# Scripting GPUs with PyOpenCL

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# Thanks

- Tim Warburton (Rice)
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- PyOpenCL, PyCUDA contributors
- Nvidia Corporation

# Outline

1. Intro: GPUs, OpenCL
2. GPU Programming with PyOpenCL
3. Additional Topics
4. Playtime!
5. Conclusions

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1 Intro: GPUs, OpenCL
- What and Why?
- Bird's eye view of OpenCL

2 GPU Programming with PyOpenCL

3 Additional Topics

4 Playtime!

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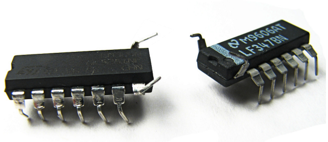
# GPU Computing?

- Design target for CPUs:
  - Make a single thread very fast
  - Hide latency through large caches
  - Predict, speculate



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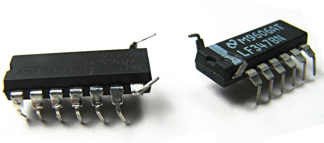
# GPU Computing?

- Design target for CPUs:
  - Make a single thread very fast
  - Hide latency through large caches
  - Predict, speculate
- GPU Computing takes a different approach:
  - Throughput matters— single threads do not
  - Hide latency through parallelism
  - Let programmer deal with "raw" storage hierarchy

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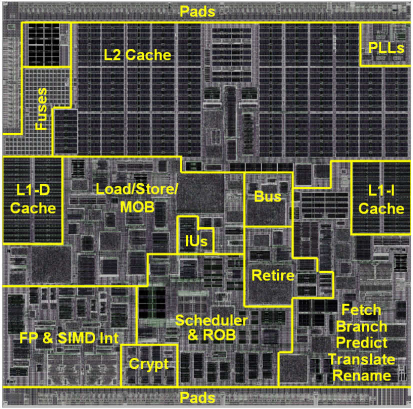
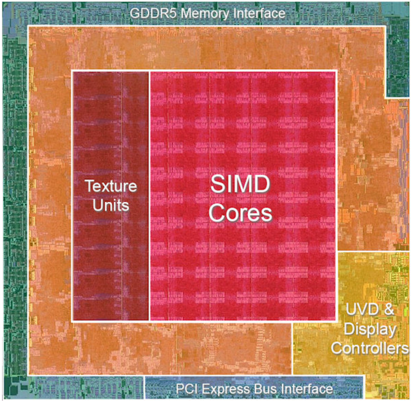
# GPU-CPU Bird's Eye Comparison

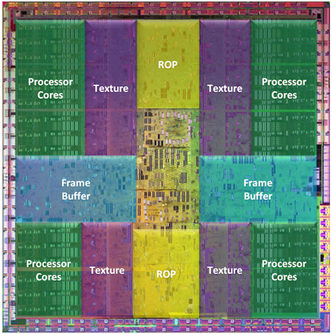



*Floorplan:* VIA Isaiah (2008)
65 nm, 4 SP ops at a time, 1 MiB L2.




*Floorplan:* AMD RV770 (2008)
55 nm, 800 SP ops at a time.

# GPU Architecture (e.g. Nvidia GT200)




- 1 GPU = 30 SIMD cores
- 1 SIMD core: $32 \times 32$ PCs, HW Sched + 1 ID (1/4 clock) + 8 SP + 1 DP + 16 KiB Shared + 32 KiB Reg
- Device $\leftrightarrow$ RAM: **140 GB/s**
- Device $\leftrightarrow$ Host: **6 GB/s**
- User manages memory hierarchy

# GPU Programming: Gains and Losses

| Gains | Losses |
|---|---|
| ⊕ Memory Bandwidth (140 GB/s vs. 12 GB/s)<br>⊕ Compute Bandwidth (Peak: 1 TF/s vs. 50 GF/s, Real: 200 GF/s vs. 10 GF/s)<br>⓪ Data-parallel programming | |

# GPU Programming: Gains and Losses

| Gains | Losses |
|---|---|
| + Memory Bandwidth (140 GB/s vs. 12 GB/s) | − Tuning hardware-specific |
| + Compute Bandwidth (Peak: 1 TF/s vs. 50 GF/s, Real: 200 GF/s vs. 10 GF/s) | − Data size ⇄ Alg. design |
| o Data-parallel programming | − Cheap branches (i.e. `ifs`) |
| | − Fine-grained `malloc` *) |
| | − Recursion *) |
| | − Function pointers *) |

*) Possibly less problematic soon.

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# What is OpenCL?

OpenCL (Open Computing Language) is an open, royalty-free standard for general purpose parallel programming across CPUs, GPUs and other processors. [OpenCL 1.1 spec]

- Vendor-neutral, unlike Nvidia CUDA
  - though rather similar to it

Defines:

- Host-side programming interface (library)
- Device-side programming language (!)

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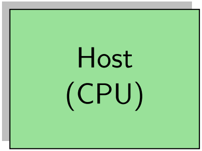
# OpenCL: Computing as a Service



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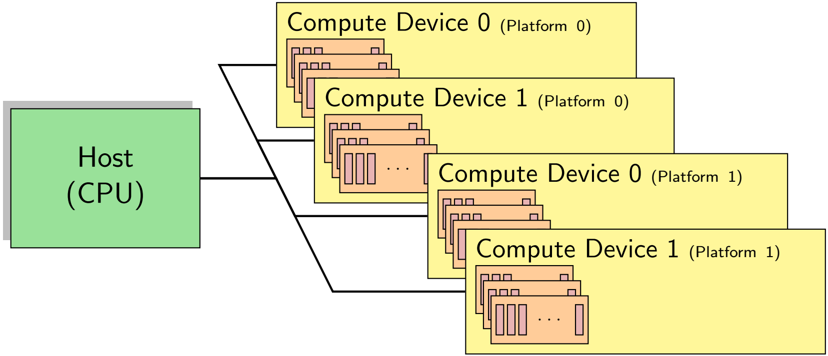

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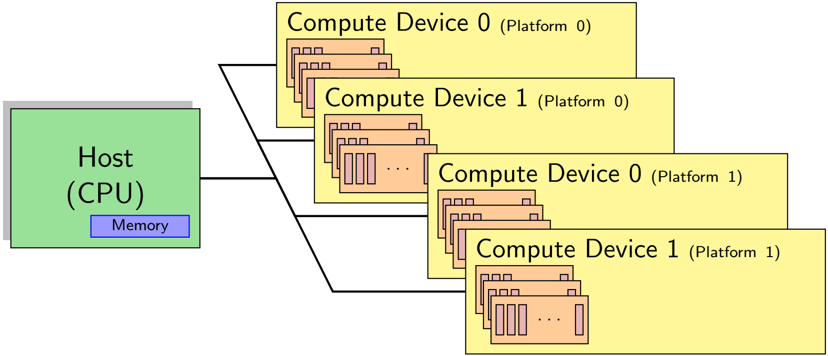

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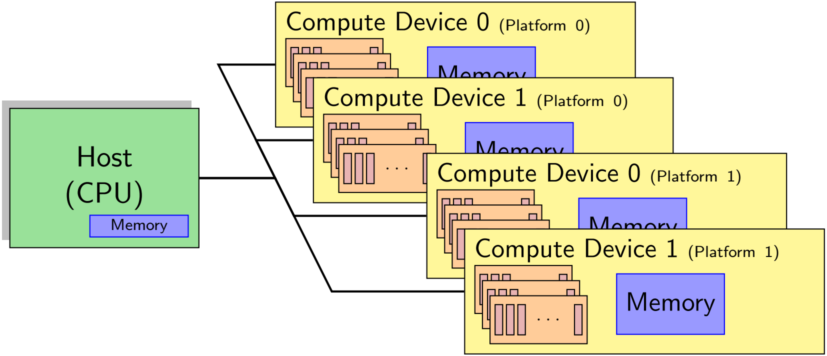

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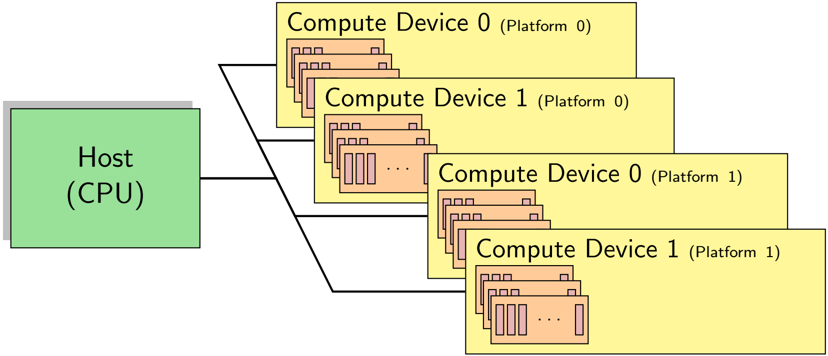

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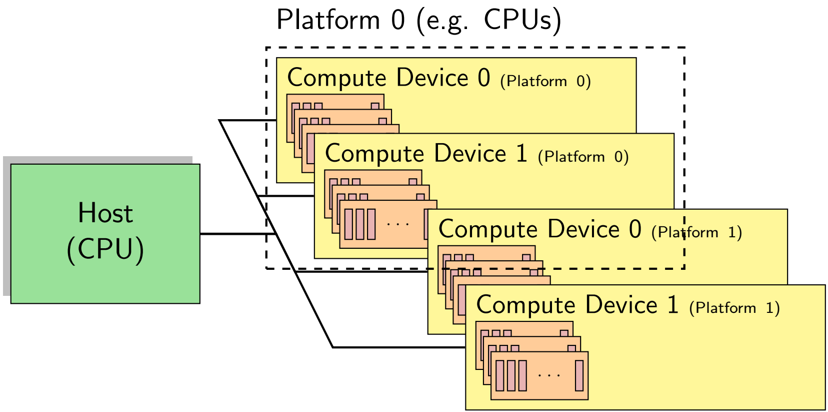

