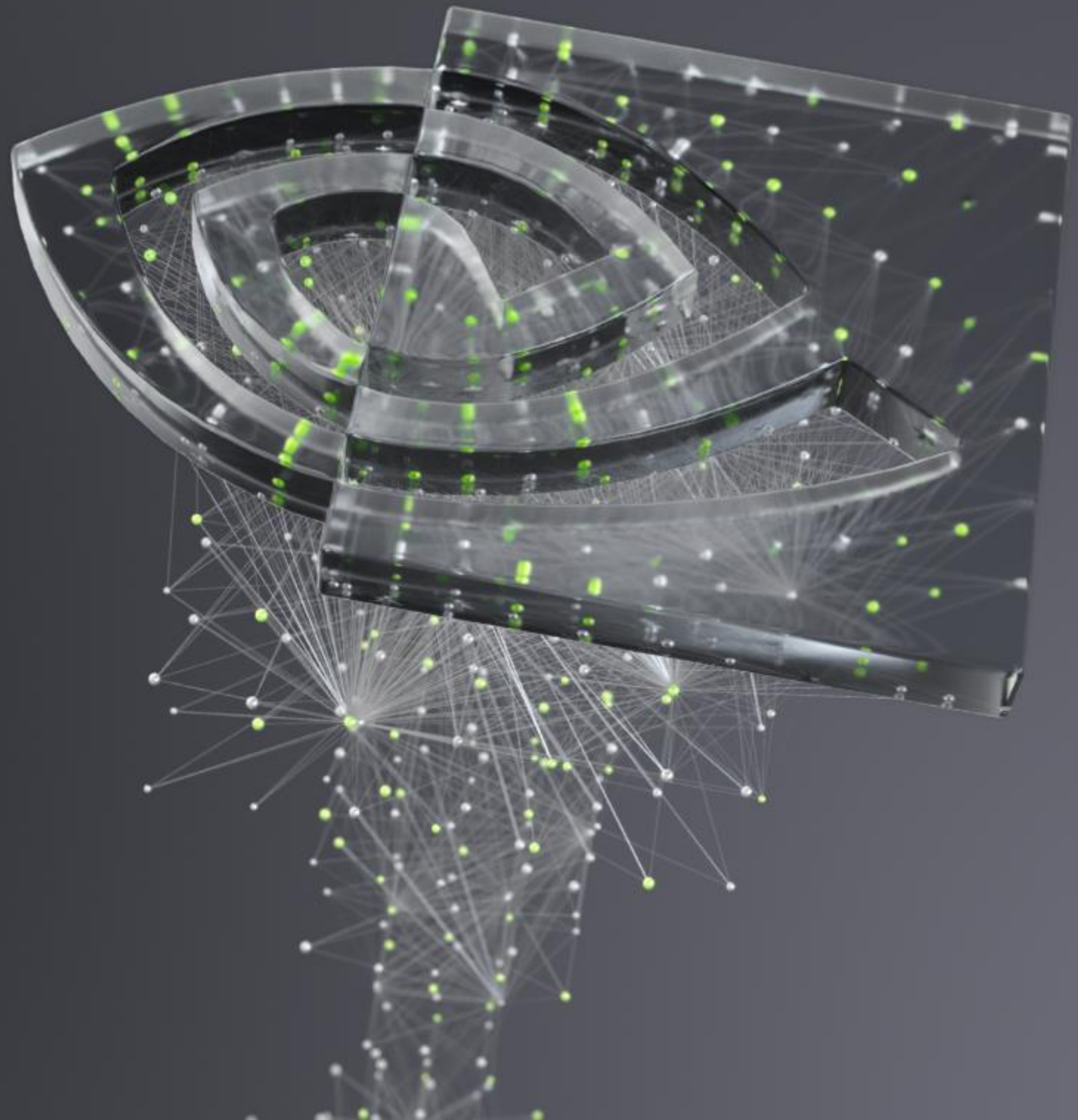


# ML FRAMEWORKS INTEROPERABILITY

Christian Hundt, Manager AI Developer Technology
Miguel Martínez, Sr. Deep Learning Data Scientist

# Today's Agenda

- About This Talk
- End-to-End Pipeline
- Common Bottlenecks:
  - *Memory Management*
  - *Data Conversion*
  - *Data Loading*
  - *Data Transfer*
- Summary

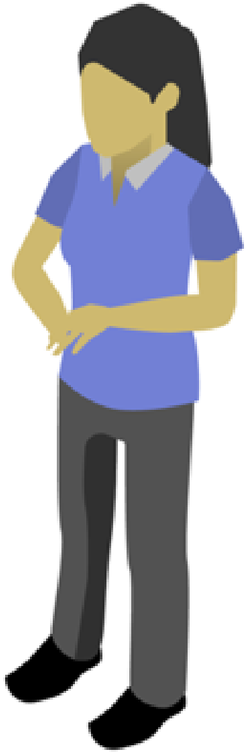
# ABOUT THIS TALK

# FRAMEWORK INTEROPERABILITY

## When a single framework is not enough

data scientist

CUDA developer



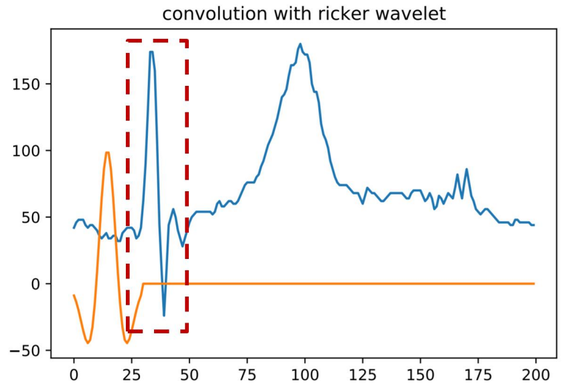
data engineer

SPOILER ALERT

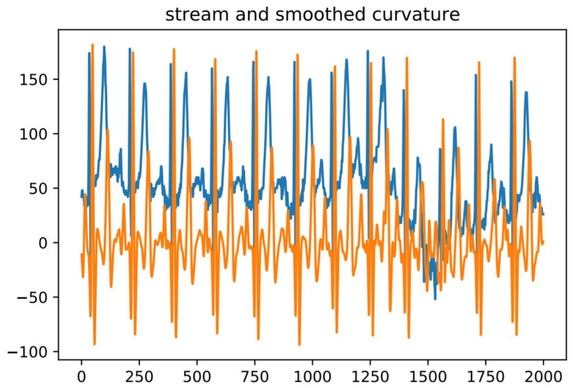
# OUTLOOK

## Things we will talk about

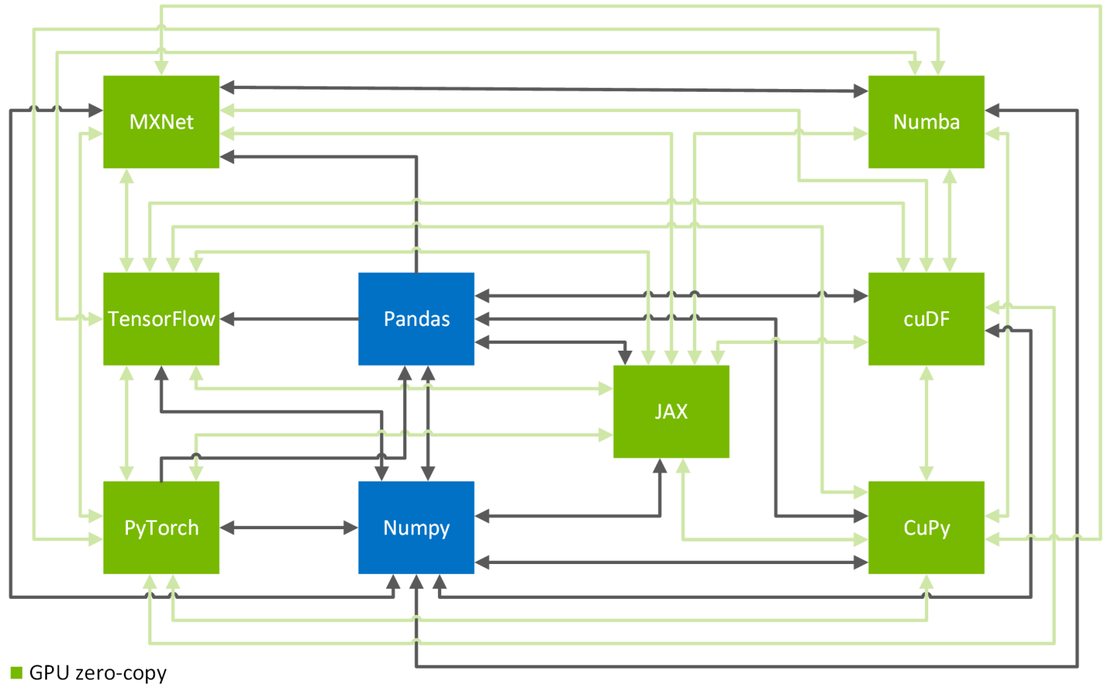
RAPIDS cuDF → CuPy → Numba → PyTorch → RAPIDS cuxfilter

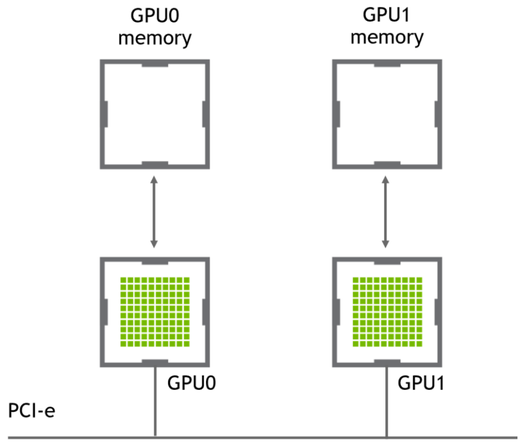


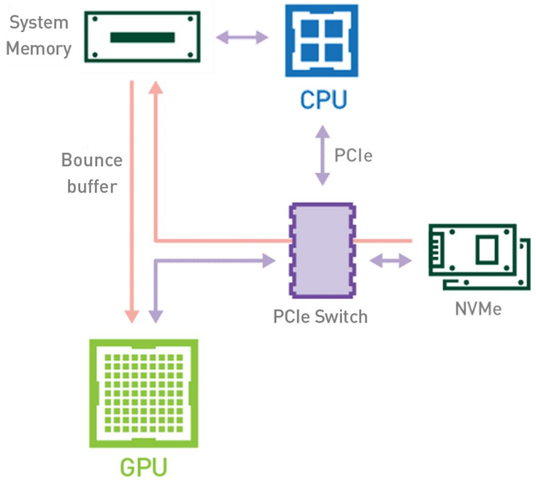

FFT based convolution

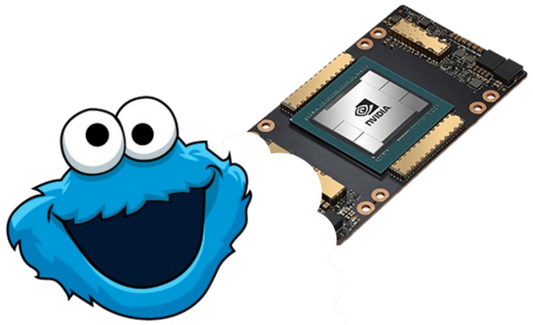



QRS Complex Detection



| | user_id | timestamp | source_ip |
|---|---|---|---|
| row_1 | 6939800 | 2021-04-12 05:31 | 42.155.123.142 |
| row_2 | 4015666 | 2021-04-12 05:47 | 67.132.212.125 |
| row_3 | 5456236 | 2021-04-12 05:52 | 81.205.129.121 |

| | Row-wise data layout |
|---|---|
| row_1 | 6939800 |
| | 2021-04-12 05:31 |
| | 42.155.123.142 |
| row_2 | 4015666 |
| | 2021-04-12 05:47 |
| | 67.132.212.125 |
| row_3 | 5456236 |
| | 2021-04-12 05:52 |
| | 81.205.129.121 |

| | Columnar data layout |
|---|---|
| user_id | 6939800 |
| | 4015666 |
| | 5456236 |
| timestamp | 2021-04-12 05:31 |
| | 2021-04-12 05:47 |
| | 2021-04-12 05:52 |
| source_ip | 42.155.123.142 |
| | 67.132.212.125 |
| | 81.205.129.121 |



