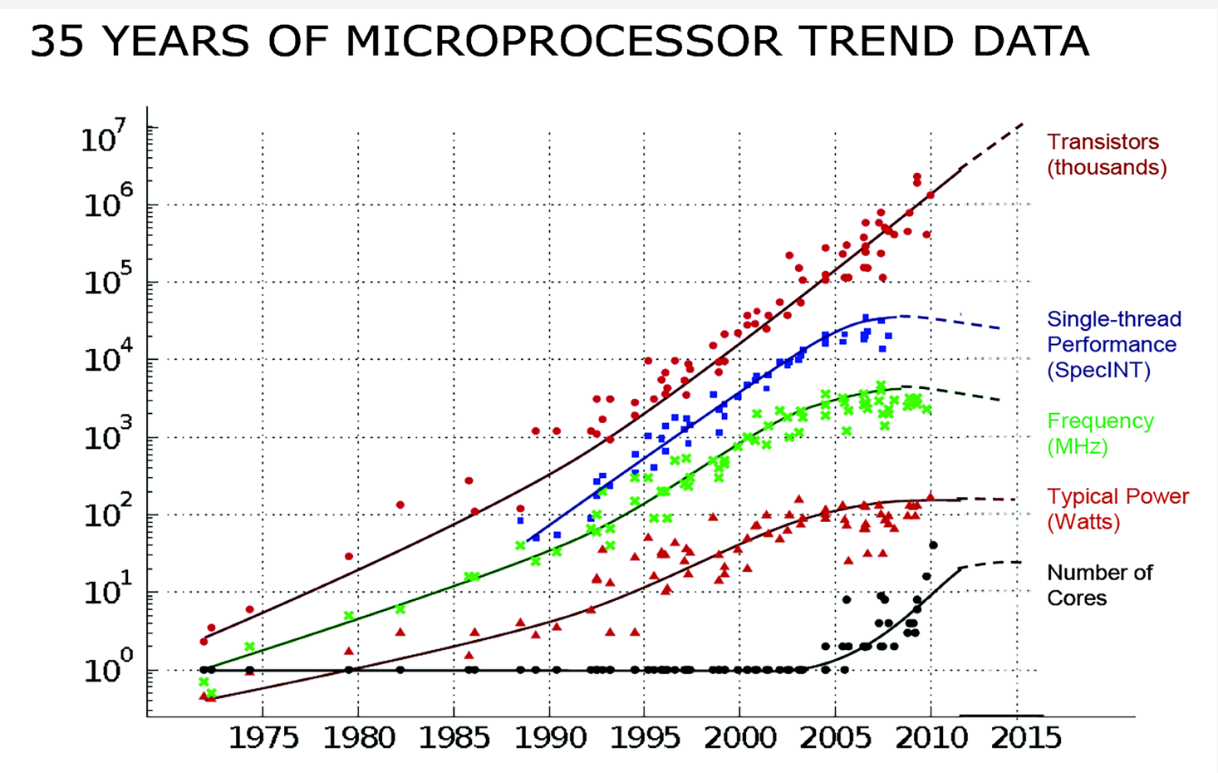
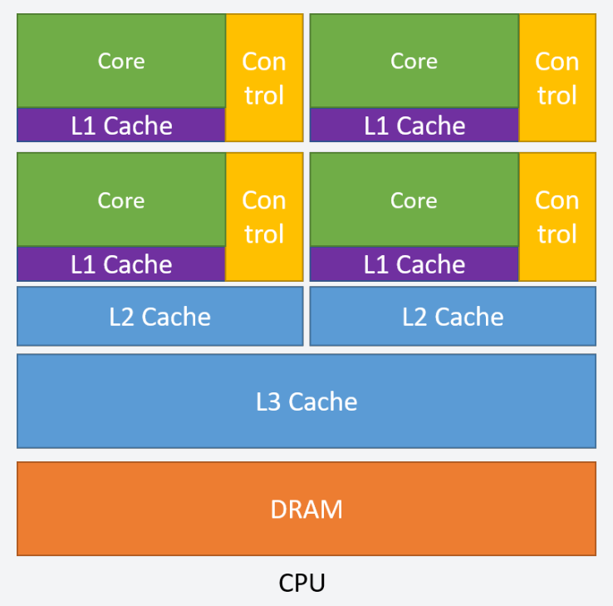
Efficiently Executing *NumPy* on GPUs via the *CUDAGraph* API

