefetch_dim_idx_1 = (int) get_local_id(1);
        prefetch_a_0[loopy_prefetch_dim_idx_0][loopy_prefetch_dim_idx_1] =
          a[loopy_prefetch_dim_idx_0 + k_outer*16 + 160*(loopy_prefetch_dim_idx_1 + i_outer*16)];
      }
      barrier(CLK_LOCAL_MEM_FENCE);

      for (int k_inner = 0; 15 - k_inner >= 0; ++k_inner)
        tmp_c_0 += prefetch_b_1[j_inner - 0][k_inner - 0]*prefetch_a_0[k_inner - 0][i_inner - 0];
    }
  }

  c[j_outer*16 + j_inner + 160*(i_outer*16 + i_inner)] = tmp_c_0;
}
```

Loo.py Example

```
knl = lp.LoopKernel(ctx.devices[0],
        "{[i,j,k]: 0<=i,j,k<1600}",
        [
            (c[i, j], a[i, k]*b[k, j])
            ],
        [
            lp.ArrayArg("a", dtype, shape=(1600, 1600), order="C"),
            lp.ArrayArg("b", dtype, shape=(1600, 1600), order="C"),
            lp.ArrayArg("c", dtype, shape=(1600, 1600), order="C"),
            ],
        name="matmul")

knl = lp.split_dimension(knl, "i", 16, outer_tag="g.0", inner_tag="l.1")
knl = lp.split_dimension(knl, "j", 16, outer_tag="g.1", inner_tag="l.0")
knl = lp.split_dimension(knl, "k", 16)
knl = lp.add_prefetch(knl, 'a', ["k_inner", "i_inner"])
knl = lp.add_prefetch(knl, 'b', ["j_inner", "k_inner", ])
```

Loo.py Example II

```
knl = lp.LoopKernel(ctx.devices[0],
        "[n] -> {[i,j,k]: 0<=i,j,k<n}",
        [
            (c[i, j], a[i, k]*b[k, j])
            ],
        [
            lp.ImageArg("a", dtype, 2),
            lp.ImageArg("b", dtype, 2),
            lp.ArrayArg("c", dtype, shape=(n_sym, n_sym), order=order),
            lp.ScalarArg("n", np.int32, approximately=1000),
            ],
        name="matmul")

ilp = 4; j_inner_split = 16
knl = lp.split_dimension(knl, "i", 2, outer_tag="g.0", inner_tag="l.1")
knl = lp.split_dimension(knl, "j", ilp*j_inner_split, outer_tag="g.1")
knl = lp.split_dimension(knl, "j_inner", j_inner_split,
    outer_tag="ilp", inner_tag="l.0")
knl = lp.split_dimension(knl, "k", 16)
knl = lp.add_prefetch(knl, 'a', ["i_inner", "k_inner"])
knl = lp.add_prefetch(knl, 'b', [("j_inner_outer", "j_inner_inner"), "k_inner"])
```

Loo.py Example II

```
knl = lp.LoopKernel(ctx.devices[0],
        "[n] -> {[i,j,k]: 0<=i,j,k<n}",
        [
            (c[i, j], a[i, k]*b[k, j])
            ],
        [
            lp.ImageArg("a", dtype, 2),
            lp.ImageArg("b", dtype, 2),
            lp.ArrayArg("c", dtype, shape=(n_sym, n_sym), order=order),
            lp.ScalarArg("n", np.int32, approximately=1000),
            ],
        name="matmul")