NVIDIA

# E2E CODE EXAMPLE + CHEAT SHEET

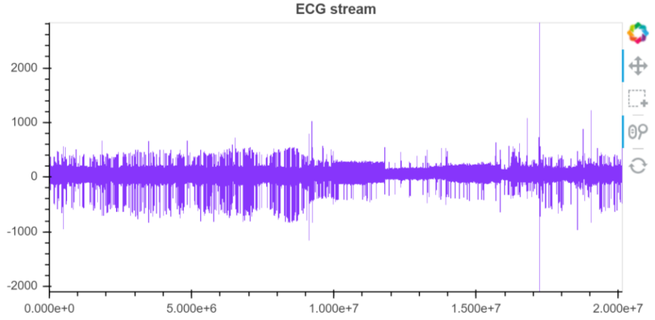
E2E Workflow.ipynb

Code | Python 3

[1]:
```
import cudf

subject_cudf = cudf.read_csv("data/subject.csv", dtype='float32')
```

[2]:
```
import cuxfilter as cux
from cuxfilter.charts.datashader import line

# Chart width and height
WIDTH=600
HEIGHT=300

# 20 hours ECG look like a mess
subject_cudf['x'] = subject_cudf.index

line_cux = line(x='x', y='data', add_interaction=False)

_ = cux.DataFrame.from_dataframe(subject_cudf).dashboard([line_cux])
line_cux.chart.title.text = 'ECG stream'
line_cux.chart.title.align = 'center'
line_cux.chart.width = WIDTH
line_cux.chart.height = HEIGHT
line_cux.view()[0]
```

[2]:



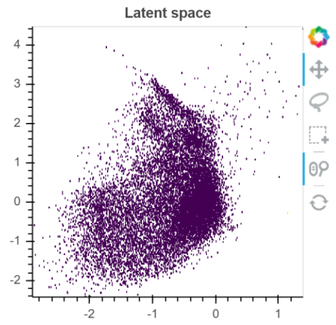

[3]:
```
import cupy as cp
from time_series_utils import smoothed_curvature_cupy

# convert to cupy
subject_cupy = cp.fromDlpack(subject_cudf['data'].to_dlpack())

# compute smoothed curvature via ricker wavelet
curvature_cupy = smoothed_curvature_cupy(subject_cupy, window=30)
```

E2E Workflow.ipynb

Code | Python 3

[15]:
```
from cuxfilter.charts import scatter

scatter_chart_cux = scatter(x='x', y='y', pixel_shade_type="linear",
                            legend=False, add_interaction=False)

_ = cux.DataFrame.from_dataframe(mu_cudf).dashboard([scatter_chart_cux])
scatter_chart_cux.chart.title.text = 'Latent space'
scatter_chart_cux.chart.title.align = 'center'
scatter_chart_cux.chart.width = WIDTH//2
scatter_chart_cux.chart.height = HEIGHT
scatter_chart_cux.view()[0]
```

[15]:




[16]:
```
print("Installing hvplot...")
!pip -q install hvplot
```

```
Installing hvplot...
```

[17]:
```
import hvplot.cudf
import panel

ROWS = 4
COLS = 4

# let's sample some fake heart beats
with torch.no_grad():
    latents = torch.empty(ROWS * COLS, 2).normal_(mean=0.0, std=0.5).to('cuda')
    samples = model.decode(latents)

heartbeats_cudf = cudf.DataFrame({'x': cp.arange(samples.shape[1])})
heartbeats_gridspec = panel.GridSpec(width=COLS*200, height=ROWS*100)
for i, (sample, latent) in enumerate(zip(samples, latents)):
    heartbeats_cudf['y_%s' % i] = sample
```

E2E Workflow.ipynb

Code | Python 3

## Index

| | Pandas | Numpy | cuDF | cuPY | JAX | Numba | TensorFlow | PyTorch | MXNet |
|---|---|---|---|---|---|---|---|---|---|
| **Pandas** | n/a | code | code | code | code | code | code | code | code |
| **Numpy** | code | n/a | code | code | code | code | code | code | code |
| **cuDF** | code | code | n/a | code | code | code | code | code | code |
| **cuPY** | code | code | code | n/a | code | code | code | code | code |
| **JAX** | code | code | code | code | n/a | code | code | code | code |
| **Numba** | code | code | code | code | code | n/a | code | code | code |
| **TensorFlow** | code | code | code | code | code | code | n/a | code | code |
| **PyTorch** | code | code | code | code | code | code | code | n/a | code |
| **MXNet** | code | code | code | code | code | code | code | code | n/a |

## From Pandas to Numpy

[25]:
```
# Option 1: Pandas DataFrame to a Numpy ndarray
src = pd.DataFrame({'x': [1, 2], 'y': [3, 4]})
dst = src.to_numpy()

print(type(dst), "\n", dst)
```

```
<class 'numpy.ndarray'>
 [[1 3]
 [2 4]]
```

[26]:
```
# Option 2: Convert a Pandas DataFrame to a Numpy ndarray
src = pd.DataFrame({'x': [1, 2], 'y': [3, 4]})
dst = src.values # "to_numpy()" is preferred to "values".

print(type(dst), "\n", dst)
```

```
<class 'numpy.ndarray'>
 [[1 3]
 [2 4]]
```

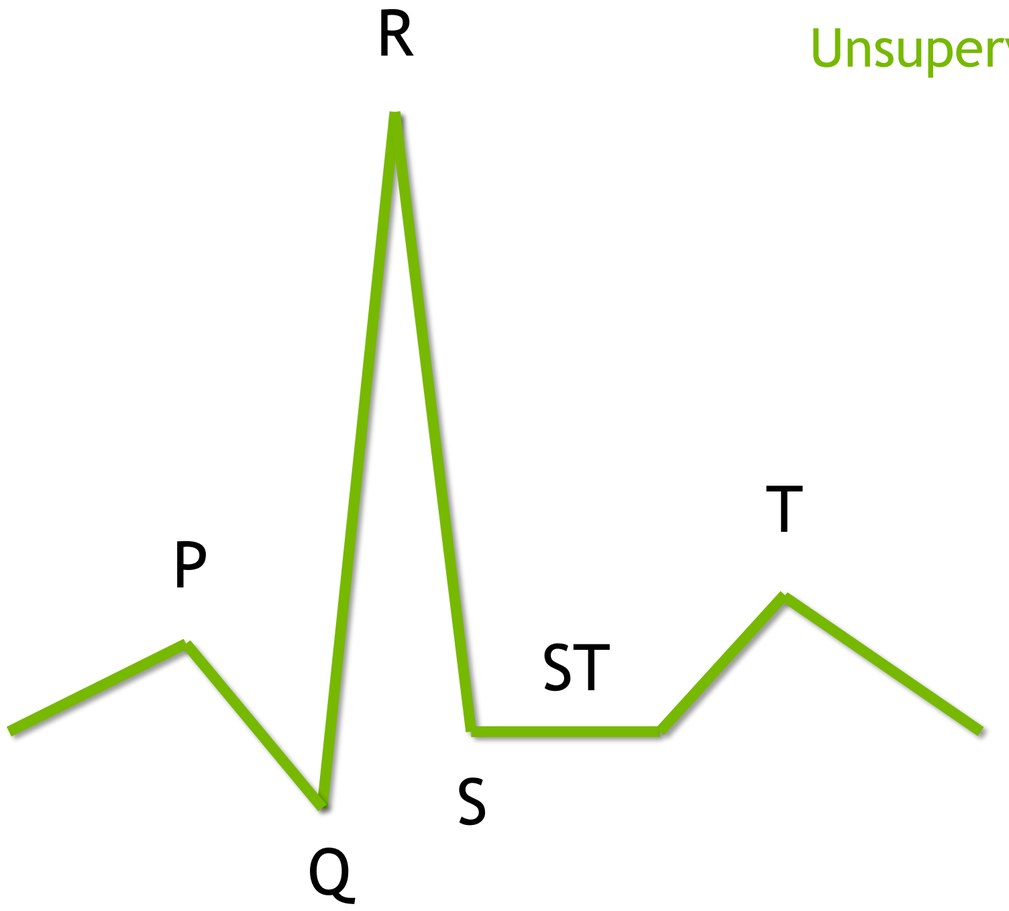
[27]:
```
# Option 3: Convert a Pandas DataFrame to a Numpy recarray
src = pd.DataFrame({'x': [1, 2], 'y': [3, 4]}, index=['a', 'b'])
dst = src.to_records()

print(type(dst), "\n", dst)
```

```
<class 'numpy.recarray'>
 [('a', 1, 3) ('b', 2, 4)]
```

# E2E PIPELINE

# TOY MODEL

## Unsupervised outlier detection




What we have:

- 20 hours stream of continuously measured electrocardiogram (ECG) data.
- Univariate and uniformly sampled time series as CSV on disk.

What we are doing:

- Unsupervised segmentation of ECG stream into ~ 100k heartbeats.
- Training of Variational Autoencoder (VAE) for outlier detection.
- Visualization of generated heartbeats

*Disclaimer*
*Technical example pipeline demonstrating framework interoperability.*
*Not suitable for production in medical environments.*

# END-TO-END PIPELINE

## Parse ECG from CSV


```
1    data
2    1.3863000000000088e+00
3    1.7349000000000109e+00
4    2.1865000000000110e+00
5    2.7471999999999864e+00
6    3.7519000000000013e+00
7    5.0231000000000342e+00
8    6.4785000000000369e+00
9    8.0025999999999270e+00
10   9.4921000000000648e+00
11   1.0825400000000013e+01
12   1.1867699999999925e+01
13   1.2486800000000057e+01
14   1.2587300000000082e+01
15   1.2142899999999914e+01
```

```
cudf.io.csv.read_csv(filepath_or_buffer,
lineterminator='\n', quotechar='"', quoting=0,
doublequote=True, header='infer',
mangle_dupe_cols=True, usecols=None,
sep=',', delimiter=None,
delim_whitespace=False,
skipinitialspace=False, names=None,
dtype=None, skipfooter=0, skiprows=0,
dayfirst=False, compression='infer',
thousands=None, decimal='.',
true_values=None, false_values=None,
nrows=None, byte_range=None,
skip_blank_lines=True, parse_dates=None,
comment=None, na_values=None,
keep_default_na=True, na_filter=True,
prefix=None, index_col=None, **kwargs)
```

