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

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PASI: The Challenge of Massive Parallelism
Lecture 2 · January 5, 2011

Motivation

```
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)
```

OpenCL: Runtime and Device

CL consists of two parts:

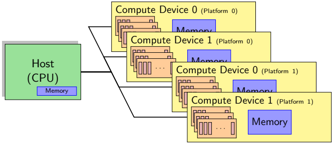
- Host-side "runtime":

  C: `#include "CL/cl.h"`, `libOpenCL.so`

  Python:
  `import pyopencl as cl`

- Device-side programming language
  A dialect of C99 (also when using PyOpenCL)

Today: A better look at both of those, with an emphasis on PyOpenCL



Outline

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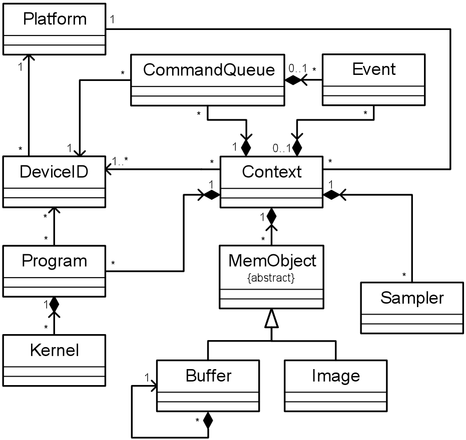
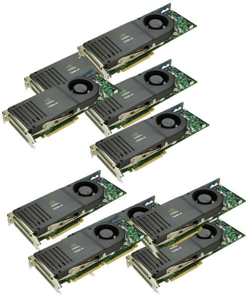
OpenCL Object Diagram



Credit: Khronos Group

CL "Platform"



- "Platform": a collection of devices, all from the same *vendor*.
- All devices in a platform use same CL driver/implementation.
- Multiple platforms can be used from one program → *ICD*.

`libOpenCL.so`: ICD loader

`/etc/OpenCL/vendors/`*`somename`*`.icd`: Plain text file with name of `.so` containing CL implementation.

CL "Compute Device"

CL Compute Devices:

- CPUs, GPUs, accelerators, ...
  - Anything that fits the programming model.
- A processor die with an interface to off-chip memory
- Can get list of devices from platform.

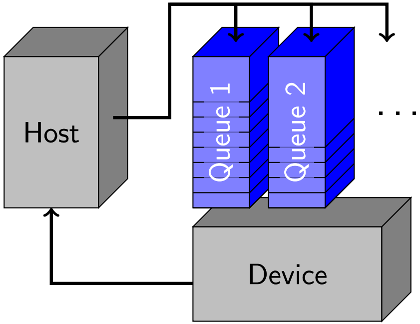
Contexts

```
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

OpenCL: Command Queues

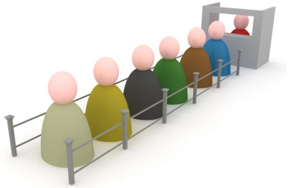
- Host and Device run asynchronously
- Host submits to queue:
  - Computations
  - Memory Transfers
  - Sync primitives
  - . . .
- Host can wait for drained queue
- Profiling



Command Queues and Events

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

- Attached to single device
- cl.command_queue_properties...
  - `OUT_OF_ORDER_EXEC_MODE_ENABLE`: Do not force sequential execution
  - `PROFILING_ENABLE`: Gather timing info



Building Blocks in Action

```python
import pyopencl as cl

platforms = cl.get_platforms()
my_platform = platforms[0]
print my_platform.vendor

devices = my_platform.get_devices()
my_device = devices[0]
print my_device.name

ctx = cl.Context([my_device])

cpq = cl.command_queue_properties
queue = cl.CommandQueue(ctx, my_device, cpq.PROFILING_ENABLE)
```

Simple version:

```python
ctx2 = cl.create_some_context()
queue2 = cl.CommandQueue(ctx)
```

Command Queues and Events

```
event = cl.enqueue_XXX(queue, ..., wait_for=[evt1, evt2])
```

Every enqueue operation returns an *Event*.

Also possible: Operation-less events ("Markers")

- Wait (`evt.wait()`), polling
- Specify dependencies

  Every enqueue operation takes a list arg `wait_for` of dependencies.
- Profile

  `event.profile....`
  - `QUEUED`, `SUBMIT`
  - `START`, `END`

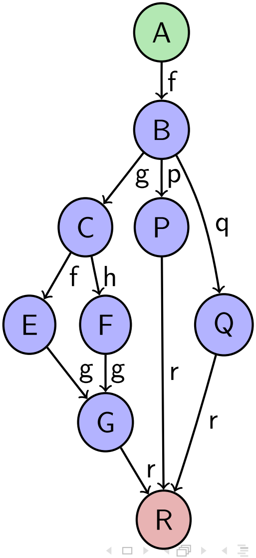
  (time stamp in ns)

Profiling example