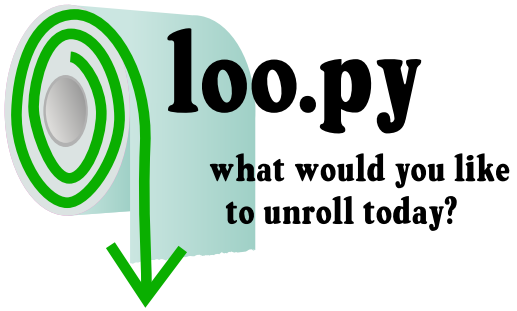
ilp = 4; j_inner_split = 16
knl = lp.split_dimension(knl, "i", 2, outer_tag="g.0", inner_tag="l.1")
knl = lp.split_dimension(knl, "j", ilp*j_inner_split, outer_tag="g.1")
knl = lp.split_dimension(knl, "j_inner", j_inner_split,
    outer_tag="ilp", inner_tag="l.0")
knl = lp.split_dimension(knl, "k", 1
knl = lp.add_prefetch(knl, 'a', ["i_i
knl = lp.add_prefetch(knl, 'b', [("j
```

Resulting code 1000+ lines long

Loo.py Summary

Can do today:

- Split dimensions
- "Tag" dimensions: GPU axes, unroll, ILP
- Lmem prefetch (with dim. merging)
- Loop schedule
- Conditional avoidance
- Warn about lmem conflicts
- Images, constant memory



Status:

- Inital goal: recipes for BLAS, DG
  - Obviously not for every computation
  - Quite general: convolutions, stencils, ...
- Public, but pre-alpha:
  `http://github.com/inducer/loopy`

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Outline

Outline

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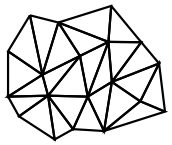
Discontinuous Galerkin Method

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



Discontinuous Galerkin Method

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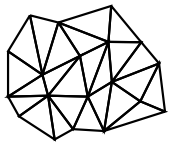

Goal

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

Discontinuous Galerkin Method

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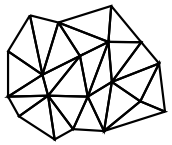


Goal

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

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:

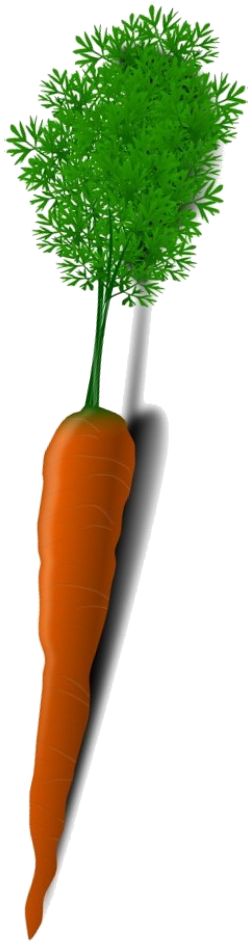
$$\begin{aligned} 0 &= \int_{\mathrm{D}_k} u_t \varphi + [\nabla \cdot F(u)] \varphi \, \mathrm{d}x \\ &= \int_{\mathrm{D}_k} u_t \varphi - F(u) \cdot \nabla \varphi \, \mathrm{d}x + \int_{\partial \mathrm{D}_k} (\hat{n} \cdot F)^* \varphi \, \mathrm{d}S_x, \end{aligned}$$