RAPIDS

GPU

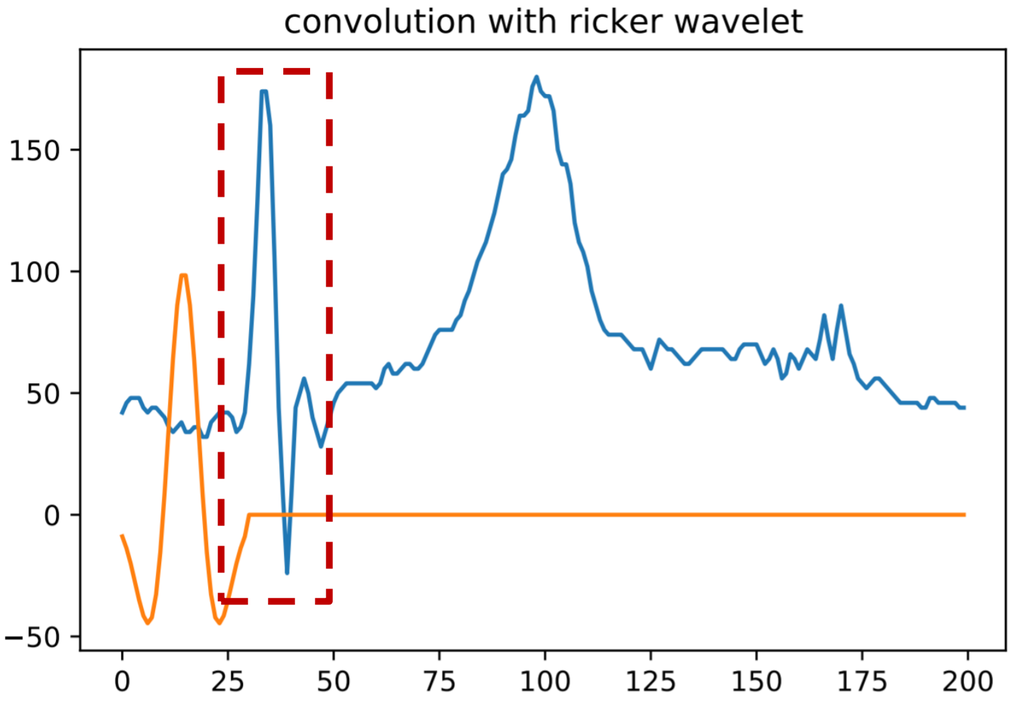
| | data |
|---|---|
| 0 | 1.3863 |
| 1 | 1.7349 |
| 2 | 2.1865 |
| 3 | 2.7472 |
| 4 | 3.7519 |
| ... | ... |