```
start_event = cl.enqueue_marker(queue)

# enqueue some commands

stop_event = cl.enqueue_marker(queue)
stop_event.wait()

elapsed_seconds = 1e-9*(
        start_event.profile.END - start_event.profile.END)

# --- OR ---

op_event = knl(queue, global_size, grp_size, args ...)
op_event.wait()
elapsed_seconds = 1e-9*(
        op_event.profile.END - start_event.profile.START)
```

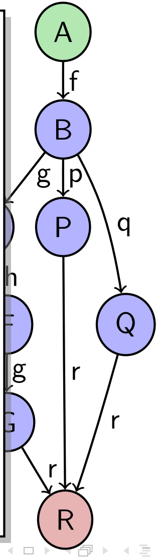
Capturing Dependencies

$$
\begin{aligned}
B &= f(A)\\
C &= g(B)\\
E &= f(C)\\
F &= h(C)\\
G &= g(E,F)\\
P &= p(B)\\
Q &= q(B)\\
R &= r(G,P,Q)
\end{aligned}
$$



Capturing Dependencies

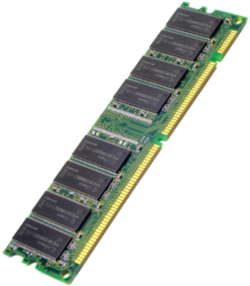
- Switch queue to out-of-order mode!
- Specify as list of events using `wait_for=` optional keyword to `enqueue_XXX`.
- Can also enqueue barrier.
- Common use case: Transmit/receive from other MPI ranks.
- Possible on Nv Fermi: Submit parallel work to increase machine use.



Memory Objects: Buffers

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

- Chunk of device memory
- No type information: “Bag of bytes”
- Observe: *Not* tied to device.
  → no fixed memory address
  → pointers do *not* survive kernel launches
  → movable between devices
- `flags`:
  - `READ_ONLY/WRITE_ONLY/READ_WRITE`
  - `{ALLOC,COPY,USE}_HOST_PTR`



Memory Objects: Buffers

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

`COPY_HOST_PTR`:

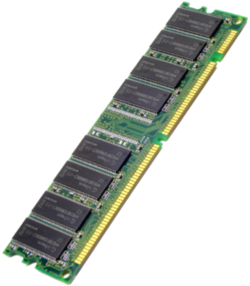
- Use `hostbuf` as initial content of buffer

`USE_HOST_PTR`:

- `hostbuf` *is* the buffer.
- Caching in device memory is allowed.

`ALLOC_HOST_PTR`:

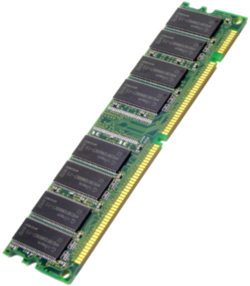
- *New* host memory (unrelated to `hostbuf`) is visible from device *and* host.



Memory Objects: Buffers

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

- Specify `hostbuf` or `size` (or both)
- `hostbuf`: Needs Python Buffer Interface e.g. `numpy.ndarray`, `str`.
  - Important: Memory layout matters
- 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`.



Command Queues and Buffers: 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=False)
```

Command Queues and Buffers: A Crashy Puzzle

✔ OK

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Command Queues and Buffers: A Crashy Puzzle

✔ OK (usually!)