Subsitute in basis functions, introduce elementwise stiffness, mass, and surface mass matrices matrices S, M, M_A:

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

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

DG on GPUs: Possible Advantages



DG on GPUs: Why?

- GPUs have deep Memory Hierarchy
  - The majority of DG is local.
- Compute Bandwidth $\gg$ Memory Bandwidth
  - DG is arithmetically intense.
- GPUs favor dense data.
  - Local parts of the DG operator are dense.
- GPUs don't like scattered access.
  - DG's cell connectivity is sparser than CG's
  - and more regular.

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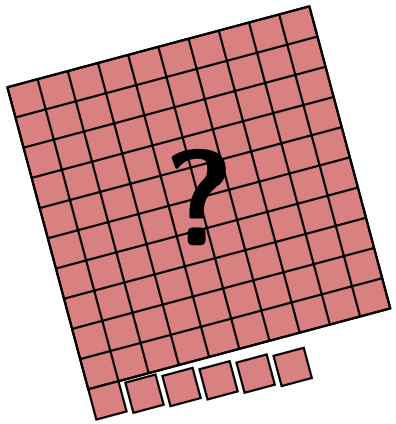
Work Partition for Element-Local Operators

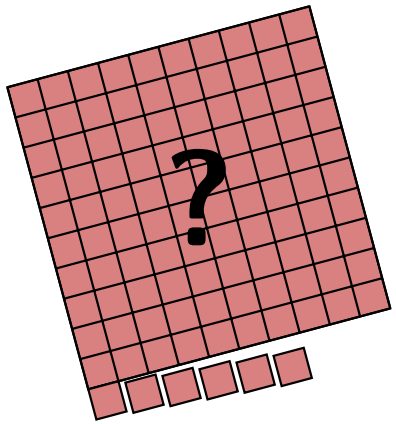
Natural Work Decomposition:
One Element per Block



Work Partition for Element-Local Operators

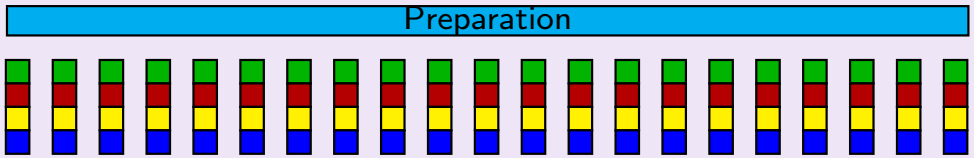
Natural Work Decomposition:
One Element per Block

- ⊕ Straightforward to implement
- ⊕ No granularity penalty
- ⊖ Cannot fill wide SIMD: unused compute power for small to medium elements
- ⊖ Data alignment: Padding wastes memory
- ⊖ Cannot amortize cost of preparation steps (e.g. fetching)



Loop Slicing for element-local parts of GPU DG

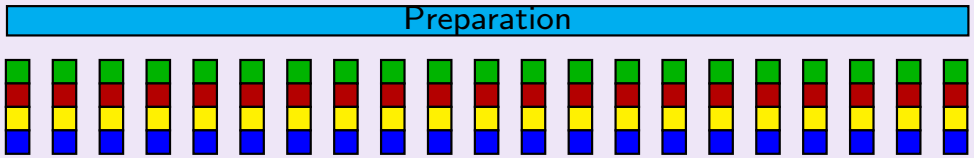
Per Block: K_L element-local mat.mult. + matrix load



Question: How should one assign work to threads?

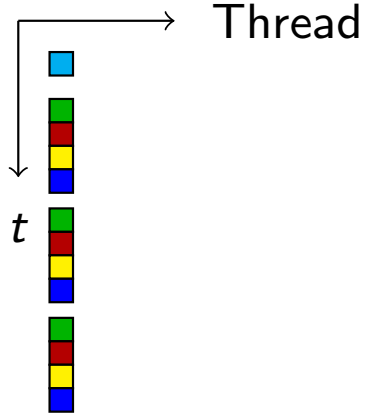
Loop Slicing for element-local parts of GPU DG

Per Block: K_L element-local mat.mult. + matrix load



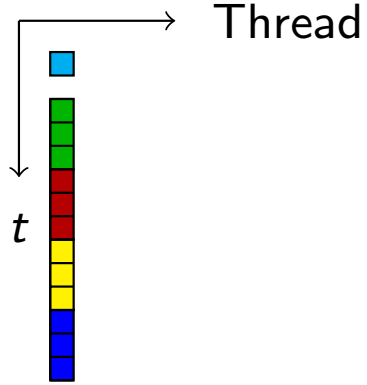
Question: How should one assign work to threads?

w_s: in sequence



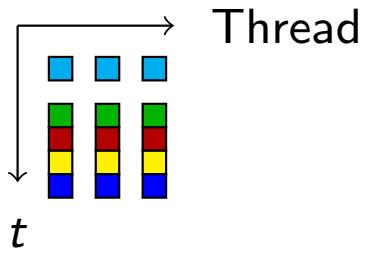
(amortize preparation)

w_i: "inline-parallel"



(exploit register space)

w_p: in parallel