Load a comma-separated-values (CSV) dataset into a DataFrame

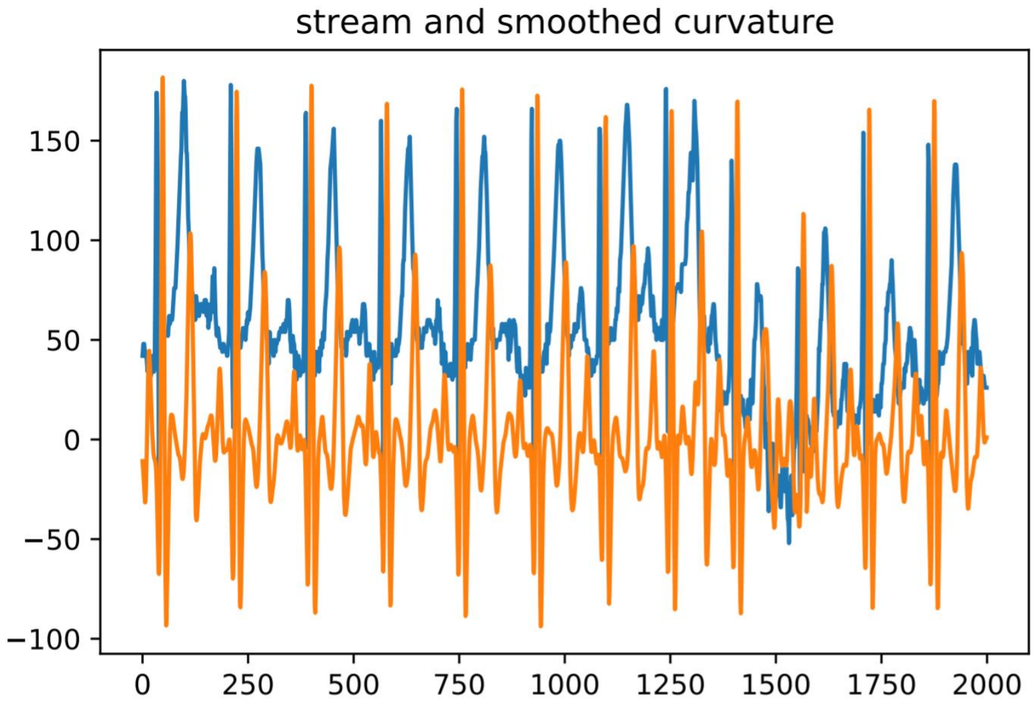
# END-TO-END PIPELINE

## Band-Pass Filter

RAPIDS cuDF → CuPy → Numba → PyTorch → RAPIDS cuxfilter




FFT based convolution

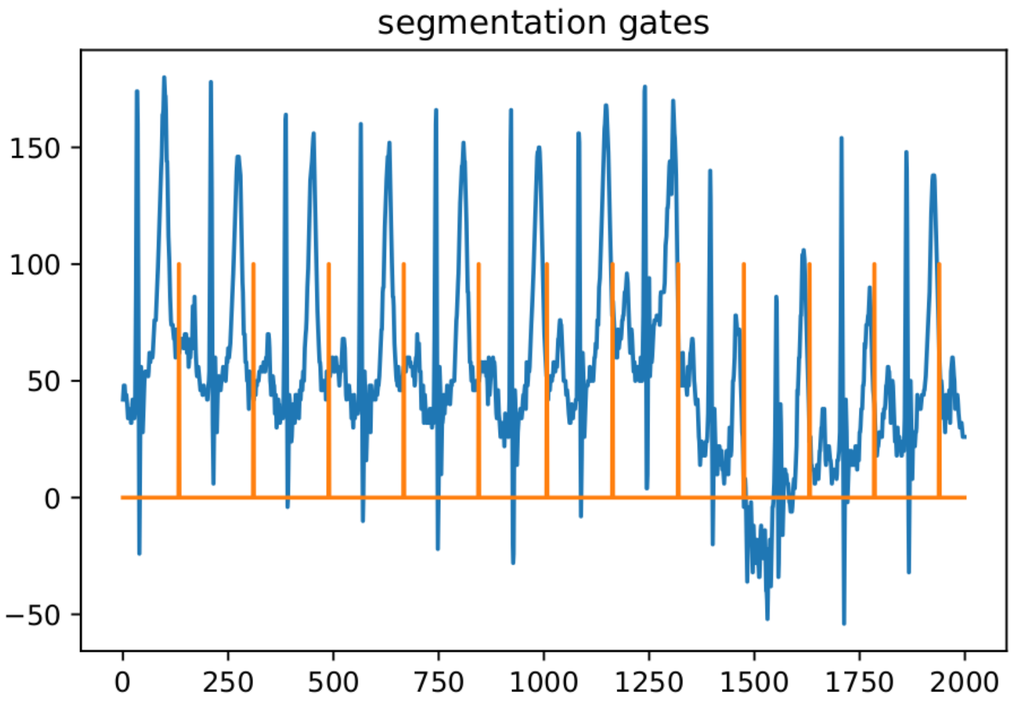


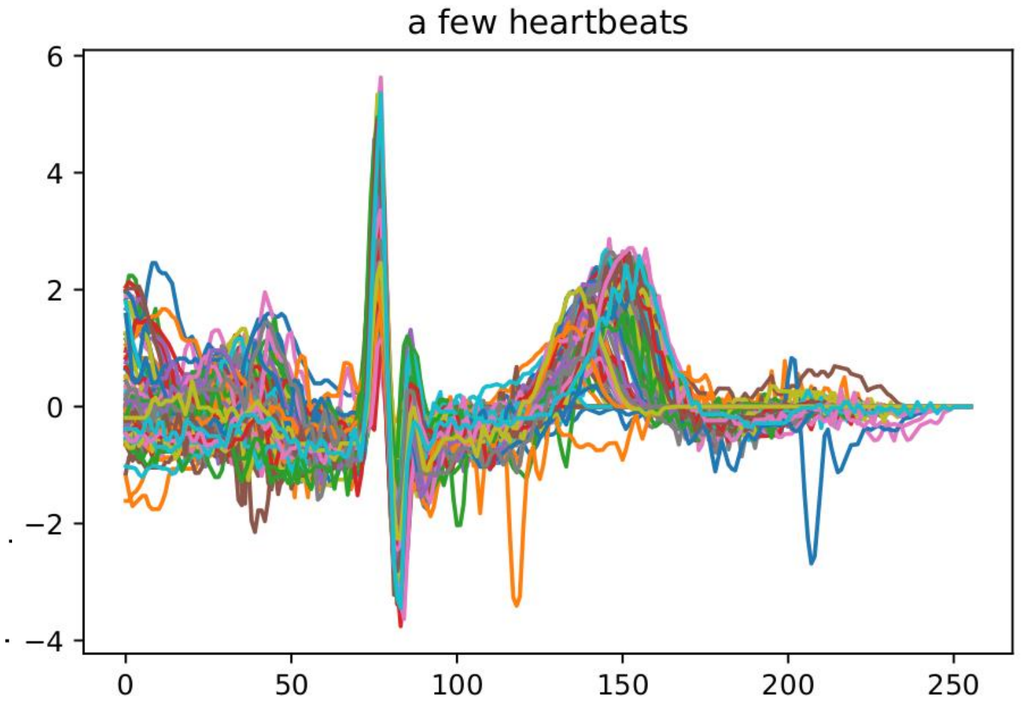

QRS Complex Detection

# END-TO-END PIPELINE

## Non-trivial Preprocessing

RAPIDS cuDF → CuPy → Numba → PyTorch → RAPIDS cuxfilter



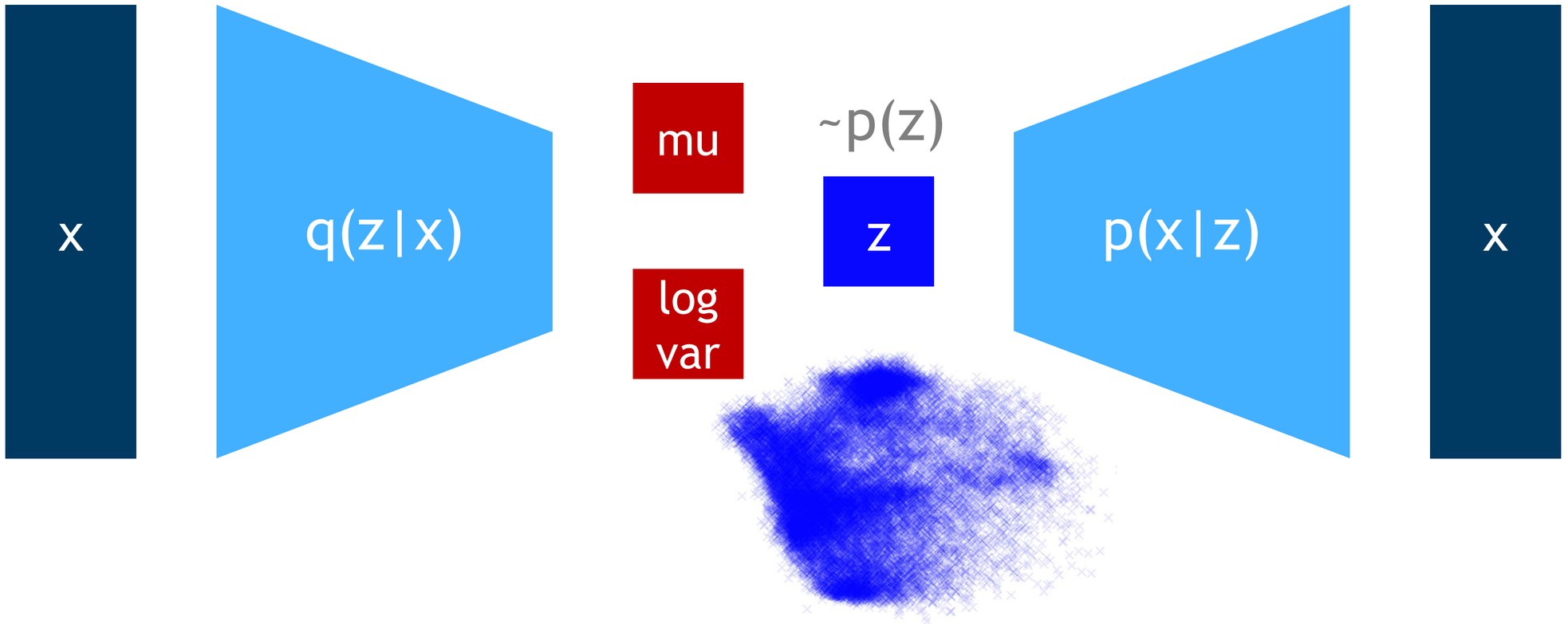

1D non-max suppression

normalization and embedding

# END-TO-END PIPELINE

## Variational Autoencoder (VAE)

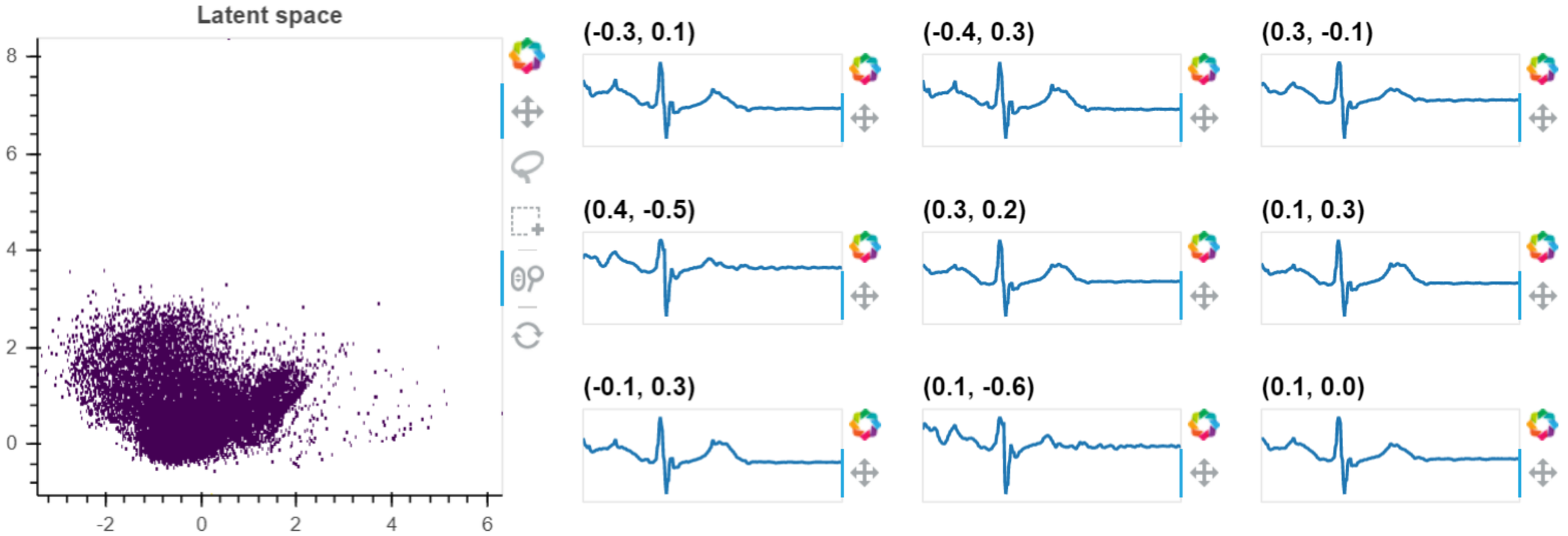
RAPIDS cuDF → CuPy → Numba → PyTorch → RAPIDS cuxfilter



# END-TO-END PIPELINE

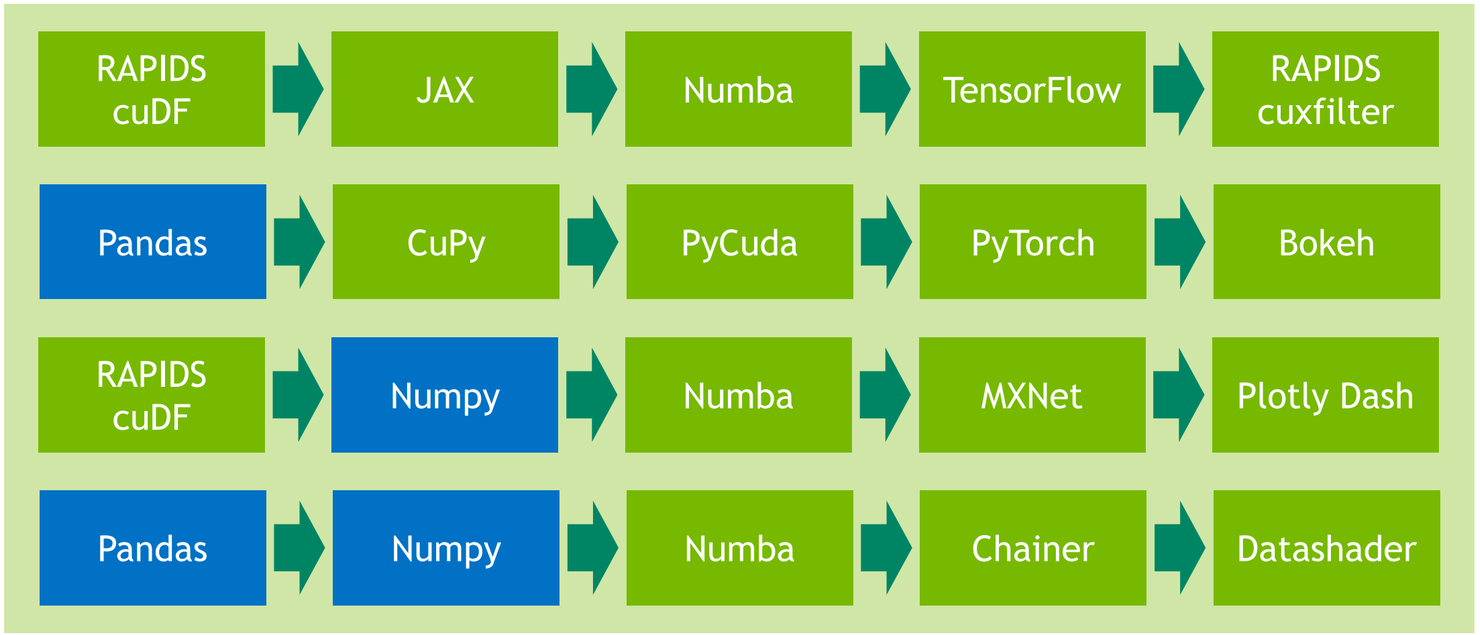
## Visualization

RAPIDS cuDF → CuPy → Numba → PyTorch → RAPIDS cuxfilter



# MIX AND MATCH WORKFLOWS

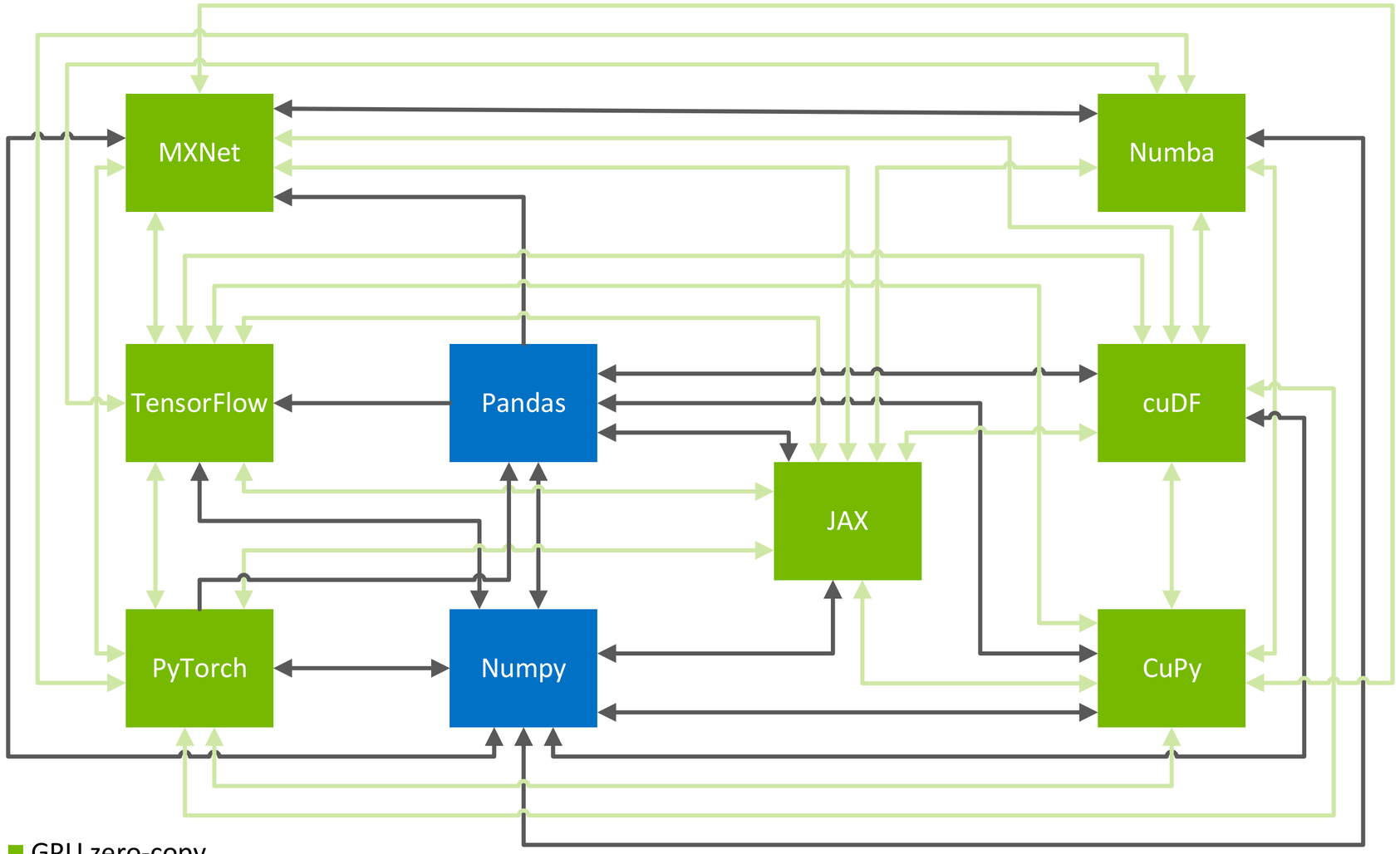
## Endless possibilities!


And many others!