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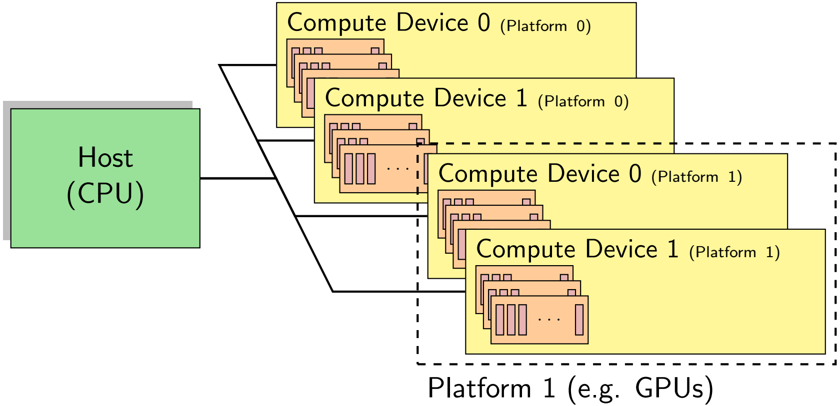

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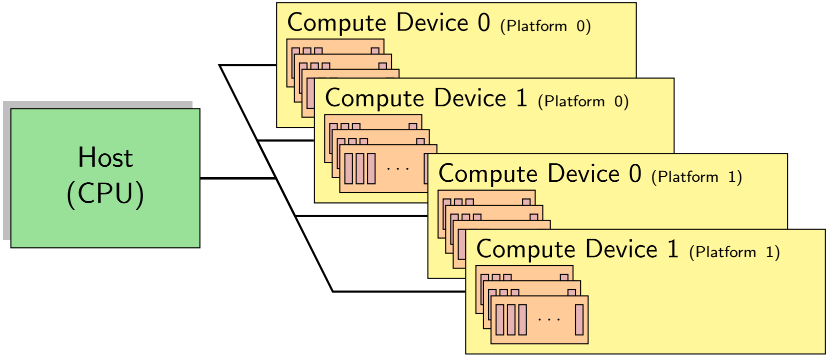

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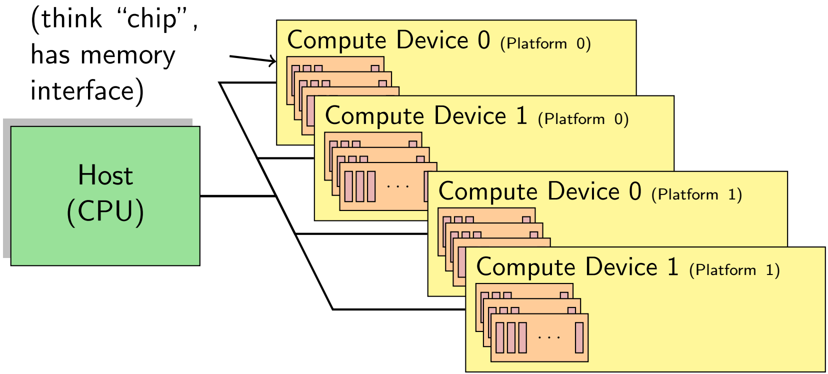

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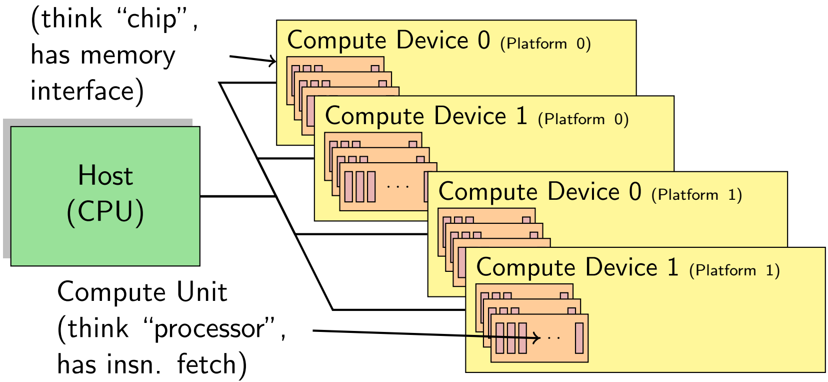

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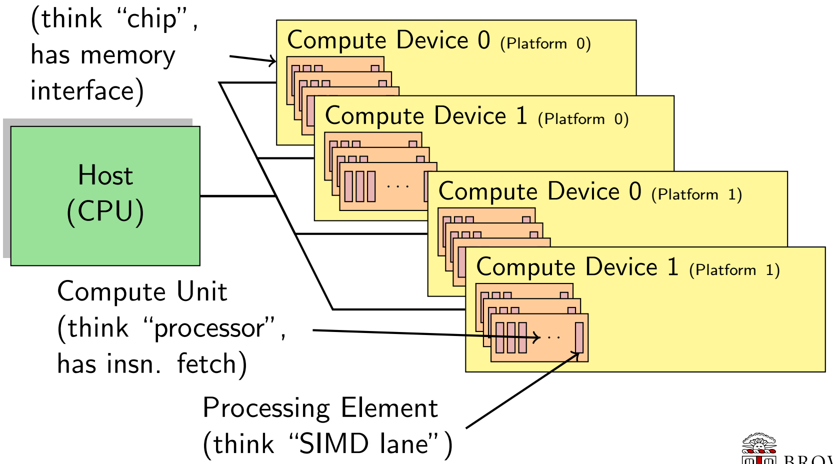

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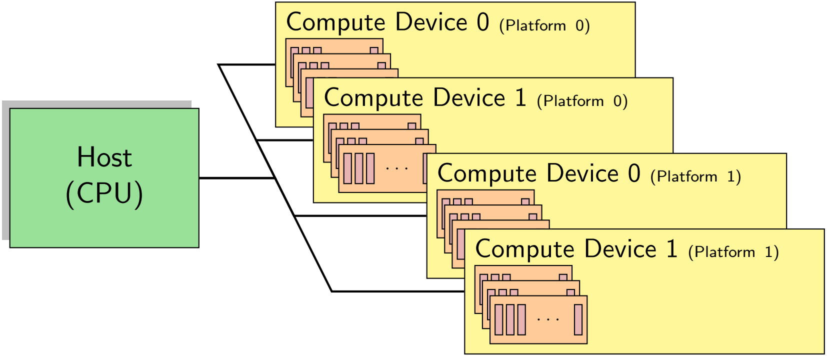

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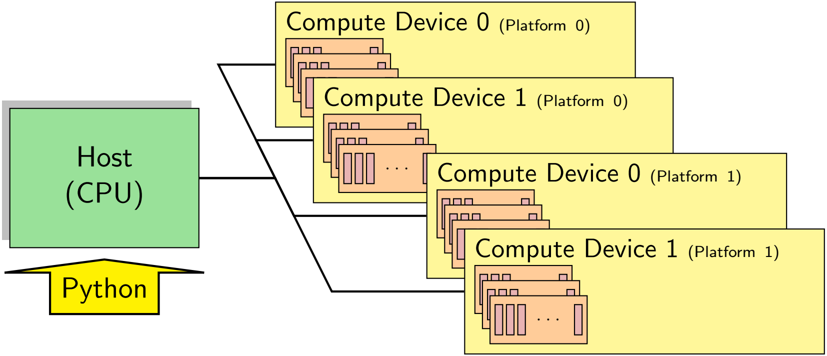

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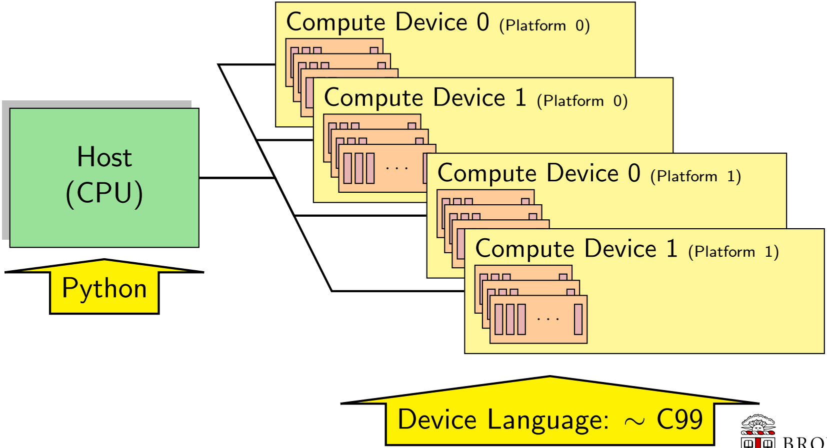
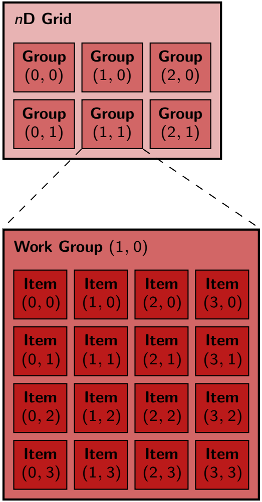


# OpenCL: Execution Model




- Two-tiered Parallelism
  - Grid $= N_x \times N_y \times N_z$ work groups
  - Work group $= S_x \times S_y \times S_z$ work items
  - Total: $\prod_{i \in \{x,y,z\}} S_i N_i$ work items

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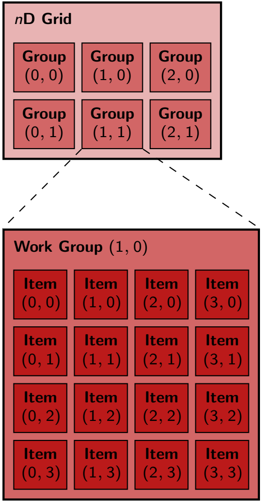


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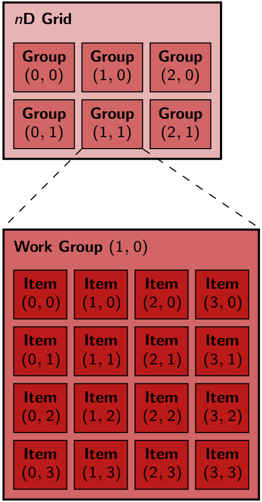


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- Comm/Sync only within work group
  - Work group maps to compute unit
- Grid/Group $\approx$ outer loops in an algorithm
- Device Language: `get_{global,group,local}_{id,size}(axis)`

# Why do Scripting for OpenCL?

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

→ complement each other

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

# Questions?

?