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Metaprogramming for GPU-DG

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

Metaprogramming for GPU-DG

- Specialize code for user-given problem:
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- Automated Tuning:
  - Memory layout
  - Loop slicing
  - Gather granularity

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Metaprogramming for GPU-DG

- Specialize code for user-given problem:
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- Constants instead of variables:
  - Dimensionality
  - Polynomial degree
  - Element properties
  - Matrix sizes

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Metaprogramming for GPU-DG

- Specialize code for user-given problem:
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Metaprogramming for GPU-DG

- Specialize code for user-given problem:
  - Flux Terms (*)
- Automated Tuning:
  - Memory layout
  - Loop slicing (*)
  - Gather granularity
- Constants instead of variables:
  - Dimensionality
  - Polynomial degree
  - Element properties
  - Matrix sizes
- Loop Unrolling

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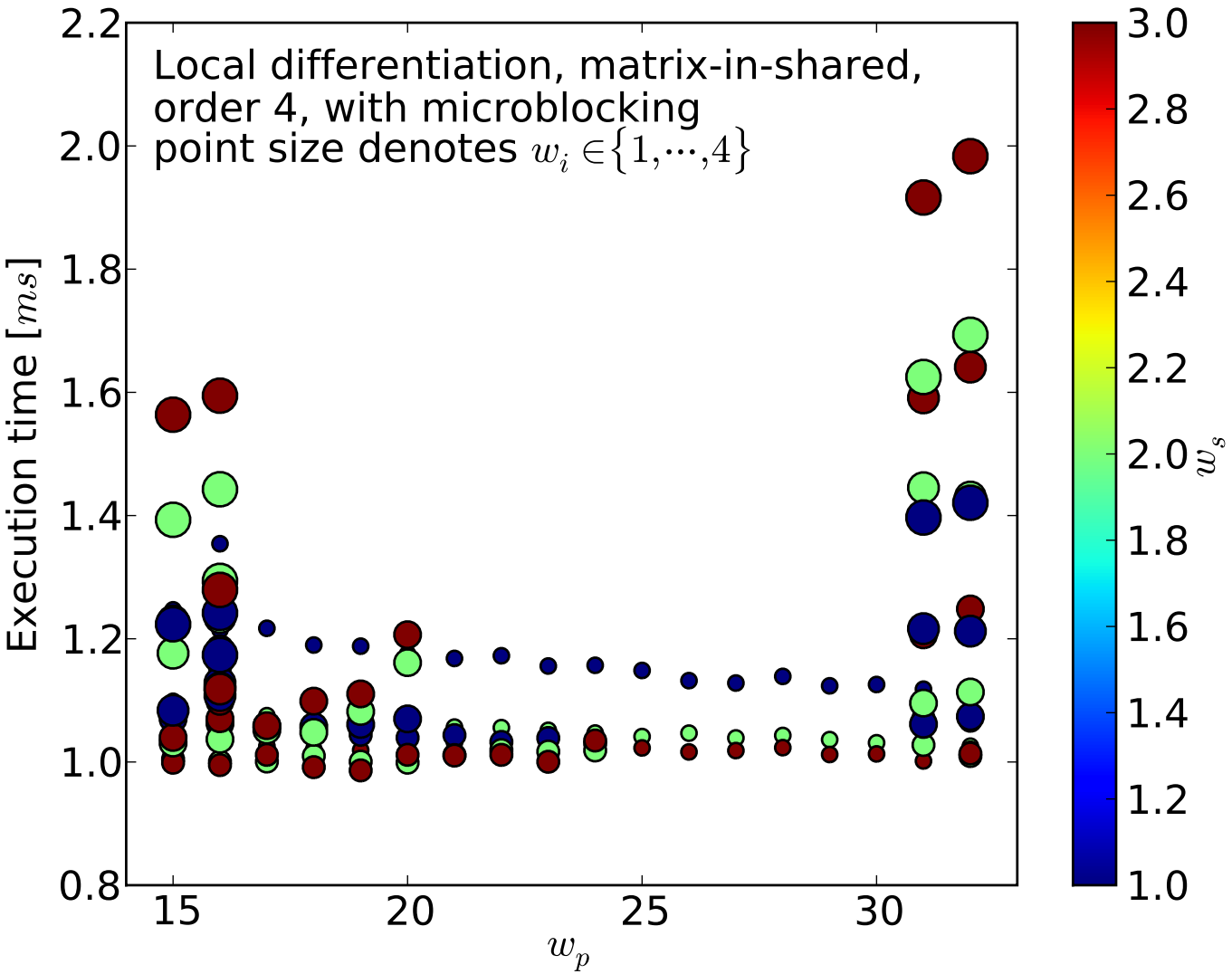
Loop Slicing for Differentiation



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Metaprogramming DG: Flux Terms

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

Metaprogramming DG: Flux Terms

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

Flux terms:

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

Metaprogramming DG: Flux Terms Example

Example: Fluxes for Maxwell's Equations

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

Metaprogramming DG: Flux Terms Example

Example: Fluxes for Maxwell's Equations

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

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);
```