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        is_blocking=True)
```
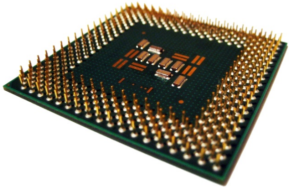

Programs and Kernels

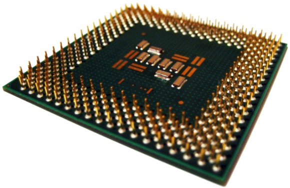
```
prg = cl.Program(context, src)
```

- `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), (L_x, L_y, L_z), `arg, ..., wait_for=None)`



Program Objects

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

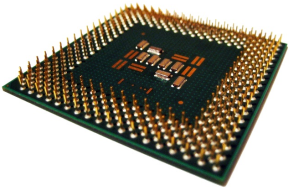


arg may be:

- `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:

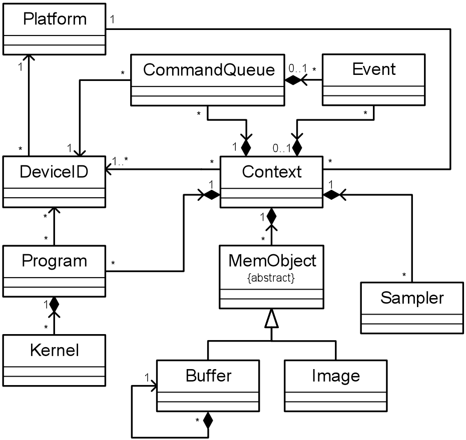
✖ Annoying, error-prone.

Better:

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

Use `None` for non-scalars.

OpenCL Object Diagram



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Outline

OpenCL Device Language

OpenCL device language is C99, with these differences:

- ⊕ Index getters
- ⊕ Memory space qualifiers
- ⊕ Vector data types
- ⊕ Many generic ('overloaded') math functions including fast `native_...` varieties.
- ⊕ Synchronization
- ⊖ Recursion
- ⊖ `malloc()`

NYU

OpenCL $\leftrightarrow$ CUDA: A dictionary

OpenCL	**CUDA**
Grid	Grid
Work Group	Block
Work Item	Thread
`__kernel`	`__global__`
`__global`	`__device__`
`__local`	`__shared__`
`__private`	`__local__`
`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)

Address Space Qualifiers

Type	Per	Access	Latency	
private	work item	R/W	1 or 1000	
local	group	R/W	2	
global	grid	R/W	1000	Not cached
`constant`	grid	R/O	1-1000	Cached
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Important

Don't "*choose one*" type of memory.
Successful algorithms combine many types' strengths.

CL vector data types

`floatn vec` (n=1,2,3,4,8,16) (also for double and integer types) Components:

- `vec.s012...abcdef` (or `xyzw`)
- `vec.s3120` (Swizzling)
- `vec.s024 = (float3)(1,2,3);` (Lvalue, Literals)

Usage:

- Elementwise operations (+,-,`sin` (generic!),...)
- `floatn vloadn/vstoren(offset, float *)` (aligned!)
- `dot/distance`

Using CPU implementation: One of the sanest ways of using SSE/vector intrinsics!

Outline

Recap: Concurrency and Synchronization

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

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GPUs have layers of concurrency.

Each layer has its synchronization primitives.

- Intra-group:
  `barrier(...)`,
  `mem_fence(...)`
  `...` =
  `CLK_{LOCAL,GLOBAL}_MEM_FENCE`
- Inter-group:
  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

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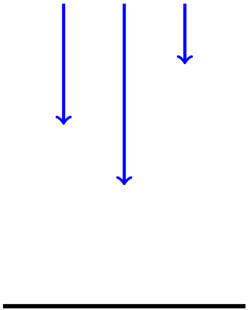