# MIX AND MATCH WORKFLOWS

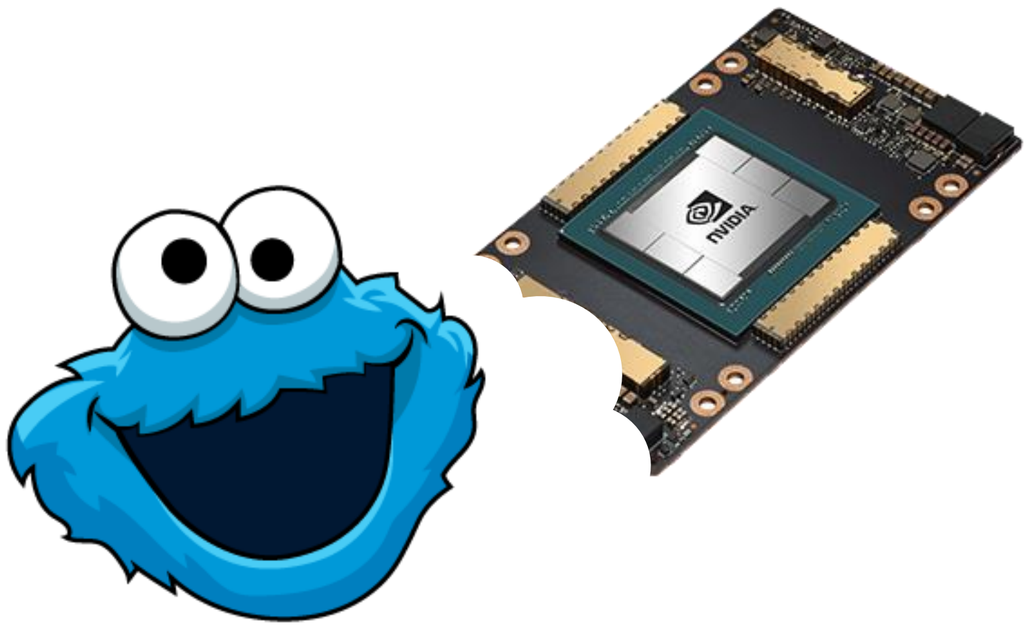
## Use the right tool, for the right job, in the right way



# MEMORY MANAGEMENT BOTTLENECK

# MEMORY MANAGEMENT BOTTLENECK

Memory managers are greedy




Gimme some more... memory!

# MEMORY MANAGEMENT ~~BOTTLENECK~~

## One memory manager to rule them all?

RAPIDS Memory Manager

CuPy

dmlc XGBoost


Numba

- Open-source external allocator interface (EAI)

```
void* allocate(std::size_t bytes, cudaStream_t stream)
void deallocate(void* p, std::size_t bytes, cudaStream_t stream)
```

- Follows open-closed principle:

  *software entities should be **open** for extension but **closed** for modification.*

- Makes it trivial to layer additional functionality like logging, leak checking, limiting, etc.

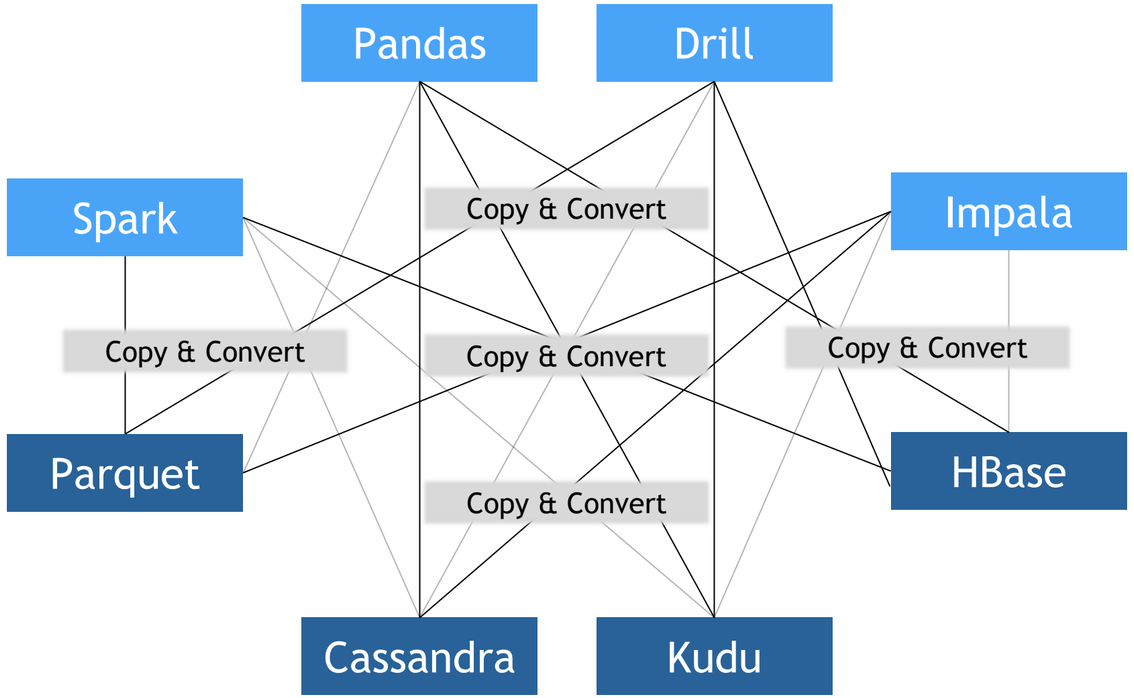
- Zero-code integration with RAPIDS:

  `import cudf` before using CuPy or Numba.

# DATA CONVERSION BOTTLENECK

# DATA CONVERSION BOTTLENECK

## Copy and convert is expensive



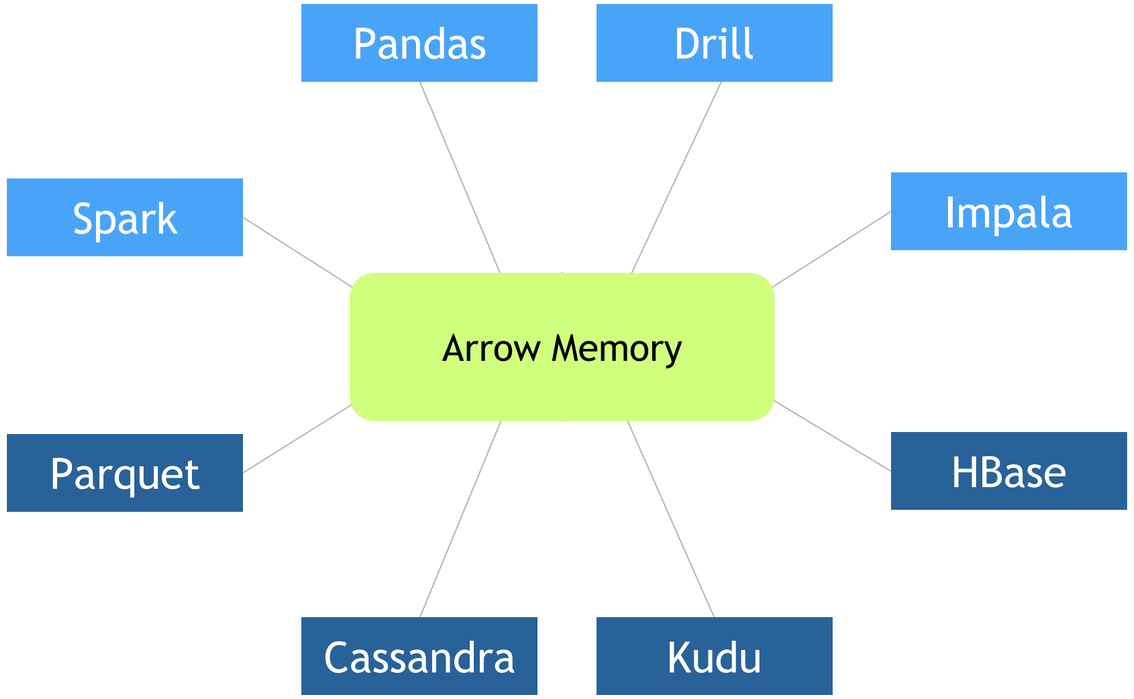

Each system has its own internal memory format.

Similar functionality implemented in multiple projects.

~70% computation wasted on serialization & deserialization.

# DATA CONVERSION ~~BOTTLENECK~~

## Learning from Apache Arrow




All systems utilize the same memory format.

Projects can share functionality.

No overhead for cross-system communication.

# COLUMNAR DATA LAYOUT

## A perfect match for data science

Columnar layout leverages GPU strengths.

CPU Single Instruction Multiple Data (SIMD) instructions also take advantage of it.

Consistency with CPU version simplifies development and conversion.

Emphasis on zero-copy and shallow-copy operations minimizes a core bottleneck.

| | user_id | timestamp | source_ip |
|---|---|---|---|
| row_1 | 6939800 | 2021-04-12 05:31 | 42.155.123.142 |
| row_2 | 4015666 | 2021-04-12 05:47 | 67.132.212.125 |
| row_3 | 5456236 | 2021-04-12 05:52 | 81.205.129.121 |

| | Row-wise data layout |
|---|---|
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| | Columnar data layout |
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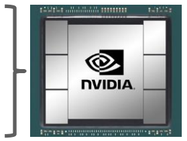



APACHE ARROW

# DLPACK

## Sharing tensors the easiest way

DLPack is an open in-memory tensor structure which enables:

- Easier sharing of tensors and operators between deep learning frameworks.
- Easier wrapping of vendor level operator implementations, allowing collaboration when introducing new devices/ops.
- Quick swapping of backend implementations, like different version of BLAS.
- For final users, this could bring more operators, and possibility of mixing usage between frameworks.

## From cuDF to CuPy

```
# Convert a cuDF DataFrame to a CuPy ndarray
src = cudf.DataFrame({'x': [1, 2], 'y': [3, 4]})
dst = cp.from_dlpack(src.toDlpack())

print(type(dst), "\n", dst)
```

```
<class 'cupy.core.core.ndarray'>
 [[1 3]
 [2 4]]
```

## From CuPy to PyTorch

```
# Convert a CuPy ndarray to a PyTorch Tensor
src = cp.array([[1, 2], [3, 4]])
dst = torch.from_dlpack(src.toDlpack())

print(type(dst), "\n", dst)
```

```
<class 'torch.Tensor'>
 tensor([[1, 2],
         [3, 4]], device='cuda:0')
```

# CUDA ARRAY INTERFACE 3.0

## Seamless Ingestion

The __cuda_array_interface__ attribute returns a dictionary (dict) that must contain the following entries:

**shape**: (integer, ...)

A tuple of int (or long) representing the size of each dimension.

**typestr**: str

The type string. This has the same definition as typestr in the numpy array interface.

**data**: (integer, boolean)

The data is a 2-tuple. The first element is the data pointer as a Python int (or long). The data must be device-accessible. For zero-size arrays, use 0 here. The second element is the read-only flag as a Python bool.

**version**: integer

An integer for the version of the interface being exported. The current version is 3.

Numba

ingests

# NUMBA INGESTION

## CuPy->Numba Example

```
from numba import cuda
import math

@cuda.jit
def segment_kernel(signal, window, out):

    base, step = cuda.grid(1), cuda.gridsize(1)
    for position in range(base, signal.shape[0]-window+1, step):
        accum = -math.inf
        for index in range(window):
            value = signal[position+index]
            accum = value if value > accum else accum
        #                  am I the maximum in my neighborhood?
        out[position] = 1 if accum == signal[position+(window+1)//2] else 0

def segment_numba(signal, window):

    out = cp.empty(signal.shape[0]-window+1, dtype=cp.int64)
    segment_kernel[80*32, 64](signal, window, out)
    cuda.synchronize()

    # fixes sequences of the following form 0000011000-> 0000010000
    out[1:] *= (cp.diff(out) == 1)

    return out
```

signal and out treated as being equivalent to numba.cuda.cudadrv.devicearray.DeviceNDArray


signal and out of type cupy.core.core.ndarray

# DataAPI

## The Consortium for Python Data API Standards

Open consortium to create n-dimensional array and dataframe API standards.

Multidimensional arrays (tensors) fragmentation:

- NumPy, CuPy, Tensorflow, PyTorch, etc.