Hedge DG Solver

- High-Level Operator Description
  - Maxwell's
  - Euler
  - Poisson
  - Compressible Navier-Stokes, ...
- One Code runs...
  - ...on CPU, CUDA
  - ...on {CPU,CUDA}+MPI
  - ...in 1D, 2D, 3D
  - ...at any order
- Uses CPU, GPU code generation
- Open Source (GPL3)
- Written in Python,

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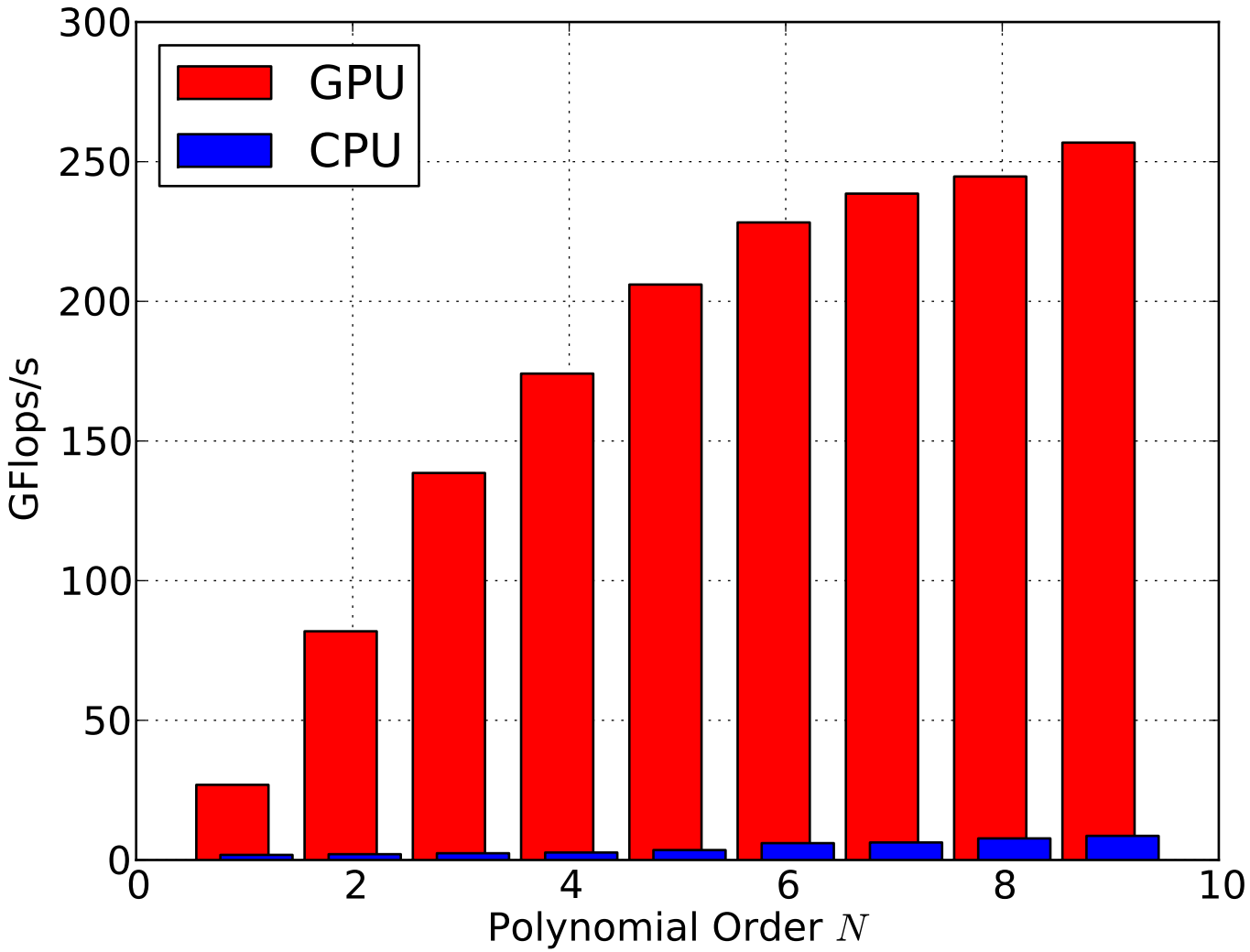
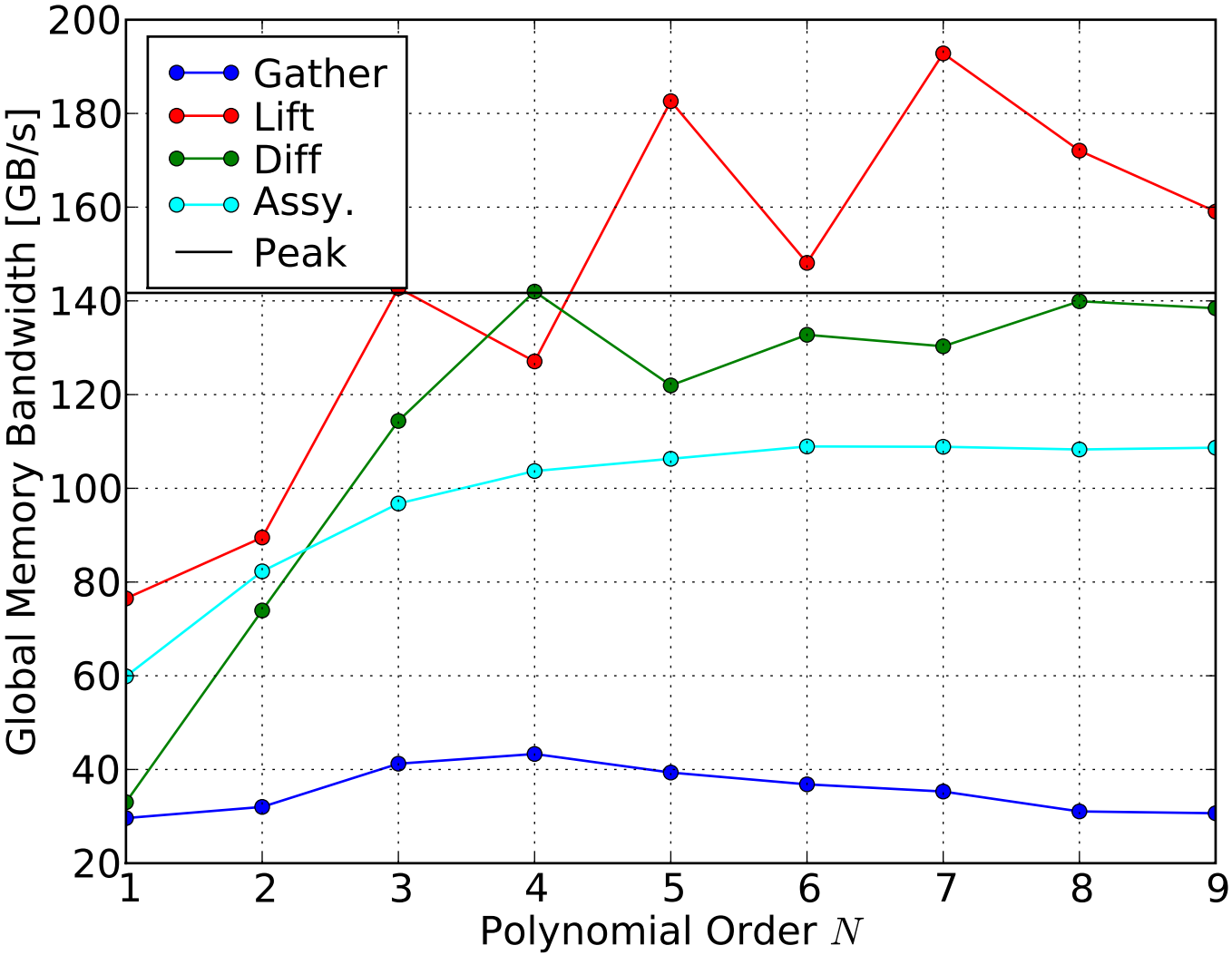
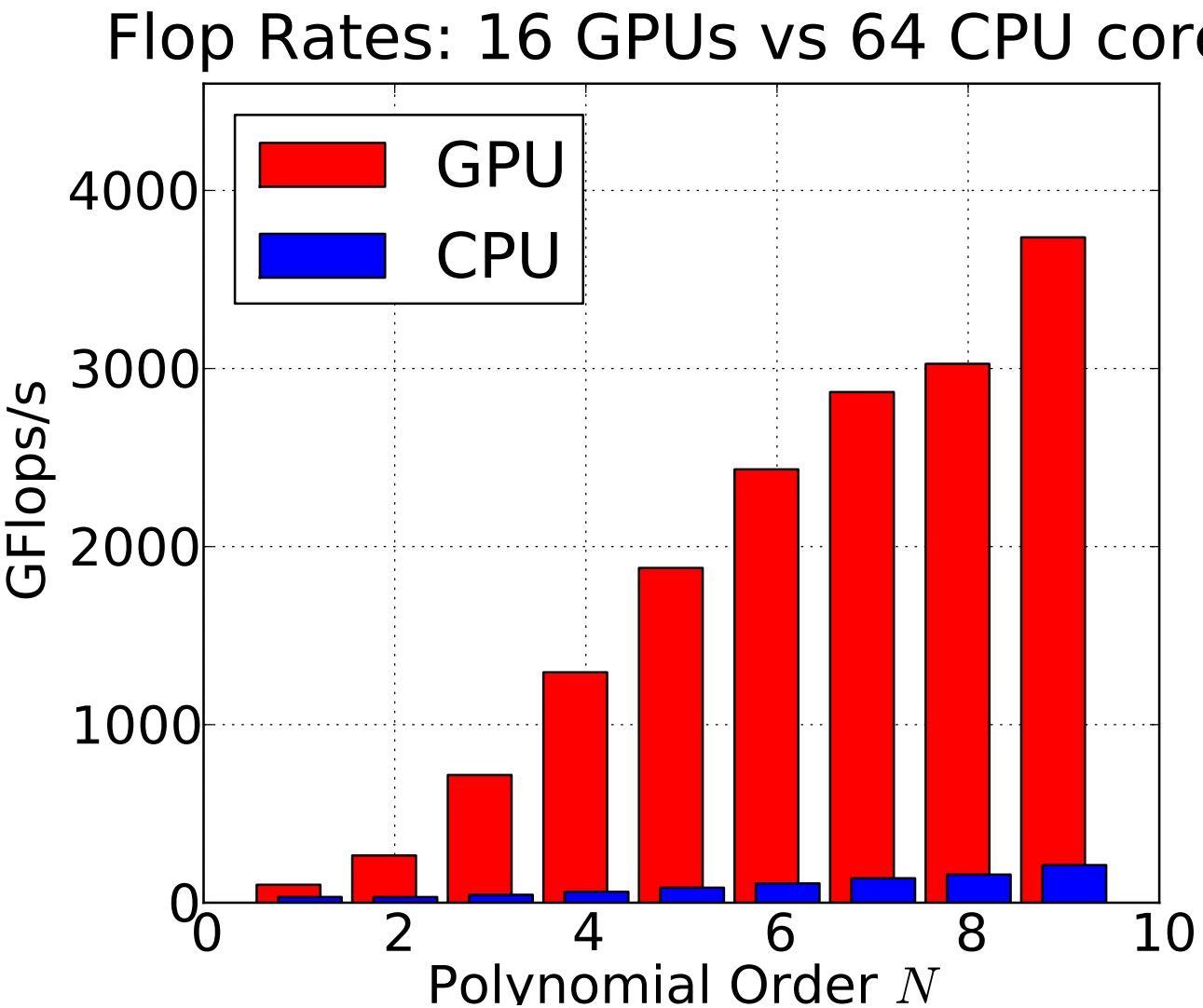
Nvidia GTX280 vs. single core of Intel Core 2 Duo E8400