# Outline

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# Dive into PyOpenCL

```python
import pyopencl as cl, numpy

a = numpy.random.rand(256**3).astype(numpy.float32)

ctx = cl.create_some_context()
queue = cl.CommandQueue(ctx)

a_dev = cl.Buffer(ctx, cl.mem_flags.READ_WRITE, size=a.nbytes)
cl.enqueue_write_buffer(queue, a_dev, a)

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

prg.twice(queue, a.shape, (1,), a_dev)
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Compute kernel

# Dive into PyOpenCL: Getting Results

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result = numpy.empty_like(a)
cl.enqueue_read_buffer(queue, a_dev, result).wait()
import numpy.linalg as la
assert la.norm(result - 2*a) == 0
```

# Dive into PyOpenCL: Grouping

```
a_dev = cl.Buffer(ctx, cl.mem_flags.READ_WRITE, size=a.nbytes)
cl.enqueue_write_buffer(queue, a_dev, a)

prg = cl.Program(ctx, """
    __kernel void twice(__global float *a)
    { a[get_local_id(0)+get_local_size(0)*get_group_id(0)] *= 2; }
    """).build()

prg.twice(queue, a.shape, (256,), a_dev)

result = numpy.empty_like(a)
cl.enqueue_read_buffer(queue, a_dev, result).wait()
import numpy.linalg as la
assert la.norm(result - 2*a) == 0
```

# Getting your feet wet

Log into your assigned machine:

1. `ssh NAME@haamster.rice.edu`
2. `ssh teramite` or `ssh slate`

In your home directory, find "`1-intro/intro.py`".
Try running it (on the right GPU).

```
http://tiker.net/tmp/scipy10-pyopencl-tut.tar.gz
```

## Thinking about GPU programming

How would we modify the program to...

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## Thinking about GPU programming

How would we modify the program to...

1. ...compute $c_i = a_i b_i$?
2. ...use groups of $16 \times 16$ work items?

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## Thinking about GPU programming

How would we modify the program to. . .

1. . . . compute $c_i = a_i b_i$?
2. . . . use groups of $16 \times 16$ work items?
3. . . . benchmark 1 work item per group against 256 work items per group? (Use `time.time()` and `.wait()`.)

# Outline

# Contexts

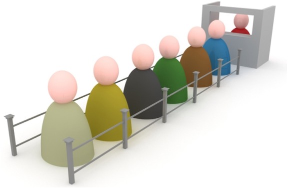
```
context = cl.Context(devices=None | [dev1, dev2], dev_type=None)
context = cl.create_some_context( interactive =True)
```

- Spans one or more Devices
- Create from device type or list of devices
  - See docs for `cl.Platform`, `cl.Device`
- `dev_type`: *`DEFAULT`*, `ALL`, `CPU`, `GPU`
- Needed to. . .
  - . . . allocate Memory Objects
  - . . . create and build Programs
  - . . . host Command Queues
  - . . . execute Grids

# Command Queues and Events

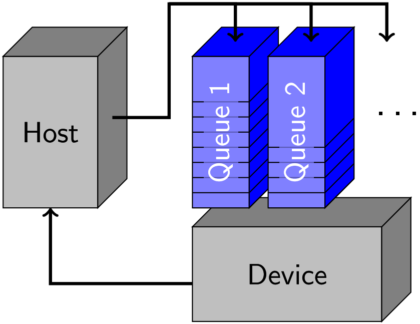
```
queue = cl.CommandQueue(context, device=None,
    properties=None | [(prop, value ),...])
```

- Attached to single device
- `event = enqueue_XXX(queue, ...,`
  `wait_for=[evt1, evt2])`
- `event.wait()`
- Command in queue implicitly waits for previous command's completion



# OpenCL: Command Queues

- Host and Device run asynchronously
- Host submits to queue:
  - Computations
  - Memory Transfers
  - Sync primitives
  - ...
- Host can wait for drained queue
- Multiple Queues: Can overlap Compute + Transfer



# Command Queues: A Crashy Puzzle

✔ OK

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```

✖ Crash

```
a_dev = cl.Buffer(ctx, cl.mem_flags.READ_WRITE, size=256**3*4)
cl.enqueue_write_buffer(queue, a_dev,
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        is_blocking=True)
```

# Command Queues: A Crashy Puzzle

✔ OK (usually!)

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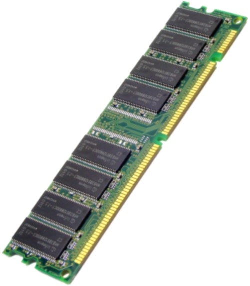
```

# Memory Objects: Buffers

```
buf = cl.Buffer(context, flags, size=0, hostbuf=None)
```

- Chunk of device memory
- No type information: “Bag of bytes”
- Specify `hostbuf` or `size` (or both)
- `hostbuf`: Needs Python Buffer Interface
  e.g. `numpy.ndarray`, `str`.
- `flags`:
  - `READ_ONLY`/`WRITE_ONLY`/`READ_WRITE`
  - `{ALLOC,COPY,USE}_HOST_PTR`



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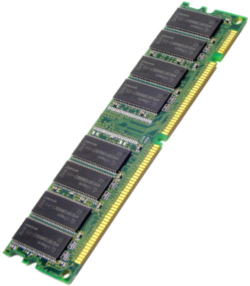
# Memory Objects: Buffers

```
buf = cl.Buffer(context, flags, size=0, hostbuf=None)
```

- Passed to device code as pointers (e.g. `float *`, `int *`)
- `enqueue_{read,write}_buffer(`
  `queue, buf, hostbuf)`
- Can be mapped into host address space: `cl.MemoryMap`.

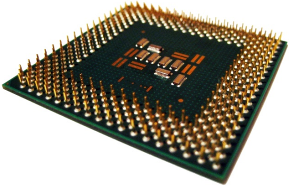


# Programs and Kernels

```
prg = cl.Program(context, src)
```

- `src`: OpenCL device code
  - Derivative of C99
  - Functions with `__kernel` attribute can be invoked from host
- `prg.build(options="", devices=None)`
- `kernel = prg.kernel_name`
- `kernel(queue,` $(G_x, G_y, G_z)$, $(S_x, S_y, S_z)$, `arg, ..., wait_for=None)`

  (Note: `local_size` used to be keyword argument.)



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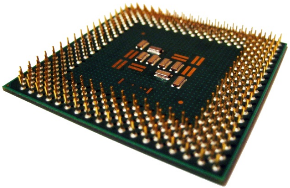
# Program Objects

kernel (queue, (Gx,Gy,Gz), (Sx,Sy,Sz), arg, ..., wait_for =None)

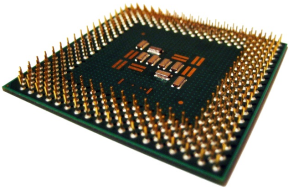


arg may be:

- `None` (a `NULL` pointer)
- numpy sized scalars: `numpy.int64,numpy.float32,...`
- Anything with buffer interface: `numpy.ndarray`, `str`
- Buffer Objects
- Also: `cl.Image`, `cl.Sampler`, `cl.LocalMemory`

# Program Objects

kernel (queue, (Gx,Gy,Gz), (Sx,Sy,Sz), arg , ..., wait_for =None)



Explicitly sized scalars:

✖ Annoying, error-prone.

Better:

```
kernel.set_scalar_arg_dtypes([
   numpy.int32, None,
   numpy.float32])
```

Use `None` for non-scalars.

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# Implicit and Explicit SIMD

## Single-Instruction Multiple-Data in OpenCL

OpenCL exposes two different forms of SIMD computing:

- Explicit: Use (e.g.) `float2`, ..., `float16`.
- Implicit: Adjacent work items get mapped to SIMD lanes (implemented in hardware or software)

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# Implicit and Explicit SIMD

## Single-Instruction Multiple-Data in OpenCL

OpenCL exposes two different forms of SIMD computing:

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```
if (get_global_id(0) % 2 == 0)
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BROWN

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BROWN

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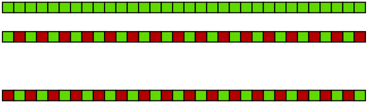

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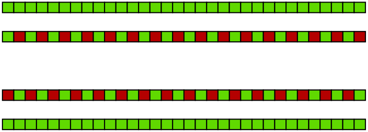

```
if (get_global_id(0) % 2 == 0)
  do_something();
else
  do_another_thing();
do_the_rest();
```

# Outline

# Example: Matrix Transpose

$$\begin{matrix} c_{1,1} & c_{1,2} & c_{1,3} & c_{1,4} \\ c_{2,1} & c_{2,2} & c_{2,3} & c_{2,4} \\ c_{3,1} & c_{3,2} & c_{3,3} & c_{3,4} \\ c_{4,1} & c_{4,2} & c_{4,3} & c_{4,4} \end{matrix} \quad \Rightarrow \quad \begin{matrix} c_{1,1} & c_{2,1} & c_{3,1} & c_{4,1} \\ c_{1,2} & c_{2,2} & c_{3,2} & c_{4,2} \\ c_{1,3} & c_{2,3} & c_{3,3} & c_{4,3} \\ c_{1,4} & c_{2,4} & c_{3,4} & c_{4,4} \end{matrix}$$

# Transpose? Simple Enough!