Dataframes fragmentation:

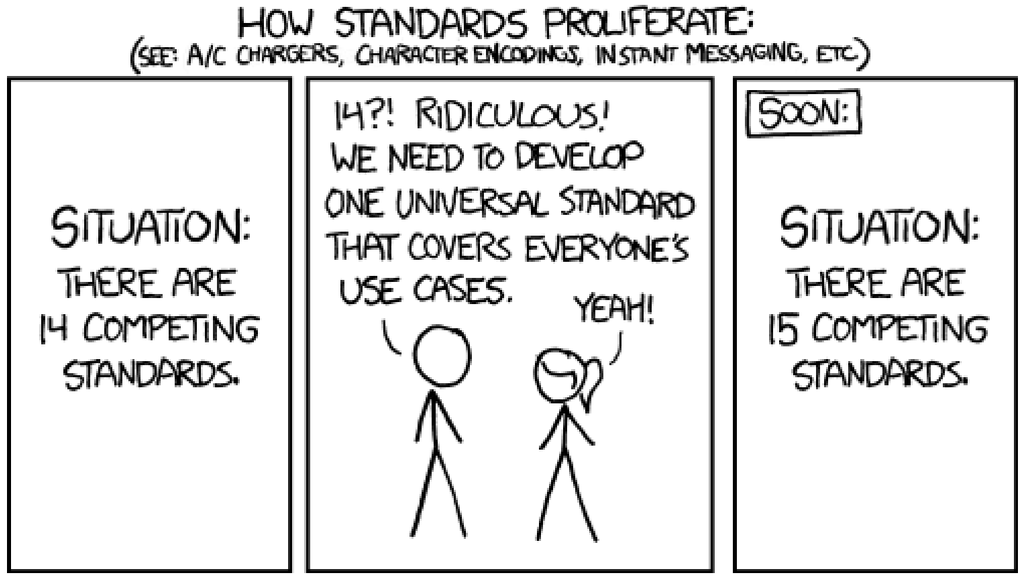
- Pandas, cuDF, Modin, Dask, Vaex, etc.

Cross-project and cross-ecosystem alignment on APIs, data exchange mechanisms and other related topics.

November 10th, 2020: Published the first version of *its* array API standard: https://data-apis.org/array-api/latest

*Consortium Members*

| | | | |
|---|---|---|---|
| Apache Arrow | GeoPandas | MXNet | PyTorch |
| Apache Spark | Ibis | NumPy | TensorFlow |
| cuDF | JAX | OmniSciDB | Vaex |
| CuPy | Koalas | ONNX | XArray |
| Dask | Modin | Pandas | … |