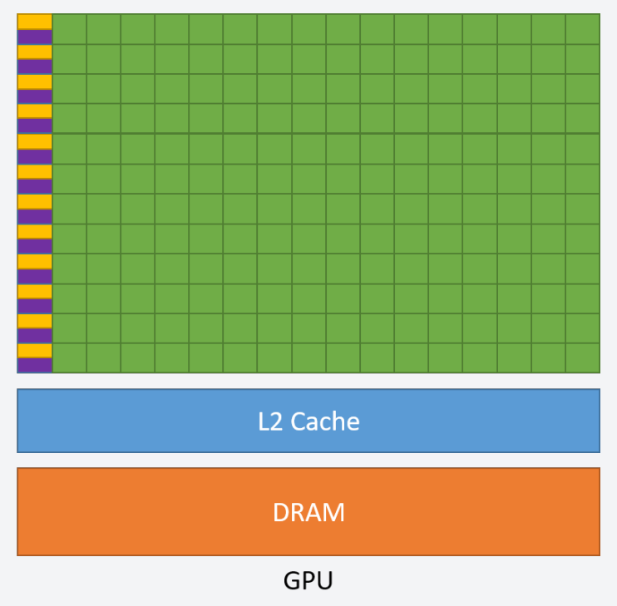
Mit Kotak · Kaushik Kulkarni · Andreas Klöckner

National Center for Supercomputing Applications · Urbana, IL

Why GPUs?







- CPU performance is flatlining
- GPUs devote more transistors to data processing

Abstract

- *NumPy* is the defacto standard for array-based numerical computations in scientific workloads (for ex. PDE solving, Image Processing, etc.)
- However, its ability to harness GPU acceleration is limited by its single-node, occasionally multi-threaded, CPU- only execution model
- Goal: Should be able to efficiently execute array operations on GPUs
- Challenges:
  - Saturating all available execution units to efficiently use the entire GPU
  - *NumPy* is a high-level programming interface, does not address performance directives such as:
    - Execution grid-size which affects data partitioning
    - User-specified local memory management
    - Kernel launch overhead costs
  - **Realizing concurrency across array operations**
- Our Approach: Use *CUDAGraph* API to concurrently launch array operations using tuned kernels that are accessed through *PyCUDA*
- Past work:
  - *Legate*: A runtime system for scheduling operations in a task graph
    - Representation lacks a global view of the program limiting the program optmizing space
  - Lazy evaluation: *Theano* | *JAX* | *PyTorch*
    - Requires expensive algorithms (ex. kernel/loop fusion)
    - Ex. *Theano*[3] claim to have super-linear codegeneration algorithm
  - Single Stream: *cuPy* | *GPUArrays.jl*

Why *CUDAGraphs*?

- *CUDA Streams*
  - Operations are enqueued in-order into the stream object
- *CUDAGraph* API
  - Takes in a task dependency graph where each node corresponds to a *CUDA* kernel
  - Scheduler realizes concurrency across nodes in the graph through multiple streams