```
self.kernel = cl.Program(ctx, """
__kernel
void transpose(
  __global float *a_t, __global float *a,
  unsigned a_width, unsigned a_height)
{
  int read_idx = get_global_id(0) + get_global_id(1) * a_width;
  int write_idx = get_global_id(1) + get_global_id(0) * a_height;

  a_t[write_idx] = a[read_idx];
}
""").build().transpose
```

```
w, h = shape
return self.kernel(queue, (w, h), (1,1),
    tgt, src, numpy.uint32(w), numpy.uint32(h))
```

# Measuring Performance

## Writing high-performance Codes

Mindset: What is going to be the limiting factor?

- Floating point throughput?
- Memory bandwidth?
  - Cache sizes?

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  - Cache sizes?

Benchmark the assumed limiting factor right away.

## Evaluate

- Know your peak throughputs (roughly)
- Are you getting close?
- Are you tracking the right limiting factor?

# Performance: Matrix transpose

Very likely: Bound by memory bandwidth.

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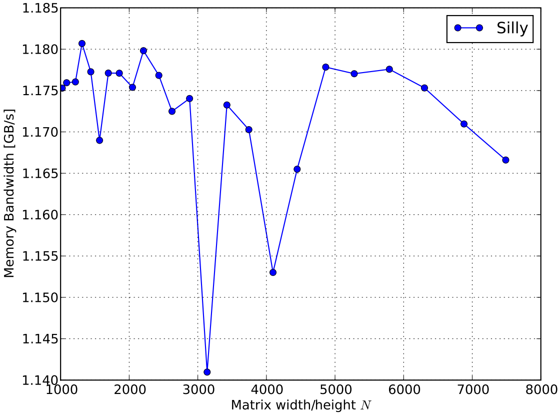



*Fantastic!* Far slower than CPU. Why?

# Intra-device Work Distribution

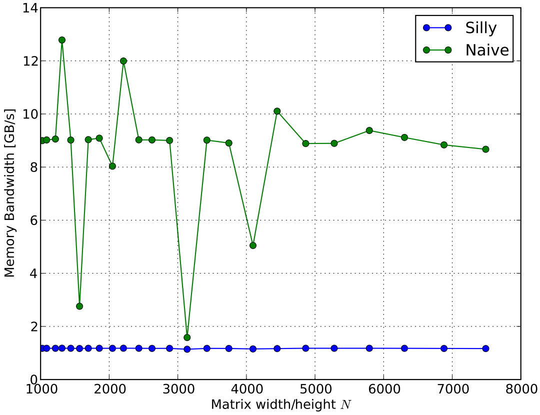
```python
w, h = shape
return self.kernel(queue, (w, h), (1,1),
    tgt, src, numpy.uint32(w), numpy.uint32(h))
```

```python
w, h = shape
return self.kernel(queue, (w, h), (16, 16),
    tgt, src, numpy.uint32(w), numpy.uint32(h))
```

## Again: Work Groups

- Work group size matters. A lot.
- Determines work distribution among processors
- Optimal size? Up to experimentation

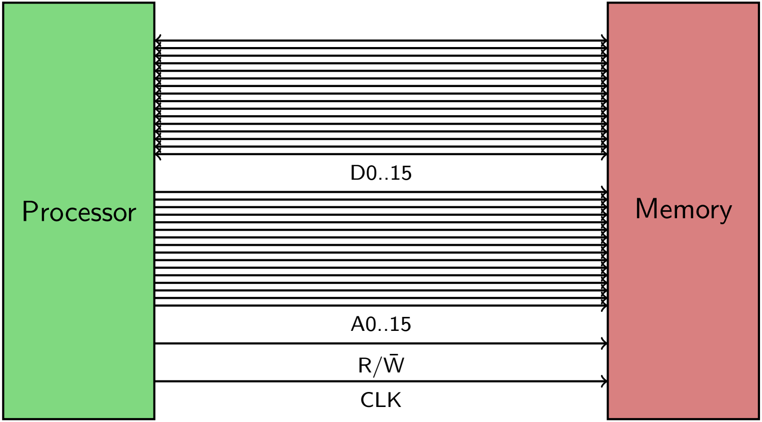
# Performance: Matrix transpose




*Better.* 1.5× faster than CPU–not great. Why?

# Aside: How does computer memory work?

One memory transaction (simplified):



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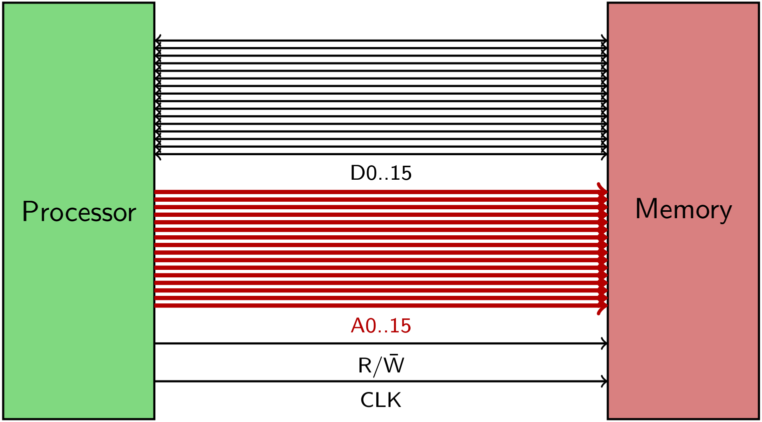

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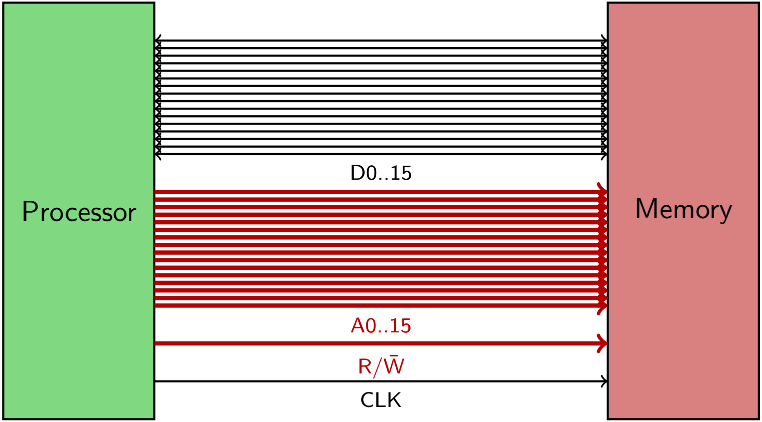

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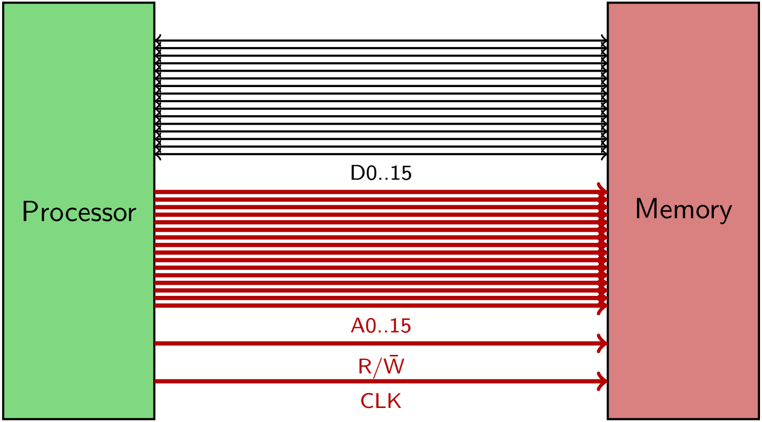

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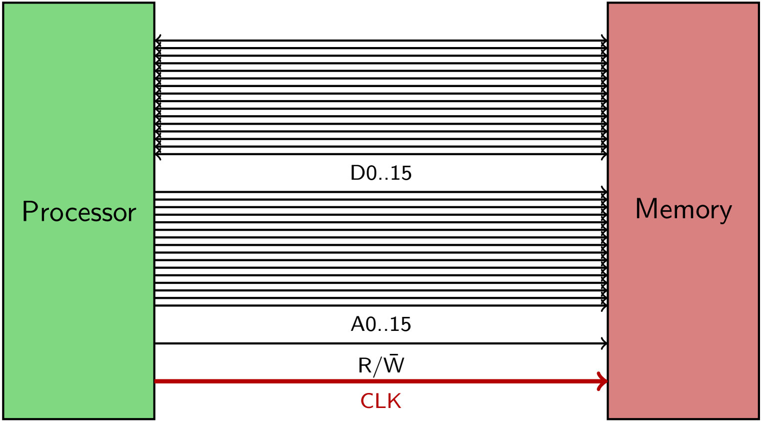

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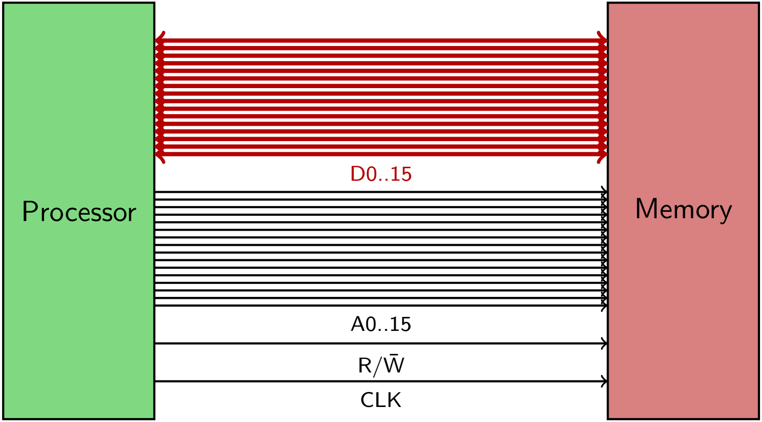

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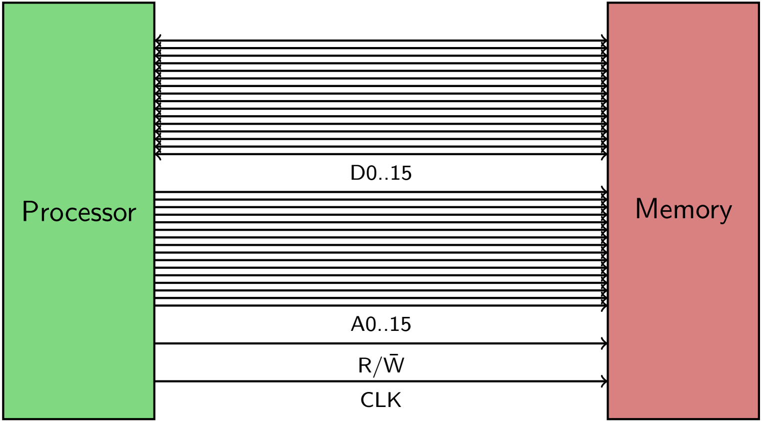


Observation: Access (and addressing) happens in bus-width-size "chunks".

# Memory for Parallel Machines

## Problem

Memory chips have only one data bus.

So how can multiple threads read multiple data items from memory simultaneously?

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Memory chips have only one data bus.

So how can multiple threads read multiple data items from memory simultaneously?

## Solutions: Parallel Access to Memory

- Split a really wide data bus, but have only one address bus
- Have many "small memories" ("*banks*") with separate data and address busses, select by address LSB.

# Naive: Using Global Memory

```python
self.kernel = cl.Program(ctx, """
__kernel
void transpose(
  __global float *a_t, __global float *a,
  unsigned a_width, unsigned a_height)
{
  int read_idx = get_global_id(0) + get_global_id(1) * a_width;
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  a_t[write_idx] = a[read_idx];
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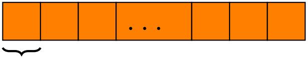
Reading from global mem:




stride: 1

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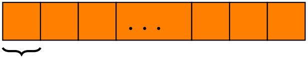


stride: 1 → one mem.trans.