https://xkcd.com/927

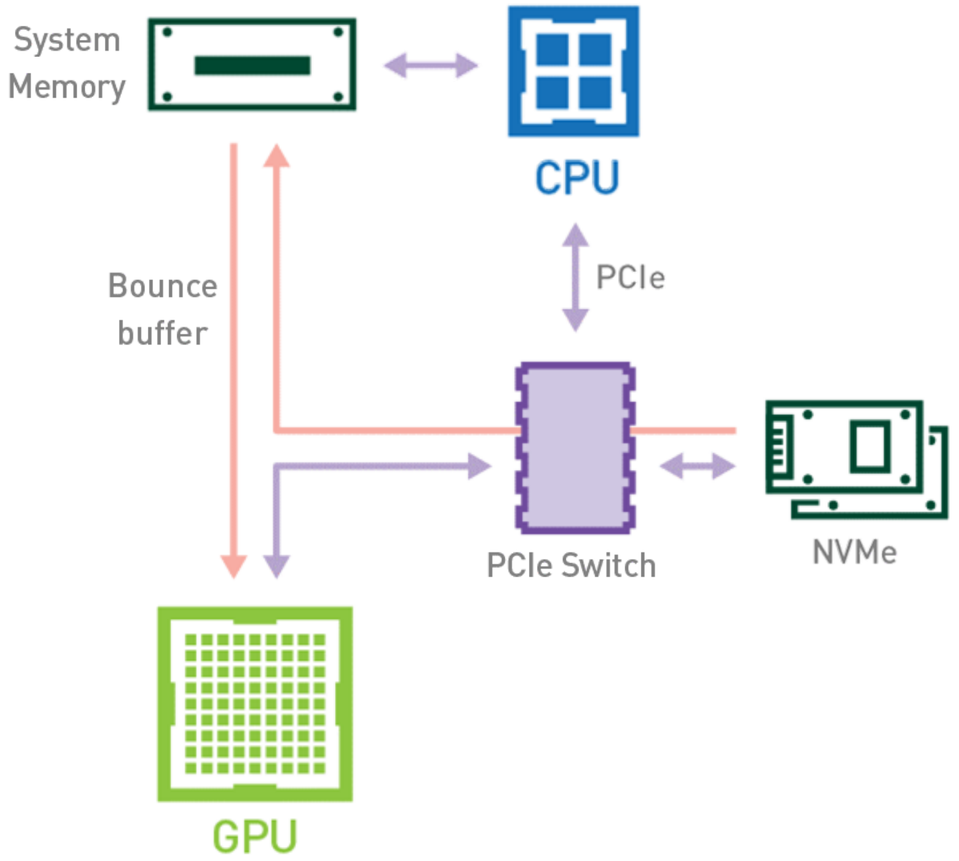


NVIDIA

# DATA LOADING BOTTLENECK

# DATA LOADING BOTTLENECK

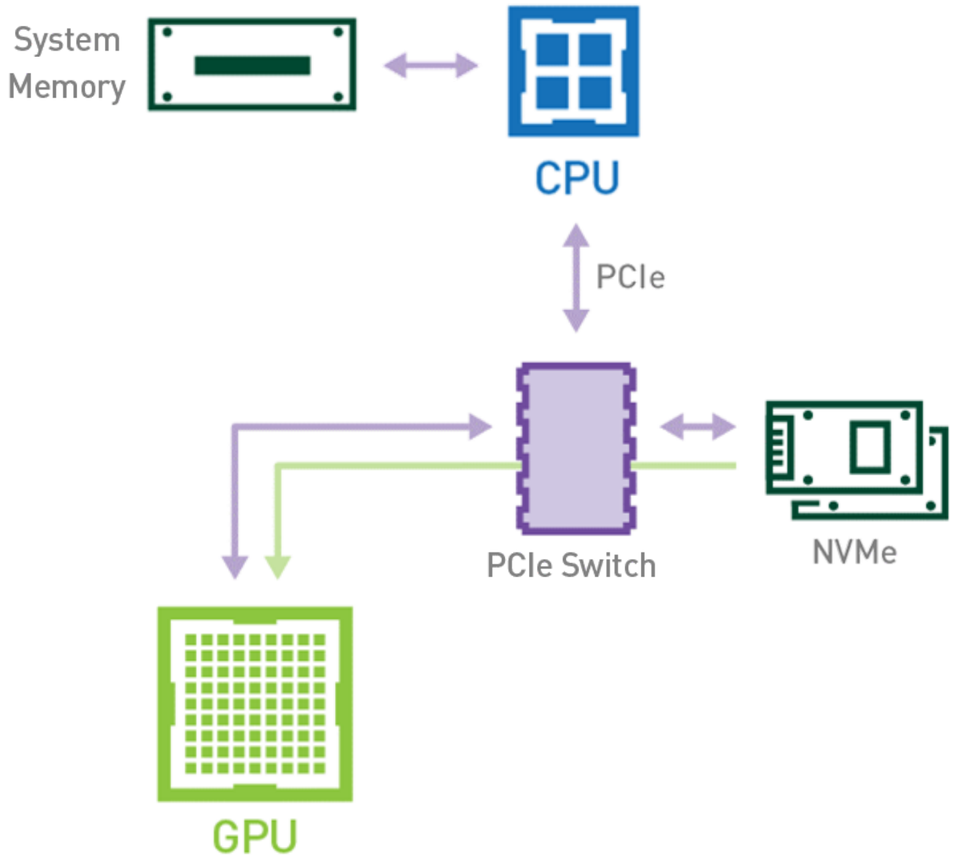
## Without GPUDirect Storage




source: https://developer.nvidia.com/blog/gpudirect

# DATA LOADING ~~BOTTLENECK~~

## With GPUDirect Storage

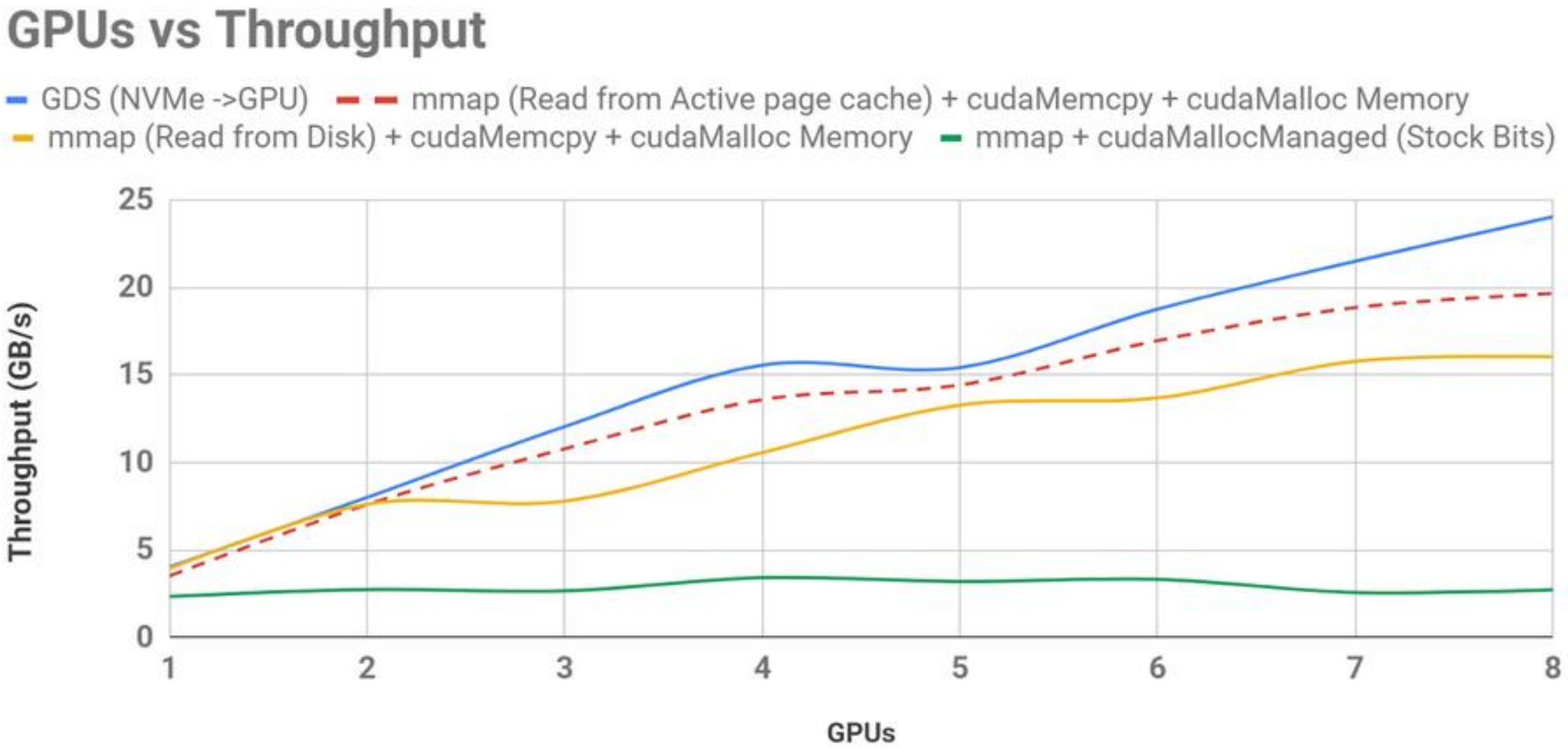



A Direct Path Between Storage and GPU Memory

source: https://developer.nvidia.com/blog/gpudirect

# DATA LOADING ~~BOTTLENECK~~

RAPIDS cuIO

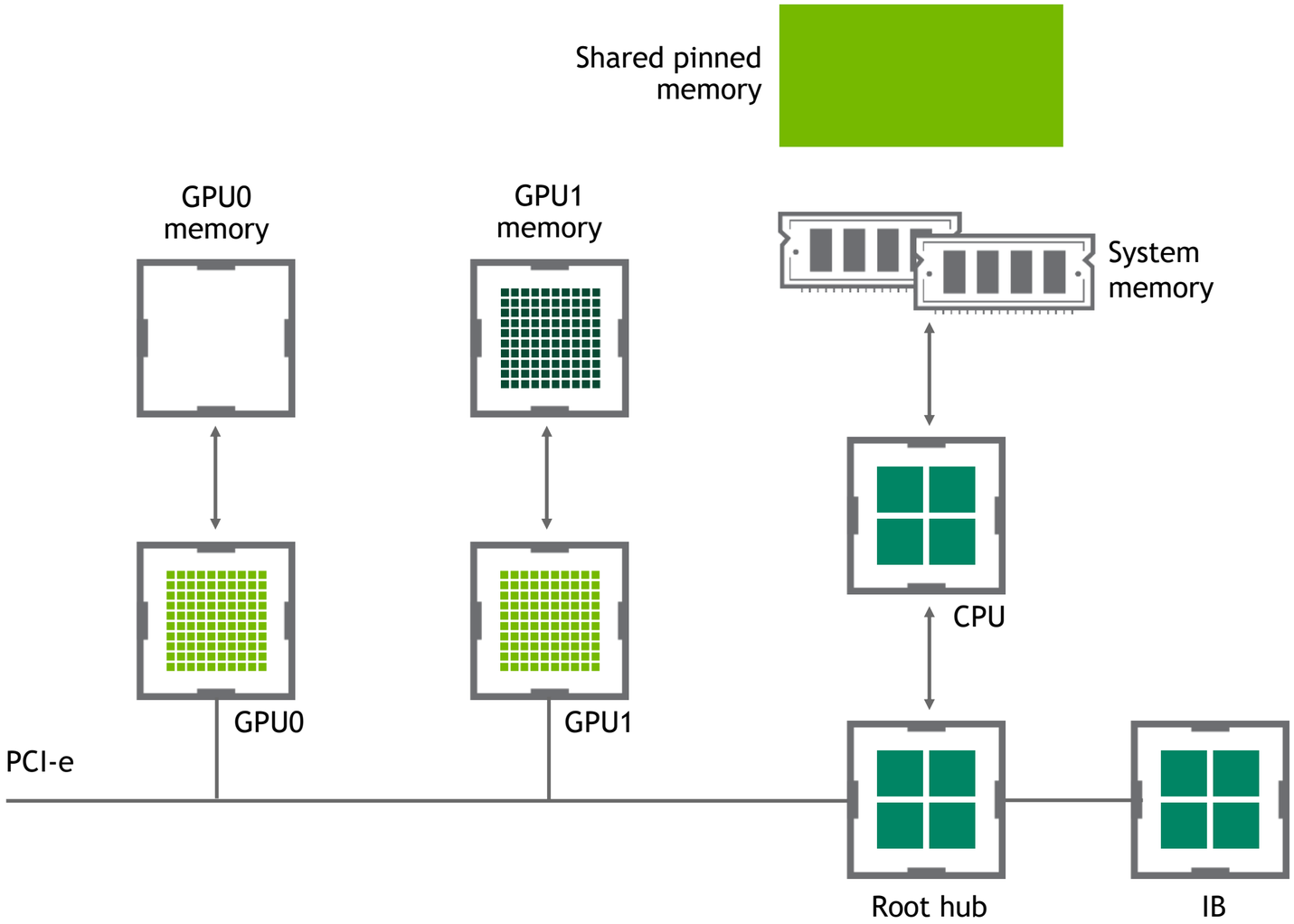



source: https://developer.nvidia.com/blog/gpudirect-storage

# DATA TRANSFER BOTTLENECK

# PEER TO PEER DATA TRANSFER BOTTLENECK

## Without GPUDirect



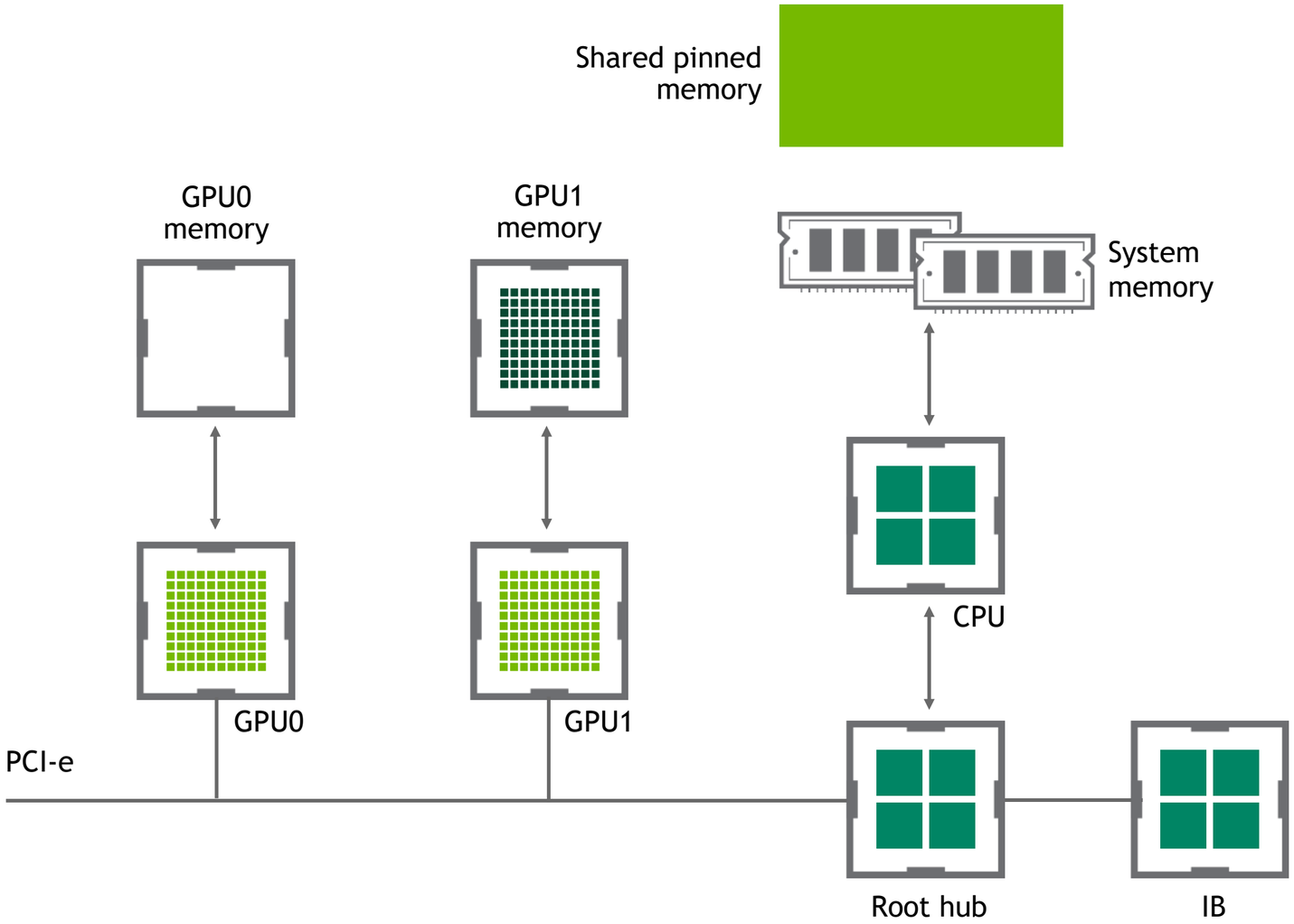

Data is copied from GPU1 to host memory.

Data is copied from host memory to GPU0.

Compute latency is high because data has to be staged in main/host memory before being transferred to gpu/device memory.

# PEER TO PEER DATA TRANSFER ~~BOTTLENECK~~

## With GPUDirect




**GPUDirect P2P Transfer:** Data is copied directly to another GPU memory.

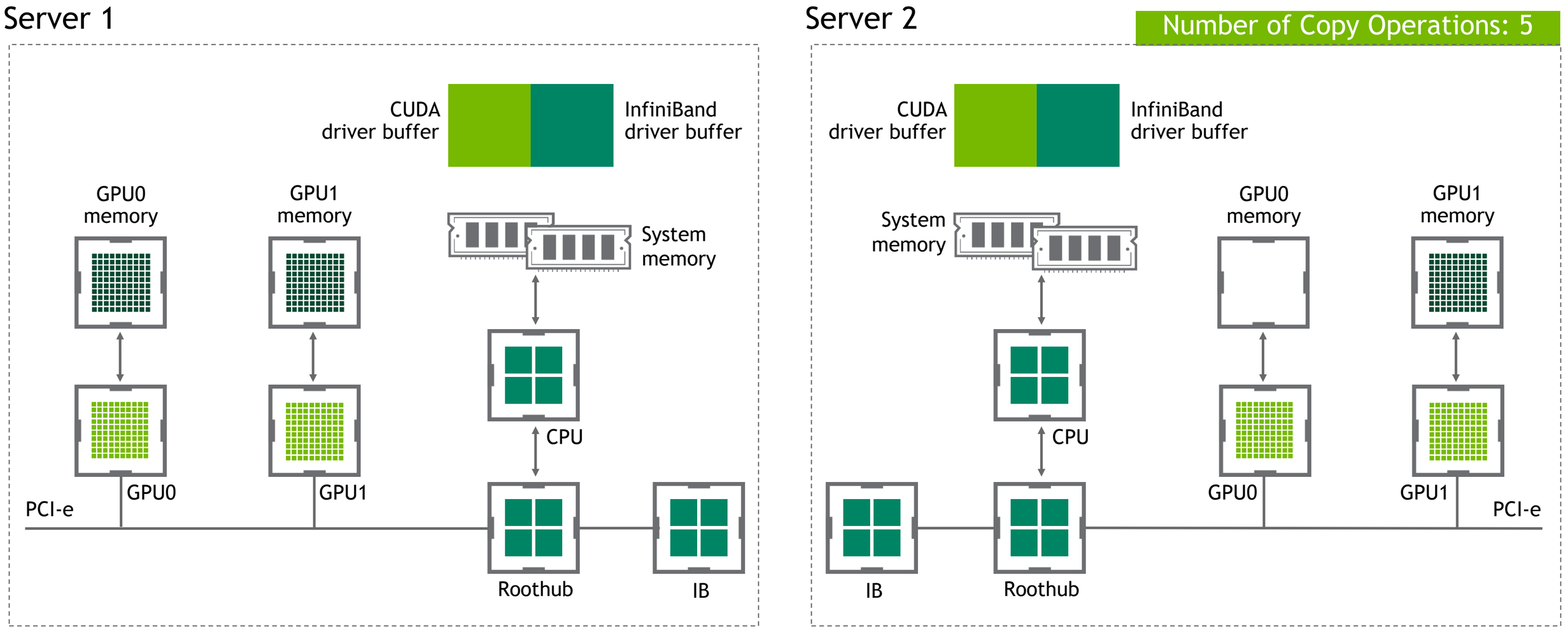
**GPUDirect P2P Access:** GPU Peers can directly access and transfer data between them if they are on the same root hub.

Compute latency is minimized because no CPU involvement is required to drive staging data.