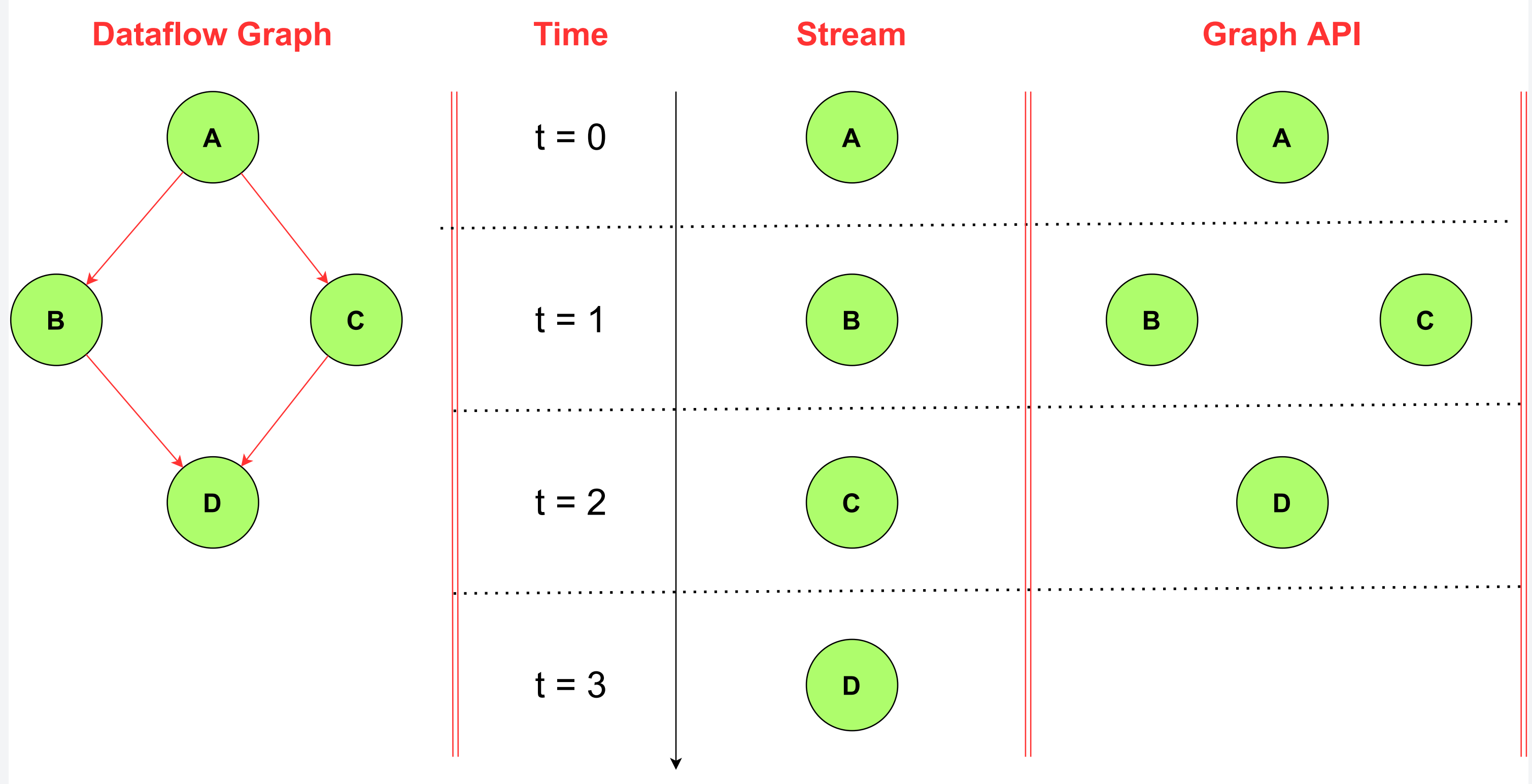
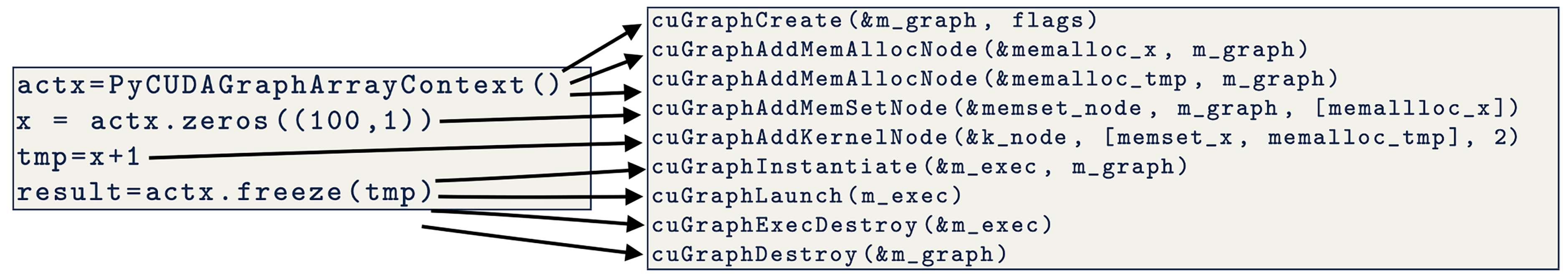