Results of the algorithm must be independent of the order in which work groups are executed.

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

Synchronization

What is a Barrier?



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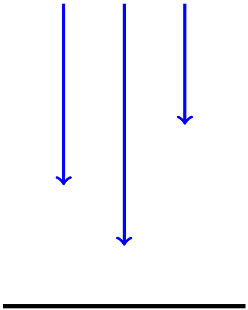

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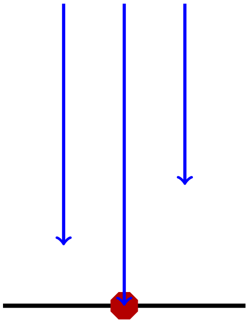

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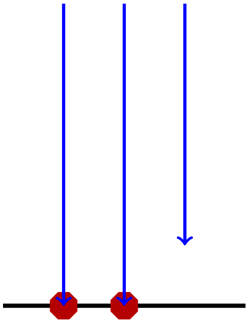

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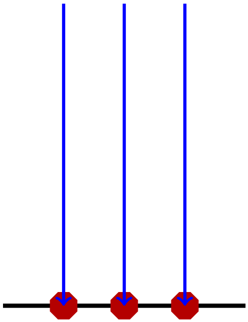

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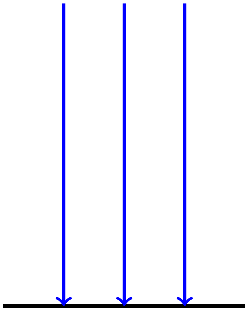

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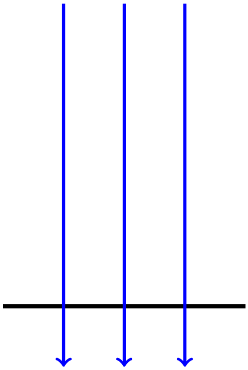

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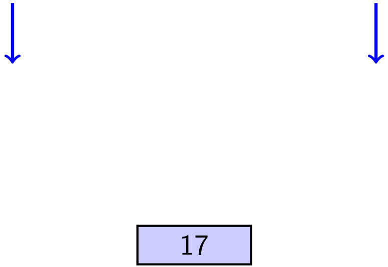

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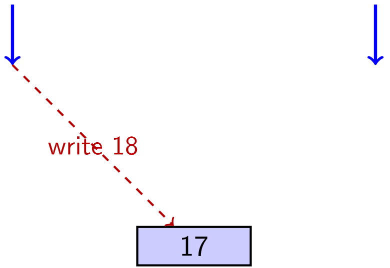

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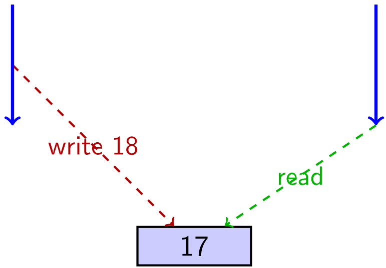

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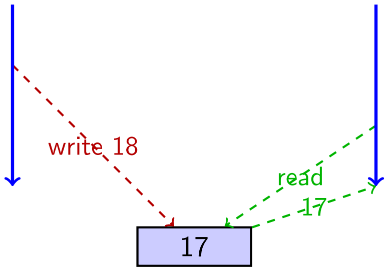

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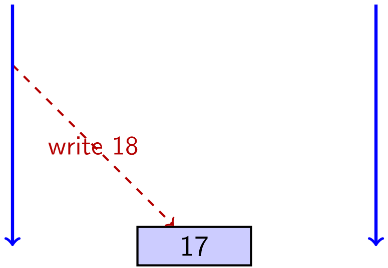

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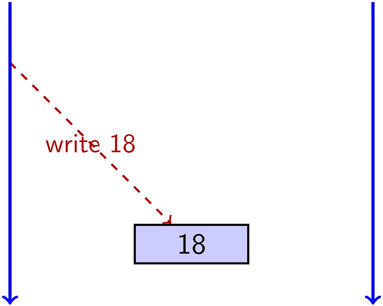

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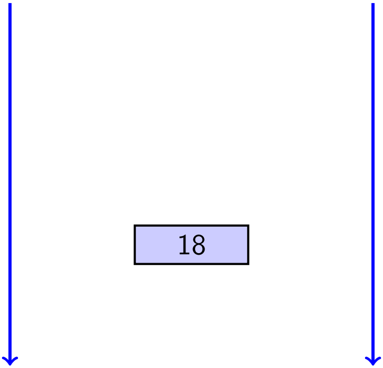

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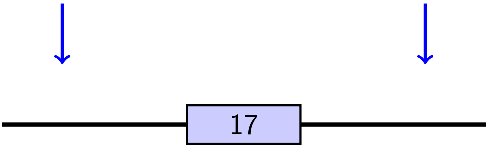
What is a Memory Fence? An ordering restriction for memory access.



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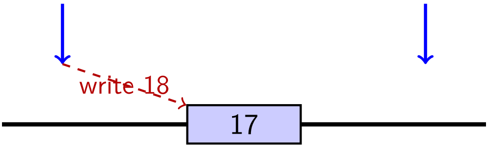

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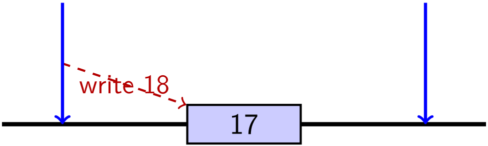

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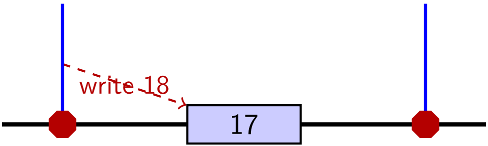

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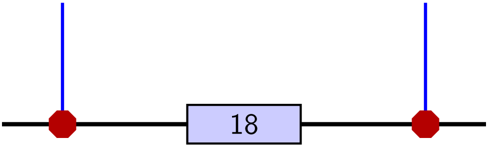

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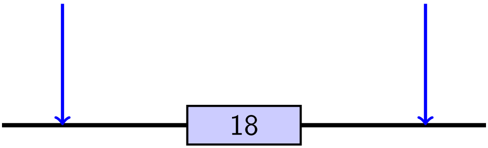

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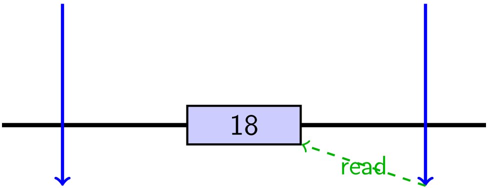

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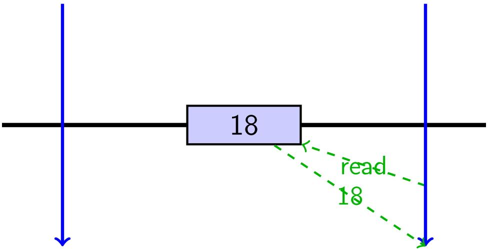

Atomic Operations

Collaborative (inter-block) Global Memory Update:

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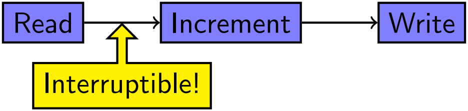

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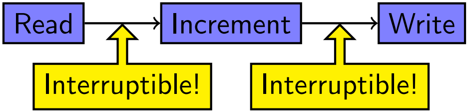