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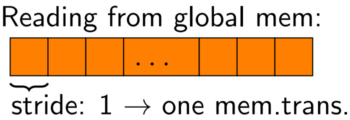


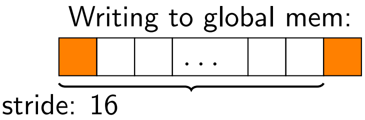

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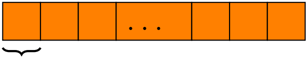


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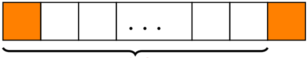
Writing to global mem:




stride: 16 → **16 mem.trans.!**

# Local Memory: Banking

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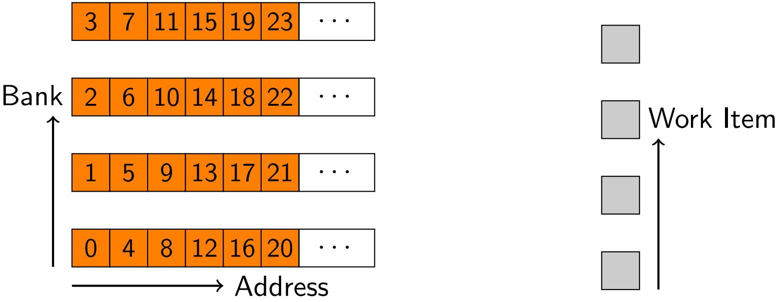

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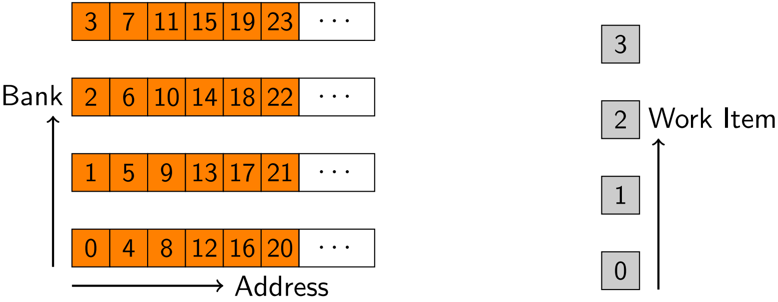

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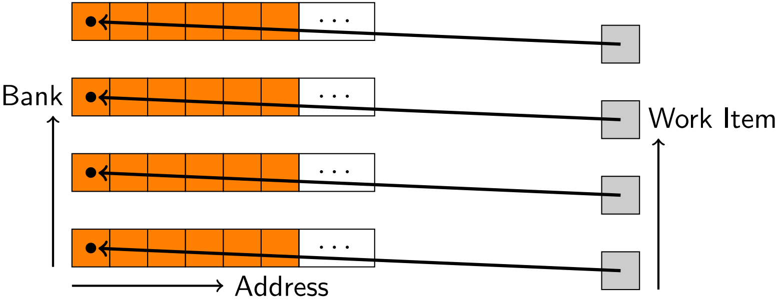


OK: `local_variable[get_local_id(0)]`,
(Single cycle)

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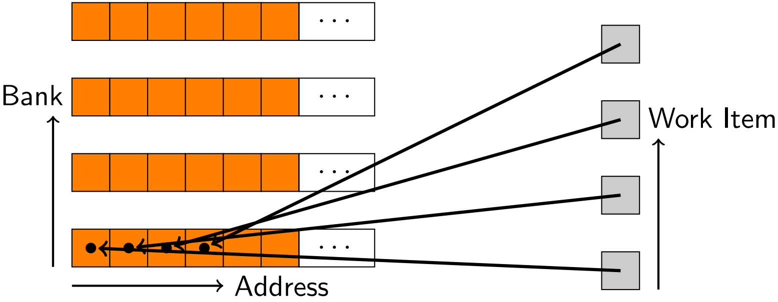


Bad: `local_variable[BANK_COUNT*get_local_id(0)]`
(`BANK_COUNT` cycles)

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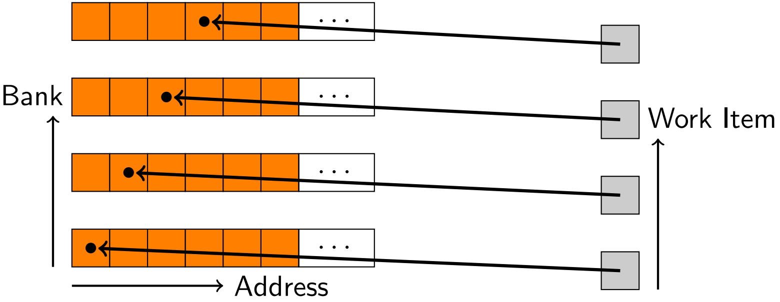
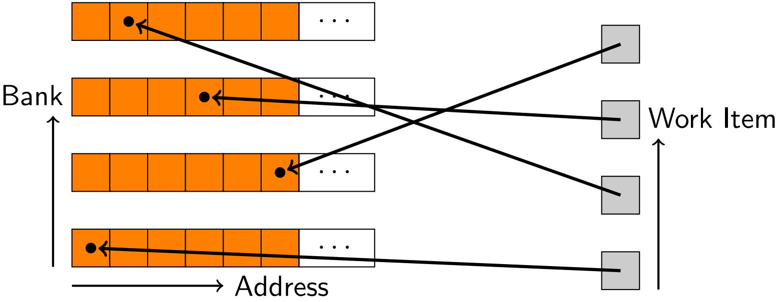



OK: `local_variable[(BANK_COUNT+1)*get_local_id(0)]`
(Single cycle)

# Local Memory: Banking




OK: `local_variable[ODD_NUMBER*get_local_id(0)]`
(Single cycle)

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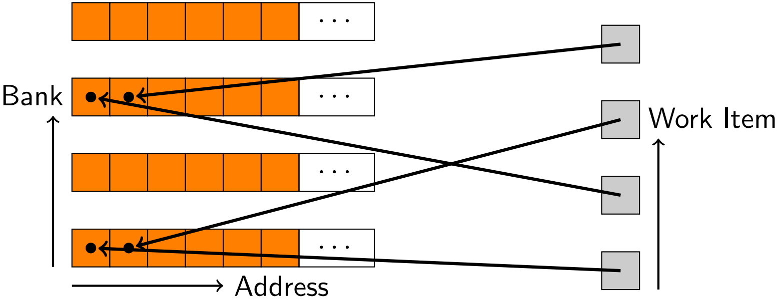
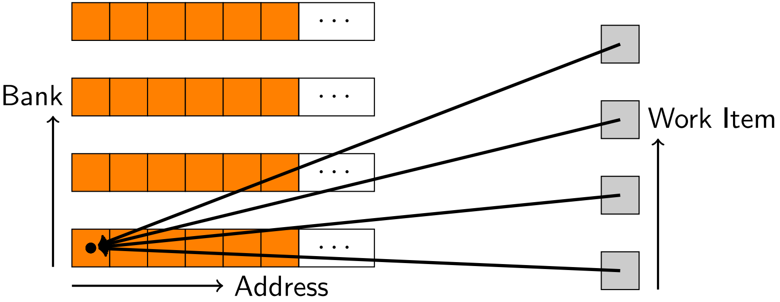



Bad: `local_variable[2*get_local_id(0)]`
(`BANK_COUNT`/2 cycles)

# Local Memory: Banking




OK: `local_variable[f(blockIdx)]`
(Broadcast–single cycle)

# Local Memory: Banking


Nvidia hardware has 16 banks.
Work item access local memory in groups of 16.

# Transpose: Idea

- Global memory dislikes non-unit strides.
- Local memory doesn't mind.

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- Don't transpose element-by-element.
- Transpose block-by-block instead.

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## Idea

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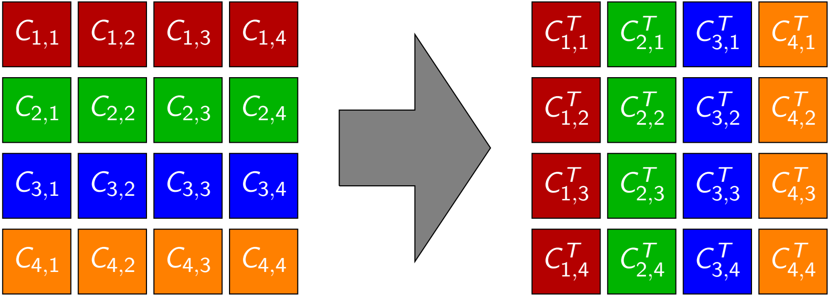
1. Read untransposed block from global and write to local
2. Read block transposed from local and write to global

# Illustration: Blockwise Transpose



# Improved: With Local Memory

Part 1/3:

```
#define BLOCK_SIZE 16
#define A_BLOCK_STRIDE (BLOCK_SIZE * a_width)
#define A_T_BLOCK_STRIDE (BLOCK_SIZE * a_height)

__kernel void transpose(
  __global float *a_t, __global float *a,
  unsigned a_width, unsigned a_height)
```

# Improved: With Local Memory

Part 2/3:

```
{
  __local float a_local [BLOCK_SIZE][BLOCK_SIZE];
  int base_idx_a =
    get_group_id (0) * BLOCK_SIZE +
    get_group_id (1) * A_BLOCK_STRIDE;
  int base_idx_a_t =
    get_group_id (1) * BLOCK_SIZE +
    get_group_id (0) * A_T_BLOCK_STRIDE;

  int glob_idx_a =
    base_idx_a + get_local_id (0)
    + a_width * get_local_id (1);
  int glob_idx_a_t =
    base_idx_a_t + get_local_id (0)
    + a_height * get_local_id (1);
```

# Improved: With Local Memory

Part 3/3:

```
    a_local [ get_local_id (1)][ get_local_id (0)] = a[glob_idx_a ];

    barrier (CLK_LOCAL_MEM_FENCE);

    a_t [ glob_idx_a_t ] = a_local [ get_local_id (0)][ get_local_id (1)];
}
```

# Improved: With Local Memory

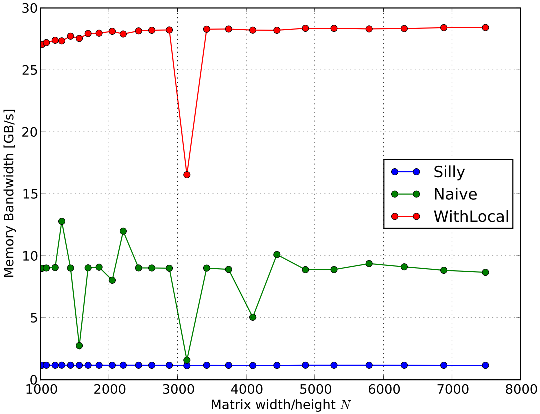
Launch Code:

```
w, h = shape

return self.kernel(queue, (w, h), (16, 16),
    tgt, src, numpy.uint32(w), numpy.uint32(h))
```

Transpose example is `2-transpose/transpose.py` in your home directory. Spot any bank conflicts? Tinker away!