Figure: Single Stream vs CUDAGraphs scheduling

Interface Implementation



```
actx=PyCUDAGraphArrayContext()
x = actx.zeros((100,1))
tmp=x+1
result=actx.freeze(tmp)
```

```
cuGraphCreate(&m_graph, flags)
cuGraphAddMemAllocNode(&memalloc_x, m_graph)
cuGraphAddMemAllocNode(&memalloc_tmp, m_graph)
cuGraphAddMemSetNode(&memset_node, m_graph, [memallloc_x])
cuGraphAddKernelNode(&k_node, [memset_x, memalloc_tmp], 2)
cuGraphInstantiate(&m_exec, m_graph)
cuGraphLaunch(m_exec)
cuGraphExecDestroy(&m_exec)
cuGraphDestroy(&m_graph)
```

Figure: User Input Program

Figure: Driver C code

- Array operations realized as a composition of *CUDA* calls (memcpy, kernel_launches, memalloc) that are added onto a task dependency graph with precise edges.
- Object cleanup tied to lifetime of objects in array operations

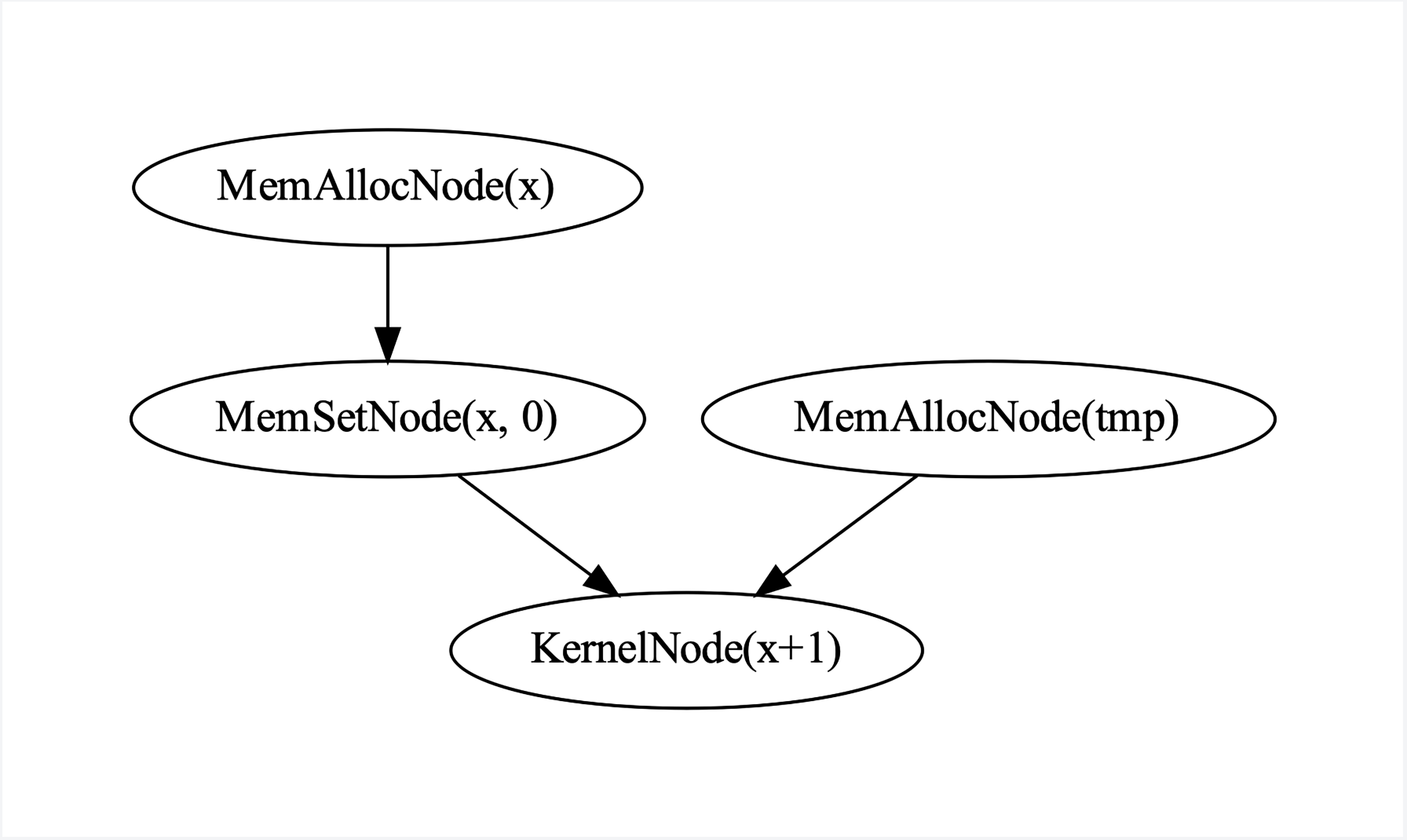
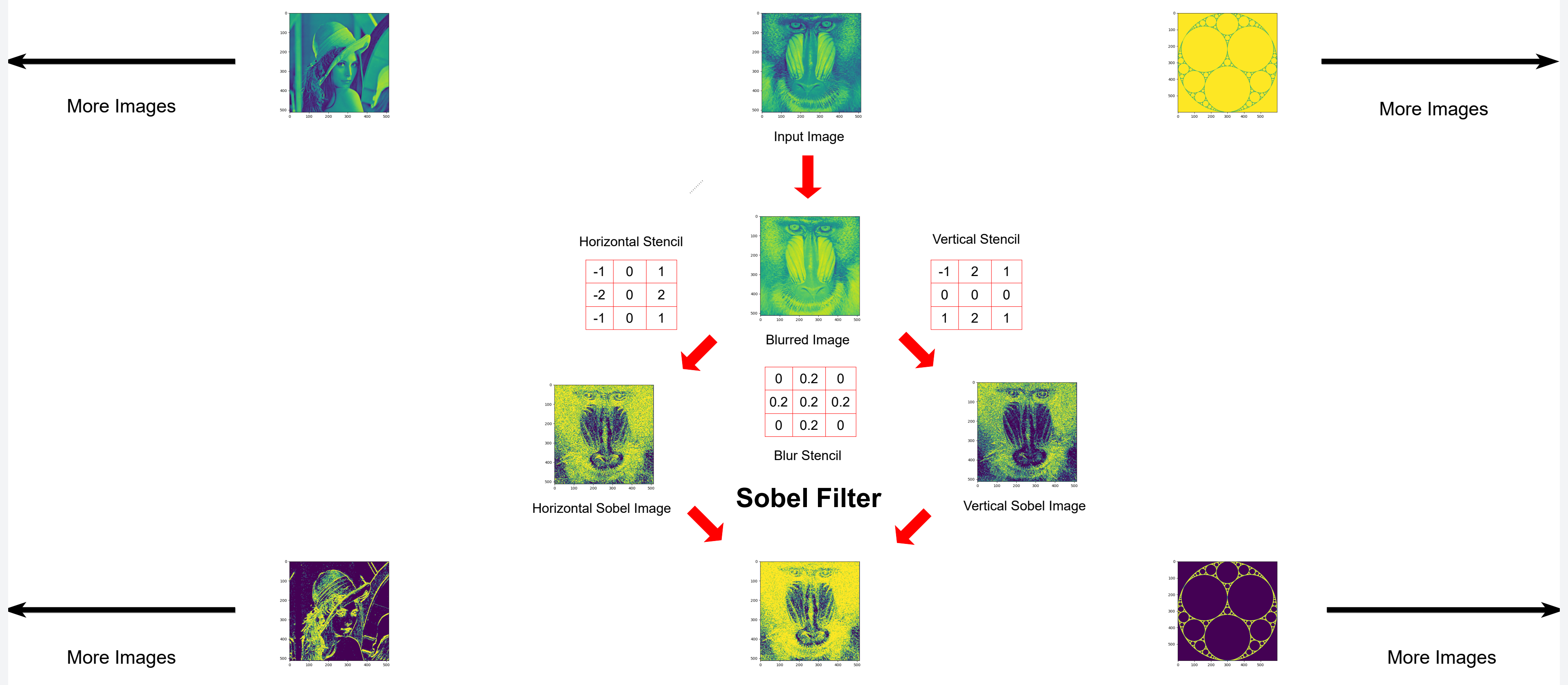