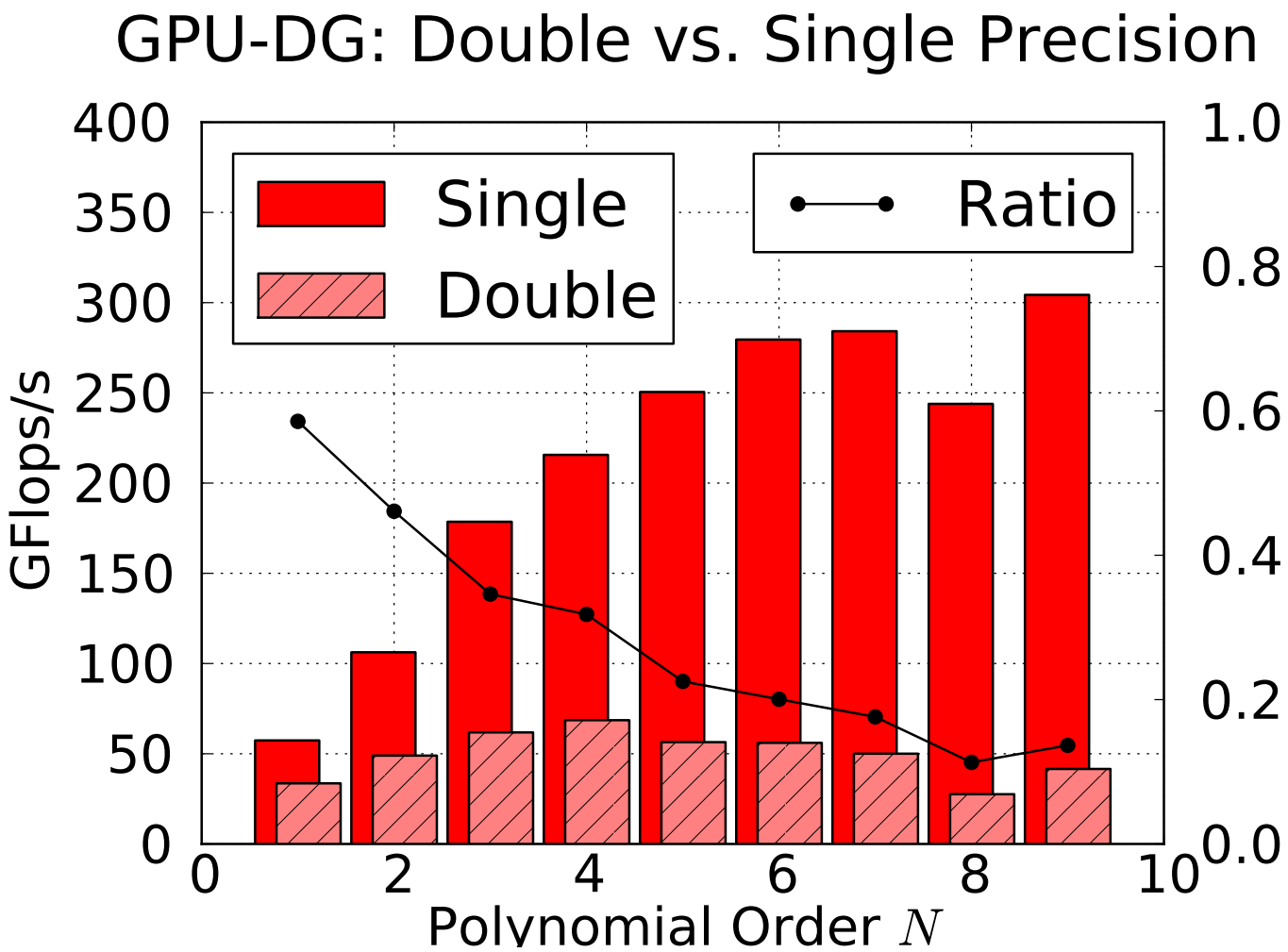
Memory Bandwidth on a GTX 280



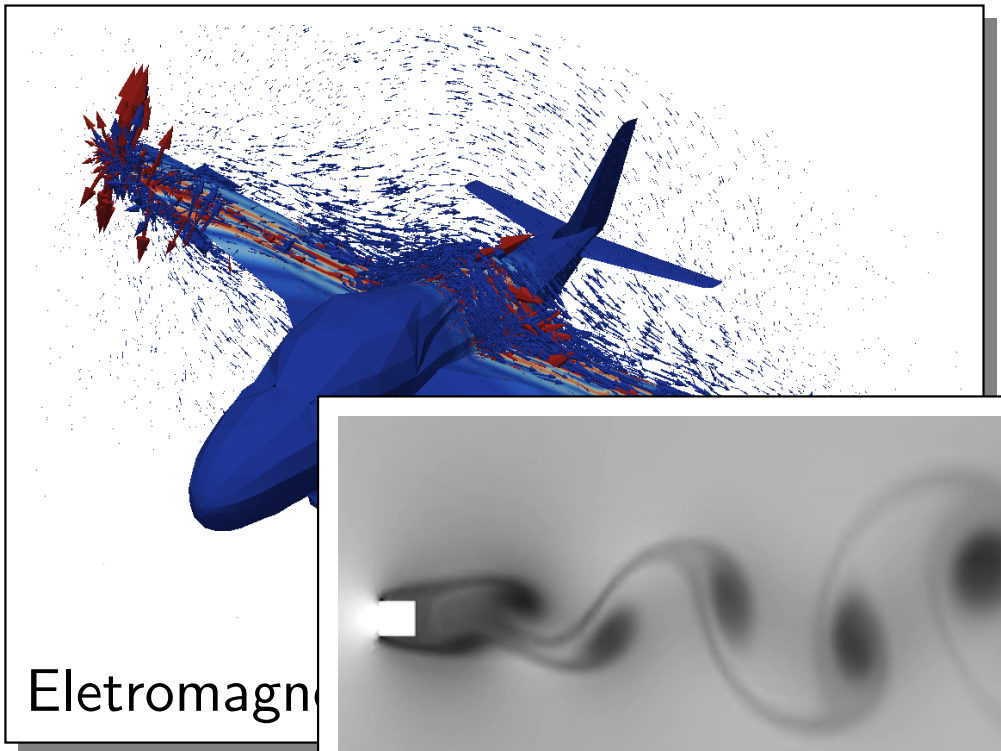
Multiple GPUs via MPI: 16 GPUs vs. 64 CPUs