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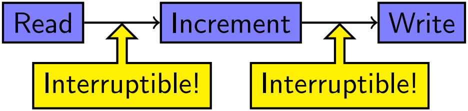

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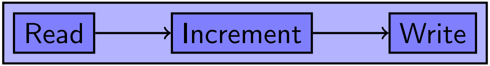

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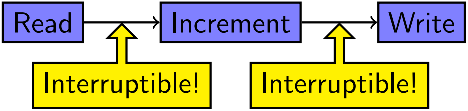

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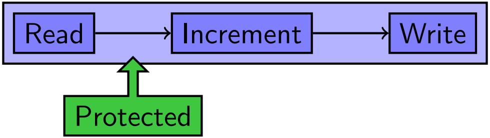

Atomic Operations

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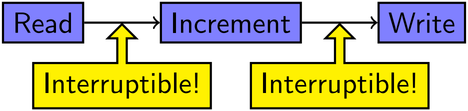

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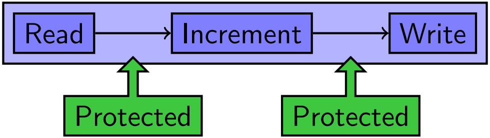

Atomic Operations

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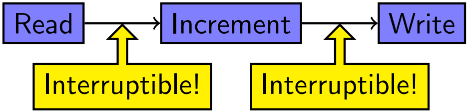

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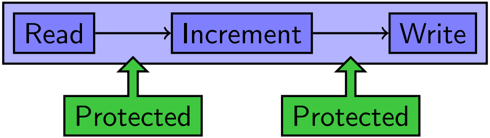

How?

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

Outline

Extensions: Future-proof CL

Similar extensions mechanism to OpenGL.

Two mechanisms:

- Runtime:
  - `cl_ext.h` header
  - availability checkable via `#ifdef`
  - `device.extensions`
- Device language:
  `#pragma OPENCL EXTENSION name : enable`

Important extension:

- cl_khr_fp64

Vendor and 'official' extensions.

Outline

The Nvidia CL implementation

Targets only GPUs

Notes:

- Nearly identical to CUDA
  - No native C-level JIT in CUDA ($\rightarrow$ PyCUDA)
- Page-locked memory:
  Use `CL_MEM_ALLOC_HOST_PTR`.
  (Careful: double meaning)
- No linear memory texturing
- CUDA device emulation mode deprecated
  $\rightarrow$ Use AMD CPU CL (faster, too!)

The Apple CL implementation

Targets CPUs and GPUs

General notes:

- Different header name `OpenCL/cl.h` instead of `CL/cl.h`
  Use `-framework OpenCL` for C access.
- Beware of imperfect compiler cache implementation
  (ignores include files)

CPU notes:

- One work item per processor

GPU similar to hardware vendor implementation.
(New: Intel w/ Sandy Bridge)

The AMD CL implementation

- Targets CPUs and GPUs (from both AMD and Nvidia)
- GPU notes:
  - Wide SIMD groups (64)
  - Native 4/5-wide vectors
    - But: very flop-heavy machine, may ignore vectors for memory-bound workloads
  - $\rightarrow$ *Both* implicit and explicit SIMD
- CPU notes:
  - Many work items per processor (emulated)
  - `cl_amd_printf`

Questions?

?

Image Credits

- Context: sxc.hu/svilen001
- Queue: sxc.hu/cobrasoft
- Check mark: sxc.hu/bredmaker
- RAM stick: sxc.hu/gobran11
- CPU: sxc.hu/dimshik
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- Dominoes: sxc.hu/rolve
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- AMD logo: AMD Corporation