Figure: Generated CUDAGraph

Experimental Setup

We ran a set of image processing algorithms with and without *CUDAGraph* API on different image batches



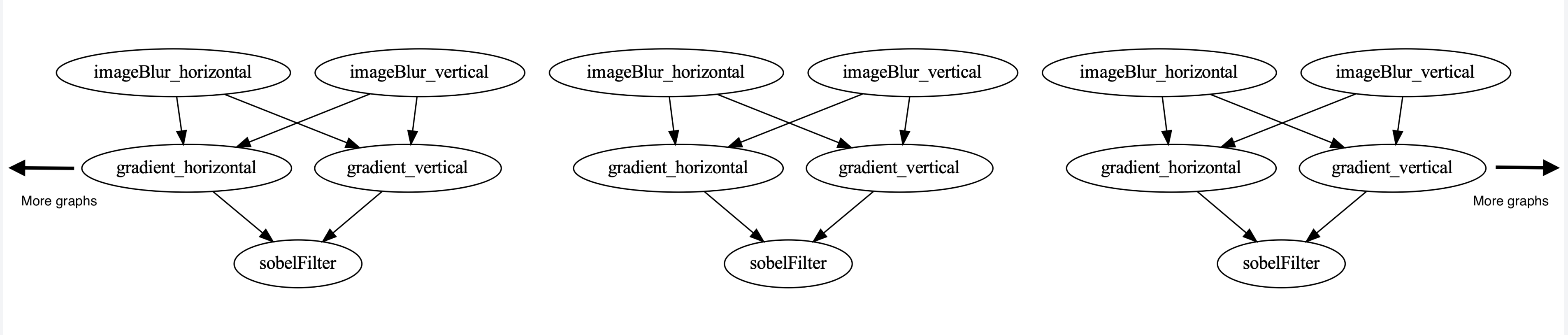


Figure: Sobel Filter Graph

Results

- We observed a speed up of upto 15% on NVIDIA Titan V for smaller problems which was attributed to high task parallelism
- We observed overlapping kernels across multiple streams for the *CUDAGraph* API program