Removes bottlenecks in PCIe topology.

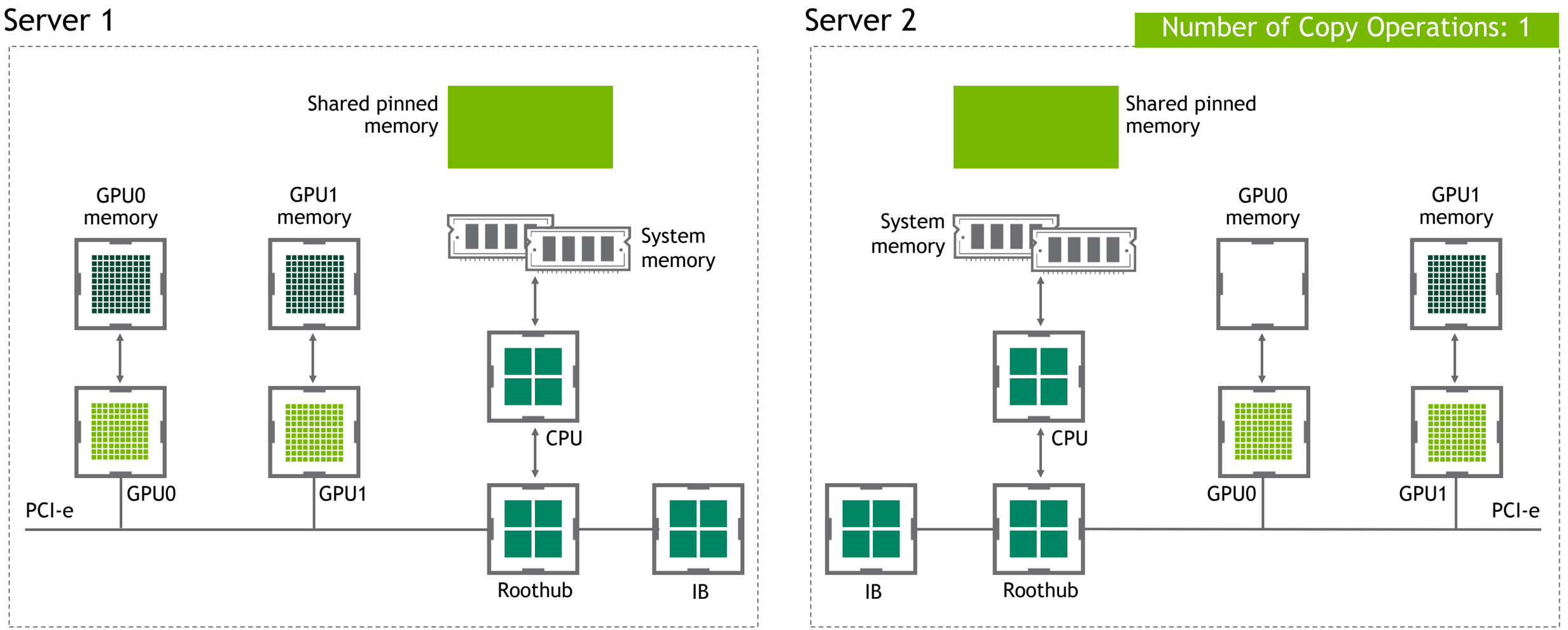
# INTER-NODE DATA TRANFER BOTTLENECK

## Without GPUDirect RDMA



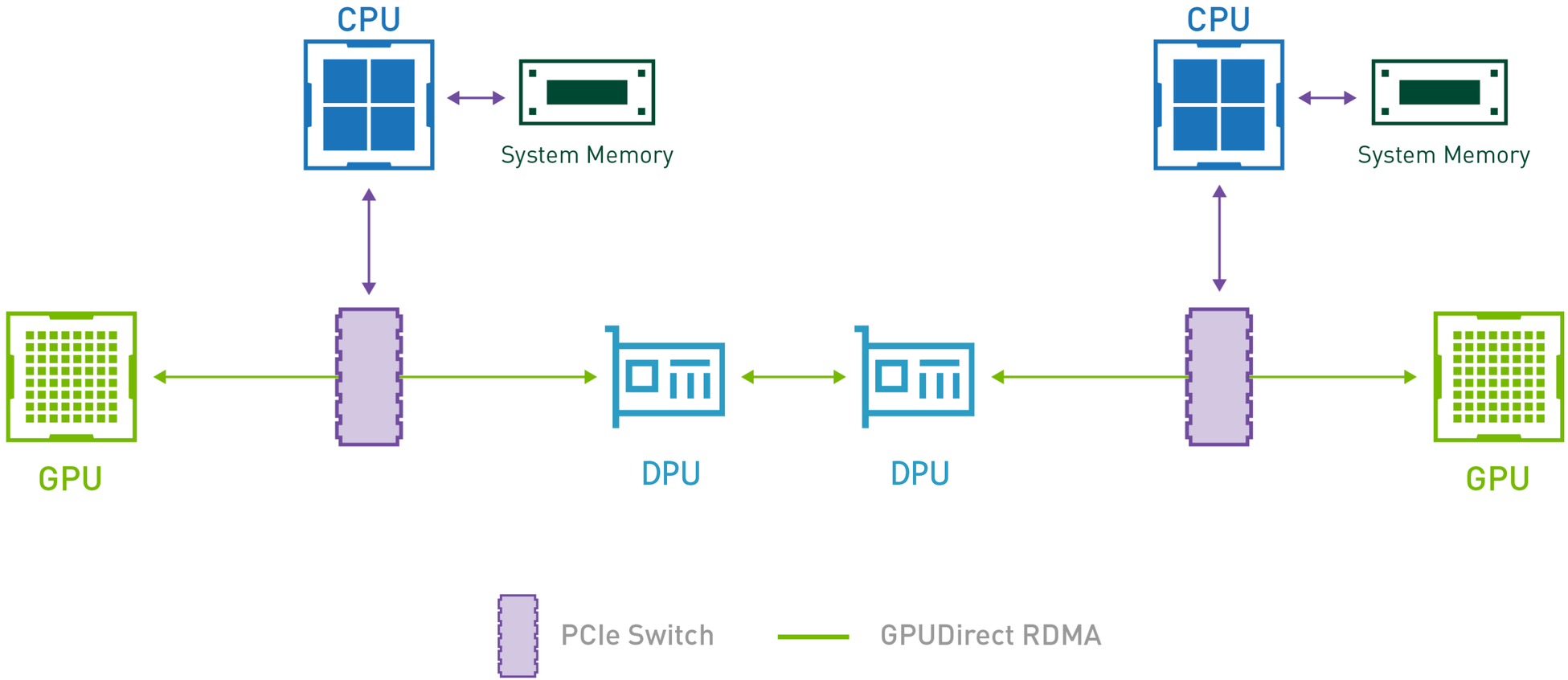
# INTER-NODE DATA TRANFER ~~BOTTLENECK~~

## With GPUDirect RDMA



# INTER-NODE DATA TRANFER ~~BOTTLENECK~~

## GPUDirect RDMA: Direct Communication between NVIDIA GPUs




source: https://developer.nvidia.com/blog/gpudirect

# SUMMARY

# ML FRAMEWORKS INTEROPERABILITY

## What we have seen today

Interoperability matters.

A single framework is not enough anymore.

Complex workloads make use of multiple libraries.

Interoperability via DLPack and CUDA Array Interface (CAI).

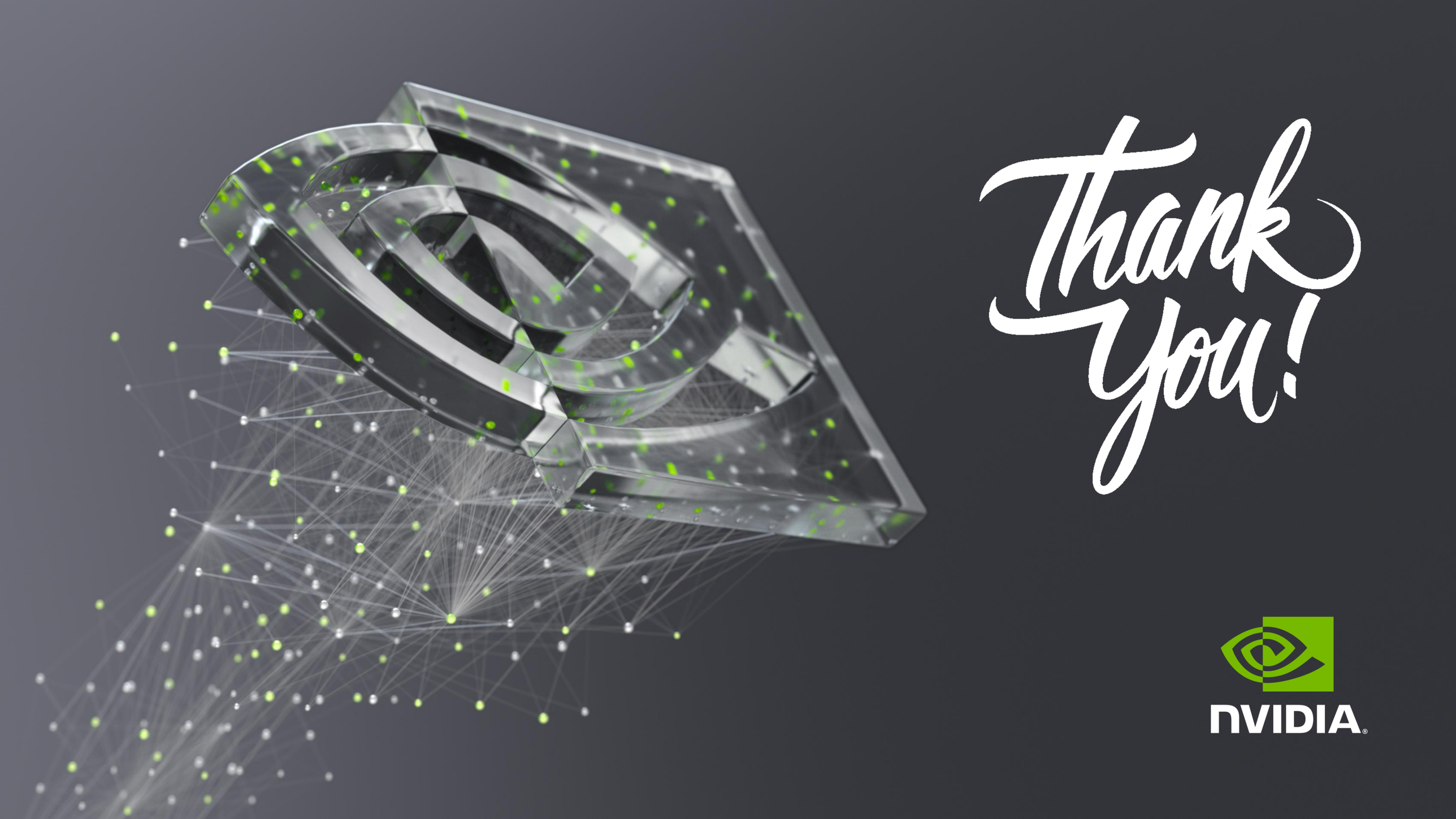
Zero-copy and no data conversion is the goal. Not always possible, yet.

Memory management, data loading and data transfer are common bottlenecks.

That’s all folks!

# RESOURCES

- Blog Post, Part 1: Memory Layouts and Memory Pools
- Blog Post, Part 2: Data Loading and Data Transfer Bottlenecks
- Blog Post, Part 3: Zero-Copy in Action using an E2E Pipeline
- GTC Video Recording | NVIDIA On-Demand
- Interoperability Cheat Sheet Notebook
- End-2-End Example Notebook


Thank You!
NVIDIA