# Performance: Matrix transpose

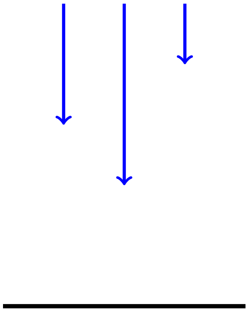



*Much better.* Not peak, but good enough.

# Outline

# Synchronization

What is a Barrier?



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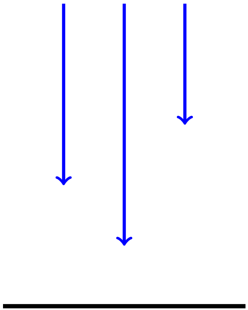

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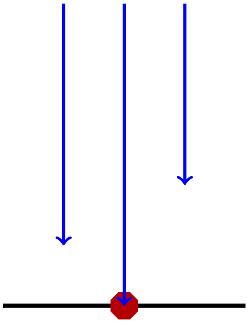

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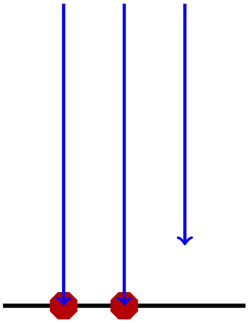

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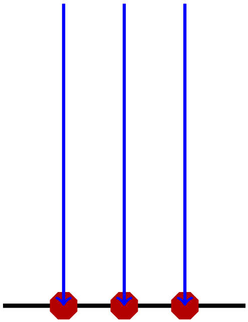

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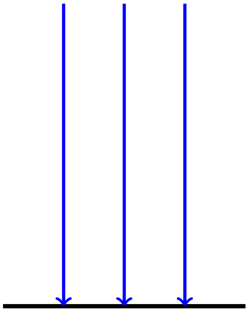

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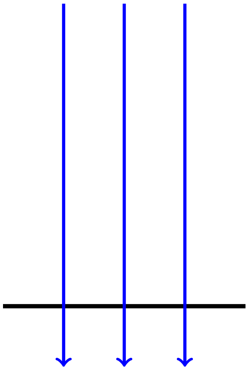

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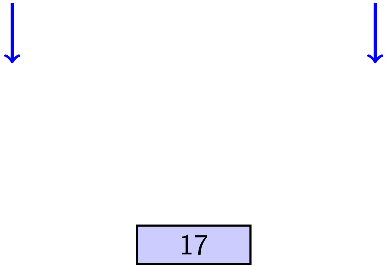
What is a Memory Fence?



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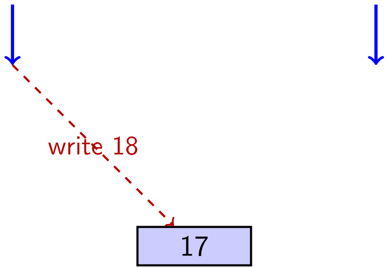

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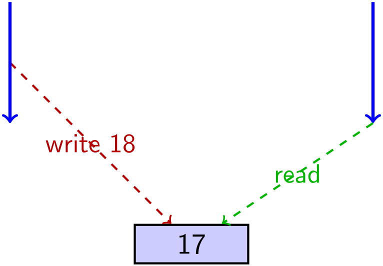

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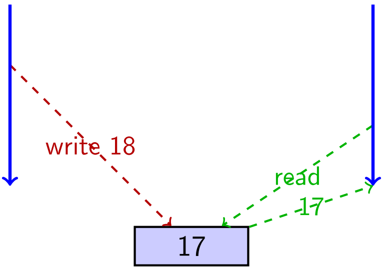

# Synchronization

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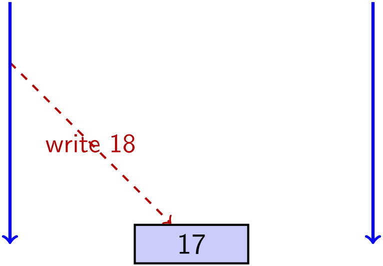

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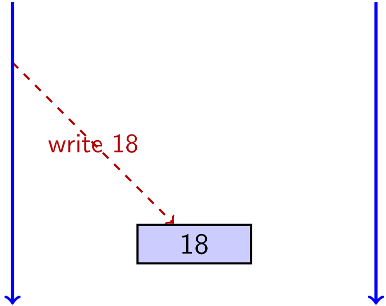

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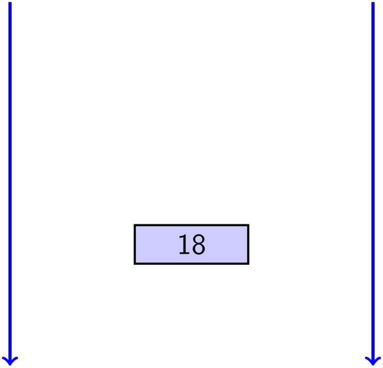

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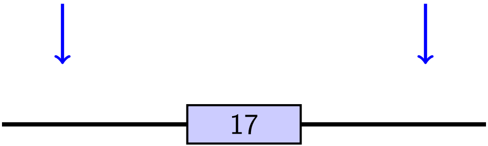

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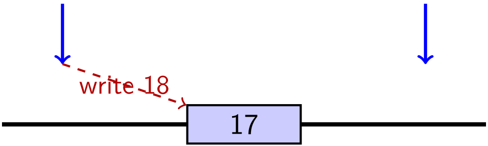

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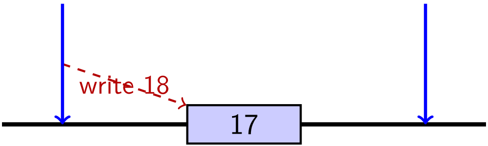

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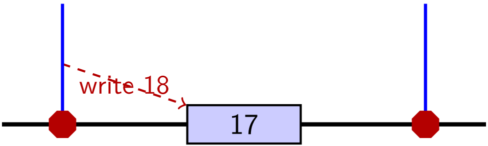

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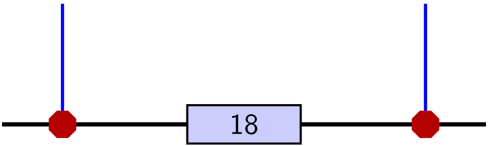

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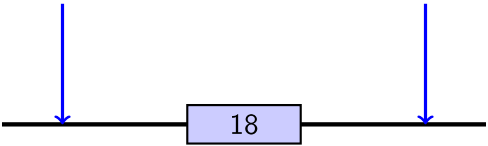

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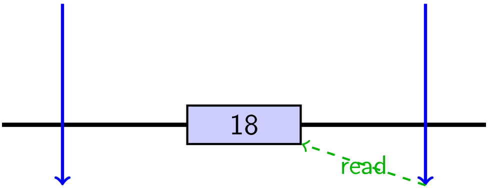

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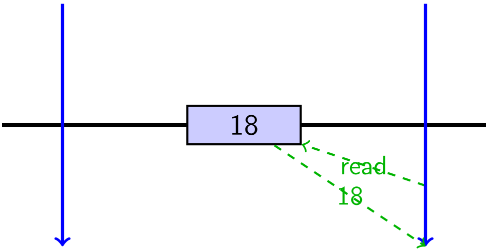


# Recap: Concurrency and Synchronization

GPUs have layers of concurrency.

Each layer has its synchronization primitives.

# Recap: Concurrency and Synchronization

GPUs have layers of concurrency.
Each layer has its synchronization primitives.

- Intra-block:
  `barrier(...)`,
  `mem_fence(...)`
  `...` =
  `CLK_{LOCAL,GLOBAL}_MEM_FENCE`
- Inter-block:
  Kernel launch
- CPU-GPU:
  Command queues, Events

# Synchronization between Groups

**Golden Rule:**

Results of the algorithm must be independent of the order in which work groups are executed.

# Synchronization between Groups

## Golden Rule:

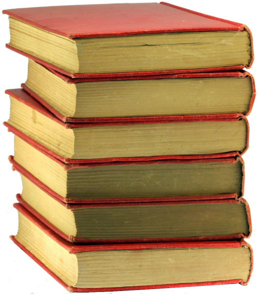
Results of the algorithm must be independent of the order in which work groups are executed.

**Consequences:**

- Work groups may read the same information from global memory.
- But: Two work groups may not validly write different things to the same global memory.
- Kernel launch serves as
  - Global barrier
  - Global memory fence

# Outline

# PyOpenCL Philosophy



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

# PyOpenCL: Completeness

PyOpenCL exposes *all* of OpenCL.

For example:

- OpenCL 1.1
- Every `GetInfo()` query
- Images and Samplers
- Memory Maps
- Profiling and Synchronization
- GL Interop (example in source)

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# PyOpenCL: Completeness

PyOpenCL supports (nearly) every OS that has an OpenCL implementation.

- Linux
- OS X
- Windows

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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.release()`)
- Correctly deals with multiple contexts and dependencies.