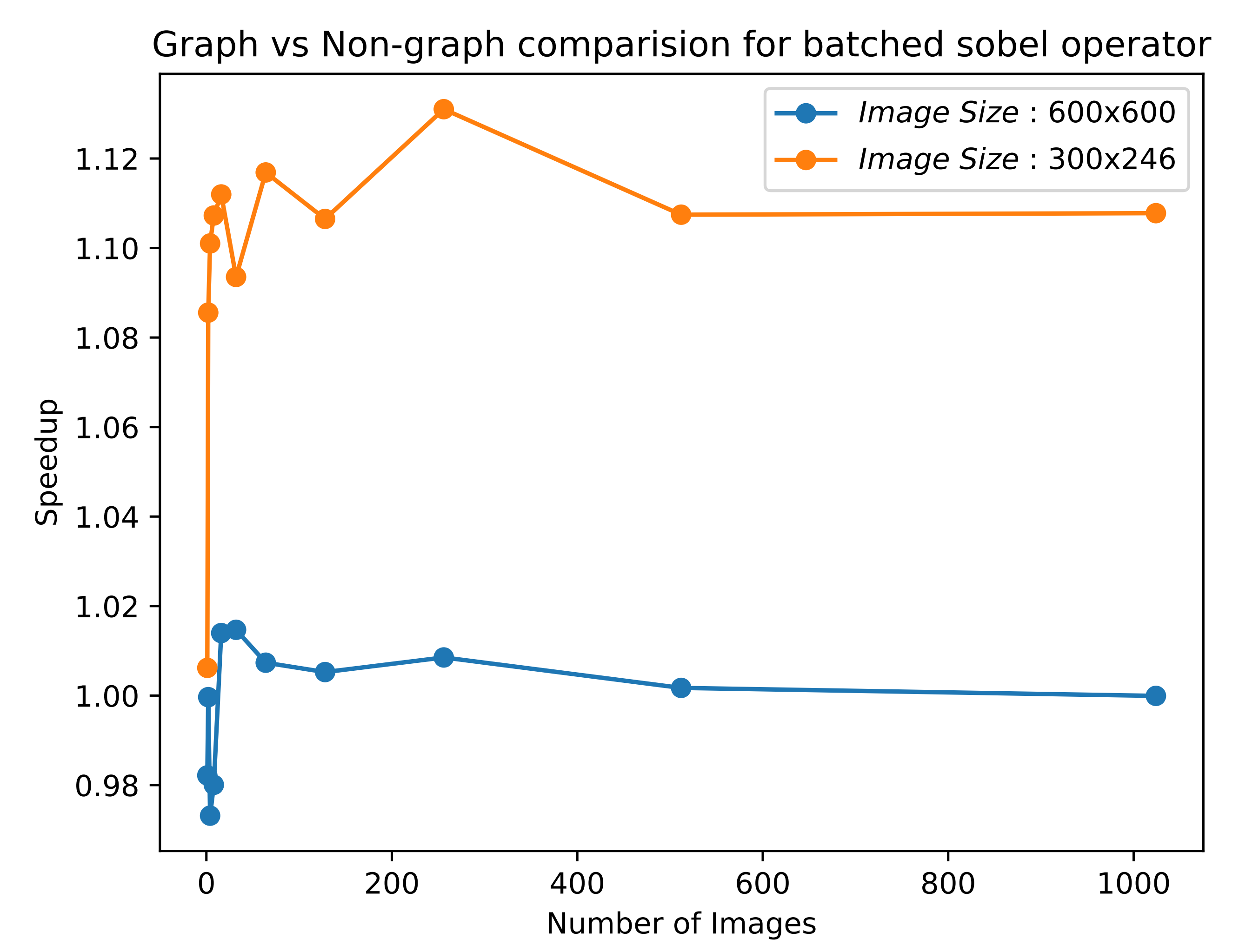


Figure: Sobel Filter on Image Batches

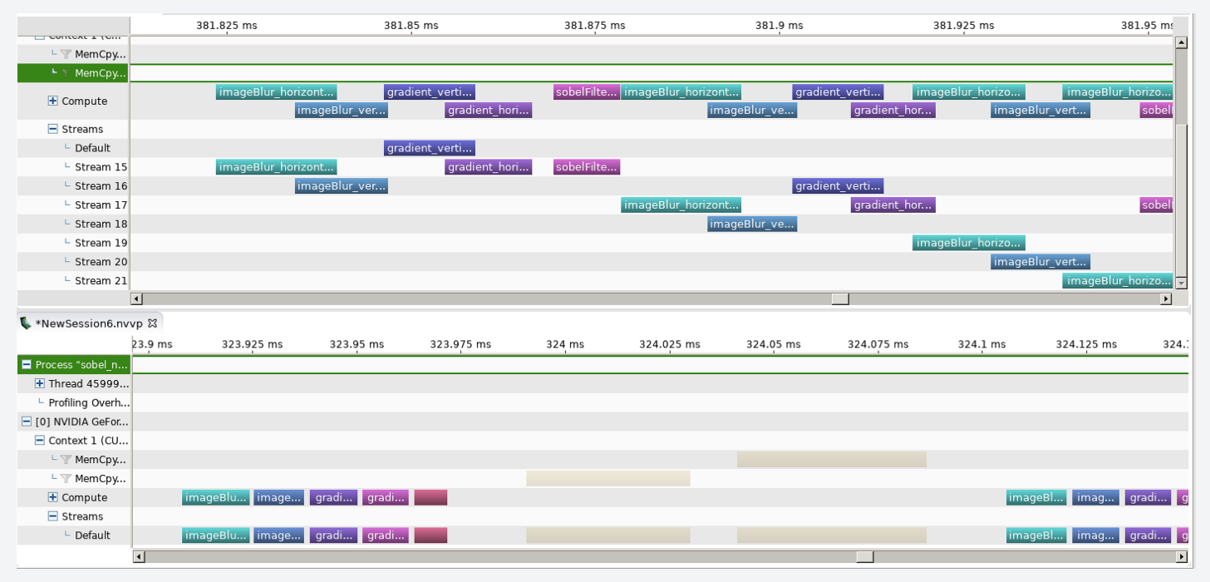


Figure: Kernel Execution timeline with (top) and without (bottom) *CUDAGraph* API Image size 300 x 246

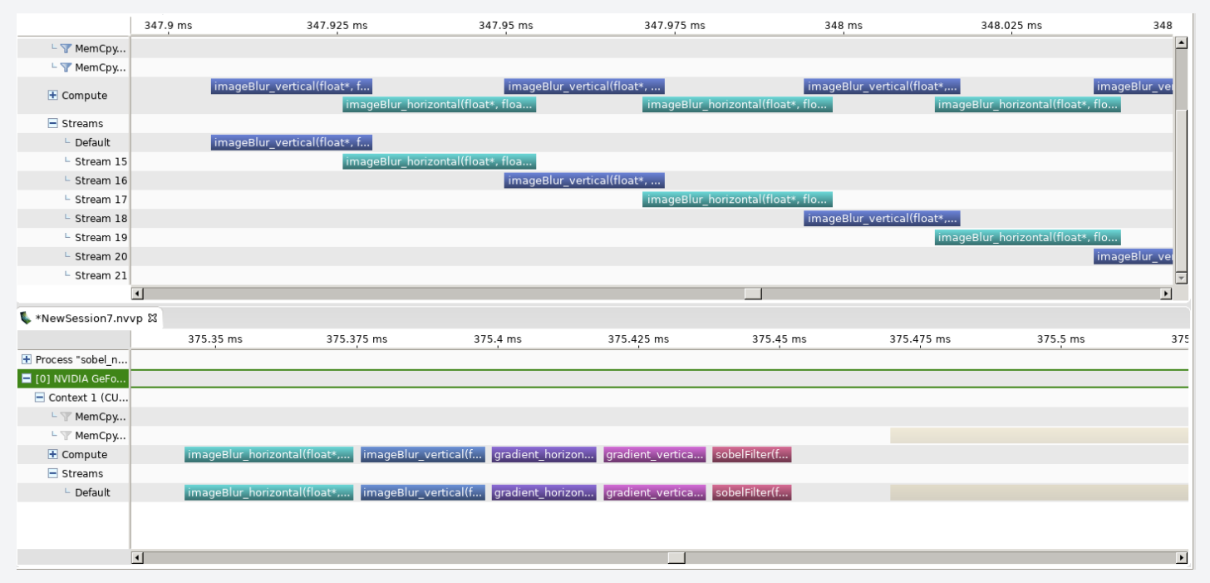


Figure: Kernel Execution timeline with (top) and without (bottom) *CUDAGraph* API Image size 600 x 600

Results, run instructions at `https://github.com/mitkotak/sobel`

Future Work

- Upstream work: Integrate with *PyCUDA* and *Arraycontext*
- Evalulate this approach on large scale scientific simulations

Acknowledgements

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References

- CUDA Programming: A Developer's Guide to Parallel Computing with GPUs (https://docs.nvidia.com/cuda/cuda-c-programming-guide/index.html)
- Chapter 27 - GPU Scripting and Code Generation with PyCUDA (https://doi.org/10.1016/B978-0-12-385963-1.00027-7)
- Theano: A Python framework for fast computation of mathematical expressions (https://doi.org/10.48550/arXiv.1605.02688)

mitak2@illinois.edu