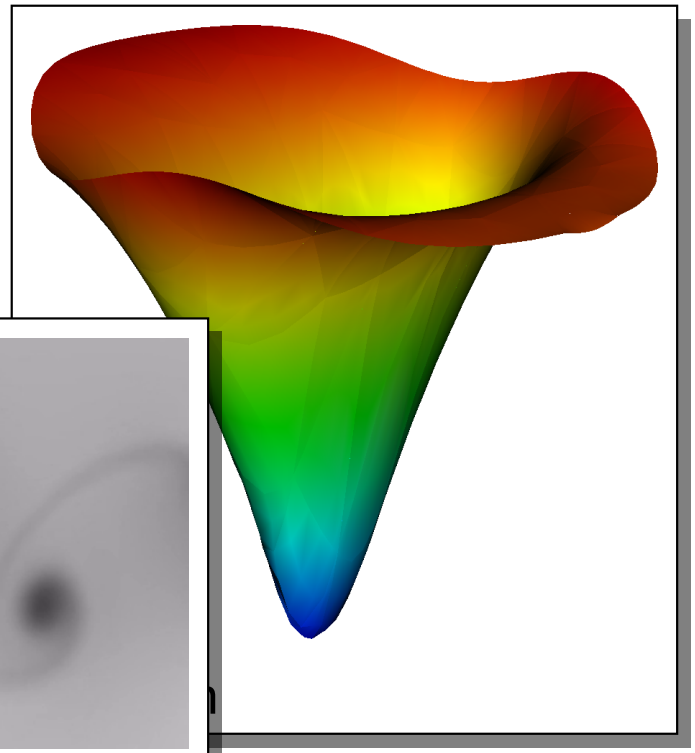


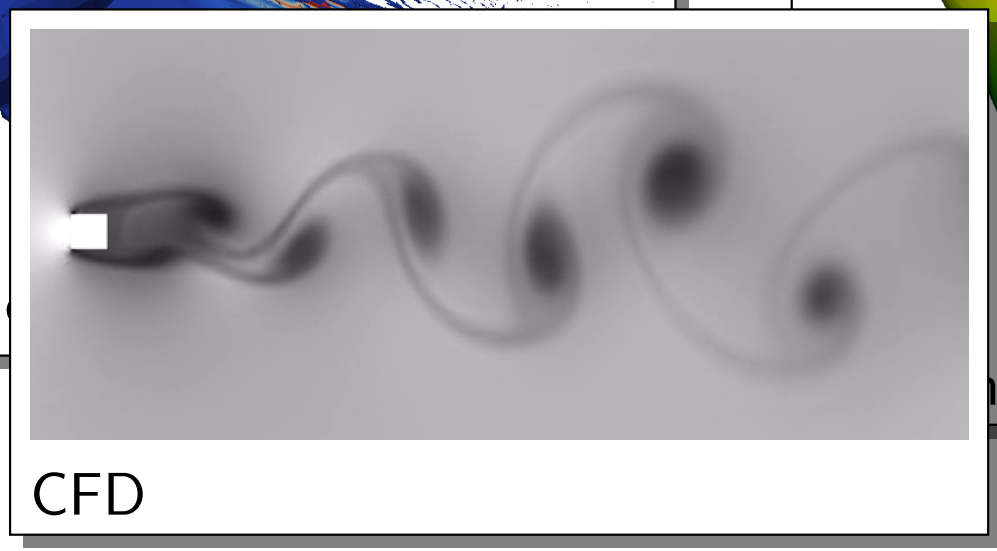
GPU-DG in Double Precision



GPU DG Showcase







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Conclusions

- OpenCL: A way to talk to *all* computing power in the box
  - Many exciting developments in/around/for CL
- OpenCL and Python scripting work surprisingly well together
  - Python/numpy connect to existing software
  - Enable run-time code generation ("RTCG")
  - Works well for tool-building
- PyOpenCL aims to realize these possibilities
  - Easy to use, safe, fast, complete

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Questions?

?

Thank you for your attention!

http://www.cims.nyu.edu/~kloeckner/

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