# PyOpenCL: Documentation





**Quick search**

Go

Enter search terms or a module, class or function name.

## Welcome to PyOpenCL's documentation!

PyOpenCL gives you easy, Pythonic access to the OpenCL parallel computation API. What makes PyOpenCL special?

- 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.
- Completeness. PyOpenCL puts the full power of OpenCL's API at your disposal, if you wish. Every obscure *get_info()* query and all CL calls are accessible.
- Automatic Error Checking. All errors are automatically translated into Python exceptions.
- Speed. PyOpenCL's base layer is written in C++, so all the niceties above are virtually free.
- Helpful Documentation. You're looking at it. ;)
- Liberal license. PyOpenCL is open-source under the *MIT license* and free for commercial, academic, and private use.

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

```
import pyopencl as cl
import numpy
import numpy.linalg as la

a = numpy.random.rand(50000).astype(numpy.float32)
b = numpy.random.rand(50000).astype(numpy.float32)

ctx = cl.Context()
queue = cl.CommandQueue(ctx)

mf = cl.mem_flags
a_buf = cl.Buffer(ctx, mf.READ_ONLY | mf.COPY_HOST_PTR, hostbuf=a)
b_buf = cl.Buffer(ctx, mf.READ_ONLY | mf.COPY_HOST_PTR, hostbuf=b)
dest_buf = cl.Buffer(ctx, mf.WRITE_ONLY, b.nbytes)

prg = cl.Program(ctx, """
    __kernel void sum(__global const float *a,
    __global const float *b, __global float *c)
    {
      int gid = get_global_id(0);
      c[gid] = a[gid] + b[gid];
    }
    """).build()

prg.sum(queue, a.shape, a_buf, b_buf, dest_buf)

a_plus_b = numpy.empty_like(a)
cl.enqueue_read_buffer(queue, dest_buf, a_plus_b).wait()

print la.norm(a_plus_b - (a+b))
```

(You can find this example as `examples/demo.py` in the PyOpenCL source distribution.)

## Contents

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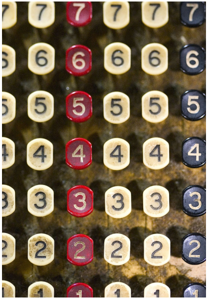
# PyOpenCL: Vital Information

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

# pyopencl.array: Simple Linear Algebra

pyopencl.array.Array:

- Meant to look and feel just like numpy.
  - `p.a.to_device(ctx, queue, numpy_array)`
  - `numpy_array = ary.get()`
- +, -, ∗, /, fill, sin, arange, exp, rand, . . .
- Mixed types (int32 + float32 = float64)
- `print cl_array` for debugging.
- Allows access to raw bits
  - Use as kernel arguments, memory maps



# Remember your first PyOpenCL program?

Abstraction is good:

```
import numpy
import pyopencl as cl
import pyopencl.array as cl_array

ctx = cl.create_some_context()
queue = cl.CommandQueue(ctx)

a_gpu = cl_array.to_device(
        ctx, queue, numpy.random.randn(4,4).astype(numpy.float32))
a_doubled = (2*a_gpu).get()
print a_doubled
print a_gpu
```

# pyopencl.elementwise: Elementwise expressions

Avoiding extra store-fetch cycles for elementwise math:

```python
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
```

# Questions?

?

# Outline

1. Intro: GPUs, OpenCL
2. GPU Programming with PyOpenCL
3. Additional Topics
   - Code Generation
   - Other GPU Gadgetry
   - GPU Architectures in more Detail
   - Automatic GPU Programming
4. Playtime!
5. Conclusions

# Outline

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

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Devices differ by

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Optimally tuned code will (often) be different for each device

# Metaprogramming

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**Idea**

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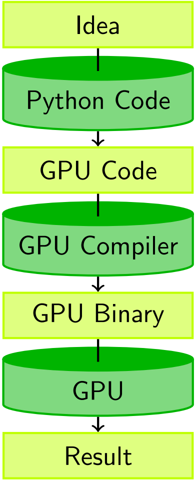


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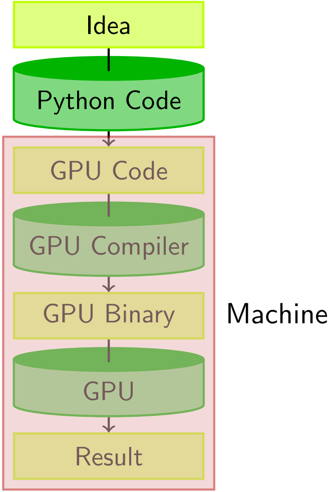


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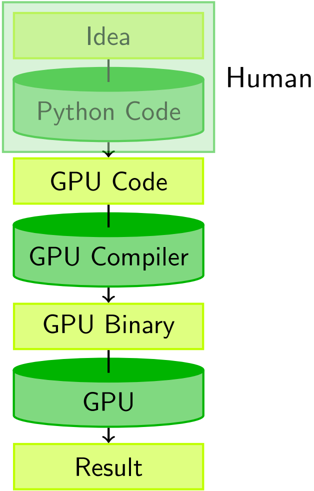


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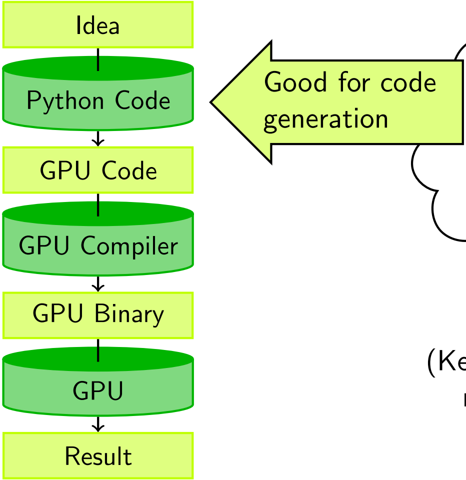


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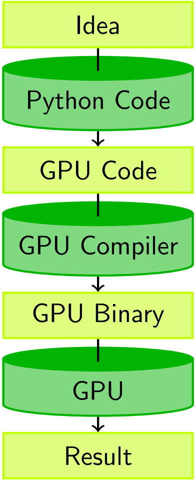


Good for code generation

*In* PyOpenCL
GPU code does
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a compile-time
constant.

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# 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

# PyOpenCL: Support for Metaprogramming

Three (main) ways of generating code:

- Simple %-operator substitution
- Use a templating engine (Jinja 2 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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# RTCG via Templates

```
from jinja2 import Template

tpl = Template("""
    __kernel void twice( __global {{ type_name }} *tgt)
    {
      int idx = get_local_id (0)
        + {{ local_size }} * {{ thread_strides }}
        * get_group_id (0);

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

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

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

# RTCG via AST Generation

```
from codepy.cgen import *
from codepy.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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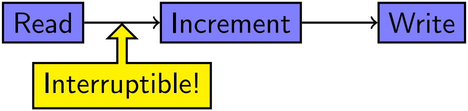

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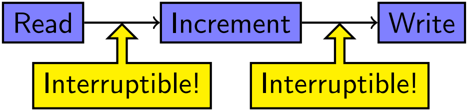

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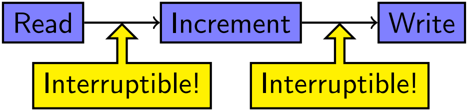


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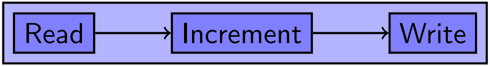

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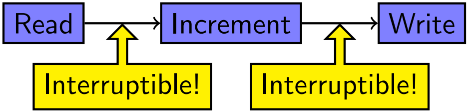


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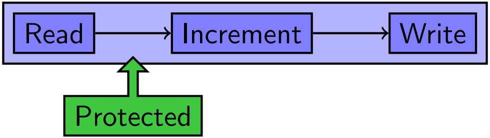

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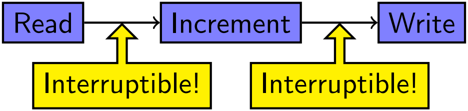


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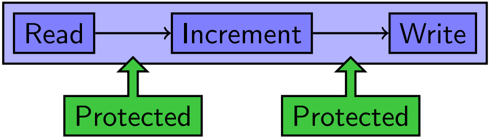

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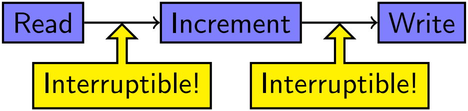


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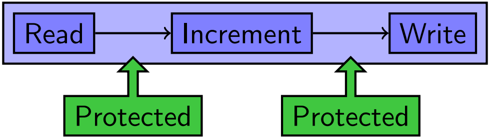


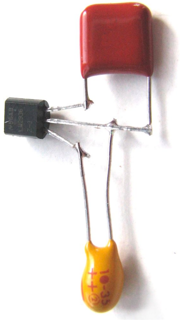

**How?**

atomic_{add,inc,cmpxchg,. . . }(int *global, int value);

# Even more GPU Gadgetry

Available in GPU code:

- Floating point intrinsics
  - `native_sin(x)`, `native_cos(x)`, etc.
  - Very fast
  - Less accurate, limited domains
- Vector types
  - `int`/`float`*n* for *n* in 1,2,3,4,8,...
  - Plus functions: load/store/sum/dot
  - Much saner than SSE intrinsics
- Images (r/w through texture units)
  - Can do filtering
  - Has some cache



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# Outline



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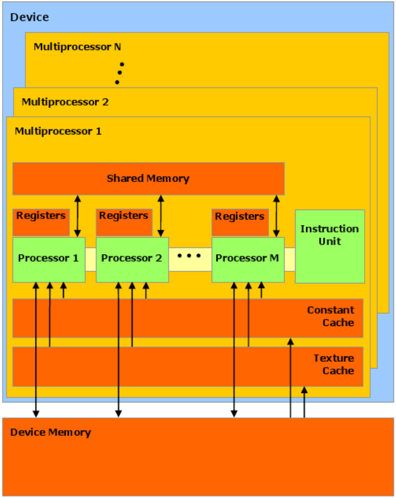
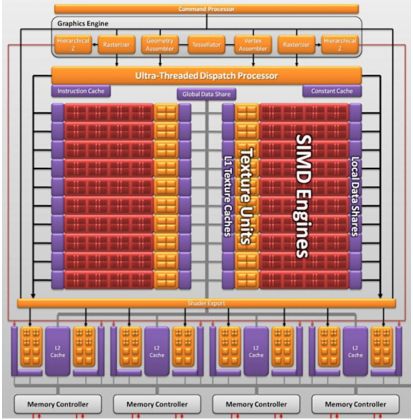
# GPU Architecture (e.g. Nvidia GT200)




- 1 GPU = 30 SIMDs
- 1 SIMD = 1 ID (1/4 clock) + 8 SP + 1 DP + 16 KiB Shared + 32 KiB Reg + HW Sched
- Scalar cores, deep pipeline
- 32 scheduling slots
- DDR3 RAM (140 GB/s)
- PCIe2 Host DMA (6 GB/s)
- Limited Caches

# GPU Architecture (e.g. ATI RV870)




- 1 GPU = 20 SIMDs
  + 64 KiB Global Share
  + 4 × 128 KiB L2
- 1 SIMD = 1 ID + 16×5 SP
  + 16 DP + 32 KiB Share
  + HW Sched + 8 KiB L1
- GDDR5 RAM (150 GB/s)
- PCIe2 Host DMA
  (6 GB/s)

# Outline

# 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:

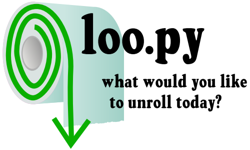
```
a, b, c, i, j, k = [var(s) for s in "abcijk"]
n = 500
k = make_loop_kernel([
    LoopDimension("i", n),
    LoopDimension("j", n),
    LoopDimension("k", n),
    ], [
    (c[i+n*j], a[i+n*k]*b[k+n*j])
    ])

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, ...



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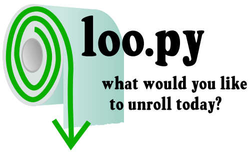
  - Require input/output separation
  - Kernels must be expressible using "loopy" model
    (i.e. indices decompose into "output" and "reduction")
  - Enough for DG, LA, FD, ...
- Kernel compilation limits trial rate
- Non-Goal: Peak performance
- Good results currently for dense linear algebra and (some)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

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# Questions?

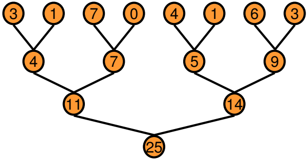
?

# Outline

# Outline

# Parallel Reduction

- **Tree-based approach used within each thread block**




- **Need to be able to use multiple thread blocks**
  - **To process very large arrays**
  - **To keep all multiprocessors on the GPU busy**
  - **Each thread block reduces a portion of the array**
- **But how do we communicate partial results between thread blocks?**

Slides by M. Harris (Nvidia Corp.)

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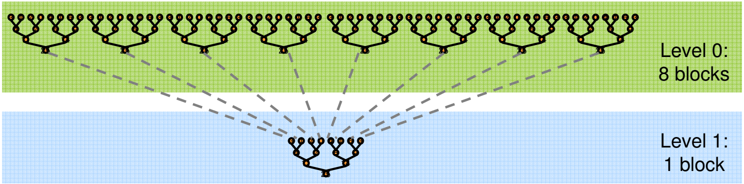
# Solution: Kernel Decomposition

- **Avoid global sync by decomposing computation into multiple kernel invocations**




- **In the case of reductions, code for all levels is the same**
  - **Recursive kernel invocation**

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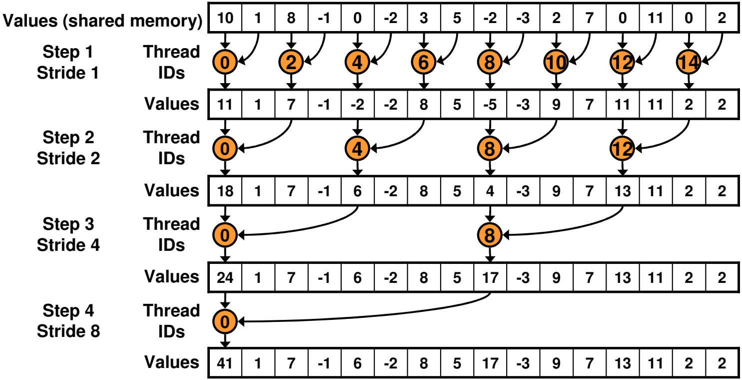
# Interleaved Addressing

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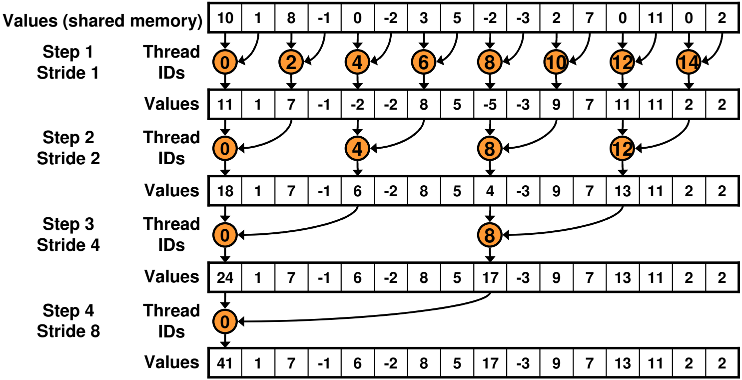
# Interleaved Addressing




**Issue:** Divergence

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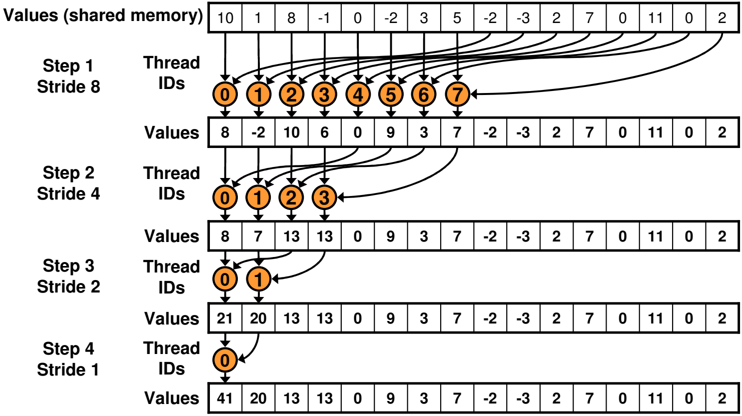
# Sequential Addressing

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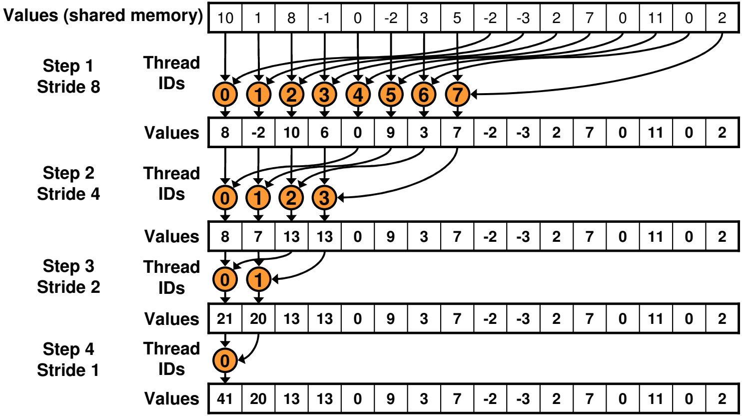
# Sequential Addressing




**Better!**

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# Reduction: Further Strategies

Further Strategies:

- Exploit SIMD synchronicity
  - Eliminate a few `barrier()`s
- Amortize cost of index calculation/preparation
  - Not just one item per thread!
- Do as much as possible at compile time
  - Unroll loops
  - Exploit compile-time knowledge of block size, etc. ($\rightarrow$ metaprogramming: PyCUDA or C++ `templates`)

Slides by M. Harris
(Nvidia Corp.)

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# Try for yourself: Performance of GPU Reduction

1. In your home directory, find and run `3-reduction/reduction.py`.
2. Add event-based timing. Compute memory throughput in GiB/s for a number of vector sizes. (e.g. $2^k$ for $k \in \{12, \ldots, 25\}$)
3. Implement and benchmark the improvements discussed previously.
4. What else is missing for peak performance? (Google?)

PyOpenCL docs: `http://documen.tician.de/pyopencl`

These slides: `http://tiker.net/tmp/scipy10-pyopencl.pdf`

# Outline

1. Intro: GPUs, OpenCL
2. GPU Programming with PyOpenCL
3. Additional Topics
4. Playtime!
5. Conclusions
   - A Brief Look at PyCUDA
   - Summary

# Outline

# OpenCL ↔ CUDA: A dictionary

| OpenCL | CUDA |
|---:|---|
| Grid | Grid |
| Work Group | Block |
| Work Item | Thread |
| __kernel | __global__ |
| __global | __device__ |
| __local | __shared__ |
| image*n*d_t | texture<type, *n*, ...> |
| barrier(LMF) | __syncthreads() |
| get_local_id(012) | threadIdx.xyz |
| get_group_id(012) | blockIdx.xyz |
| get_global_id(012) | – (reimplement) |

# PyOpenCL ↔ PyCUDA: A (rough) dictionary

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

# Whetting your appetite

```python
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;
      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
```

Compute kernel

# Whetting your appetite, Part II

Did somebody say "Abstraction is good"?

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# 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
```

# Outline

# Concluding Remarks

- GPU Computing is maturing.
  Now is a great time to start looking at GPUs.
- First factor of 5-10 is usually easy to reach.
- Second factor of 5-10 is a bit harder
  - Usually involves rethinking the algorithm
- Fun time to be in computational science
- Python makes GPUs even more fun
  - With no compromise in performance
- OpenCL presents a huge opportunity:
  - A JIT compiler in a library
  - CPU backends exist (AMD, Apple)
  - → Like weave/codepy/Cython's pyximport, but un-hacky

# Questions?

?

Thank you for your attention!

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

image credits

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# Image Credits

- Fighting chips: flickr.com/oskay (cc)
- Isaiah die shot: VIA Technologies
- RV770 die shot: AMD Corp.
- Nvidia Tesla Architecture: Nvidia Corp.
- C870 GPU: Nvidia Corp.
- Context: sxc.hu/svilen001
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- Dictionary: sxc.hu/topfer

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