ACCELERATED GENERAL DATA SCIENCE IN MEDICINE WITH CUPY, RAPIDS & NUMBA

HUIWEN JU - HJU@NVIDIA.COM - SOLUTIONS ARCHITECT, HIGHER EDUCATION & RESEARCH

4/17/2024 @ MOUNT SINAI

AGENDA

Overview of GPU Computing

GPU-Accelerated Numerical Computing with ***CuPy***

GPU-Accelerated Data Science with ***RAPIDS***

Custom GPU Kernels with ***Numba***

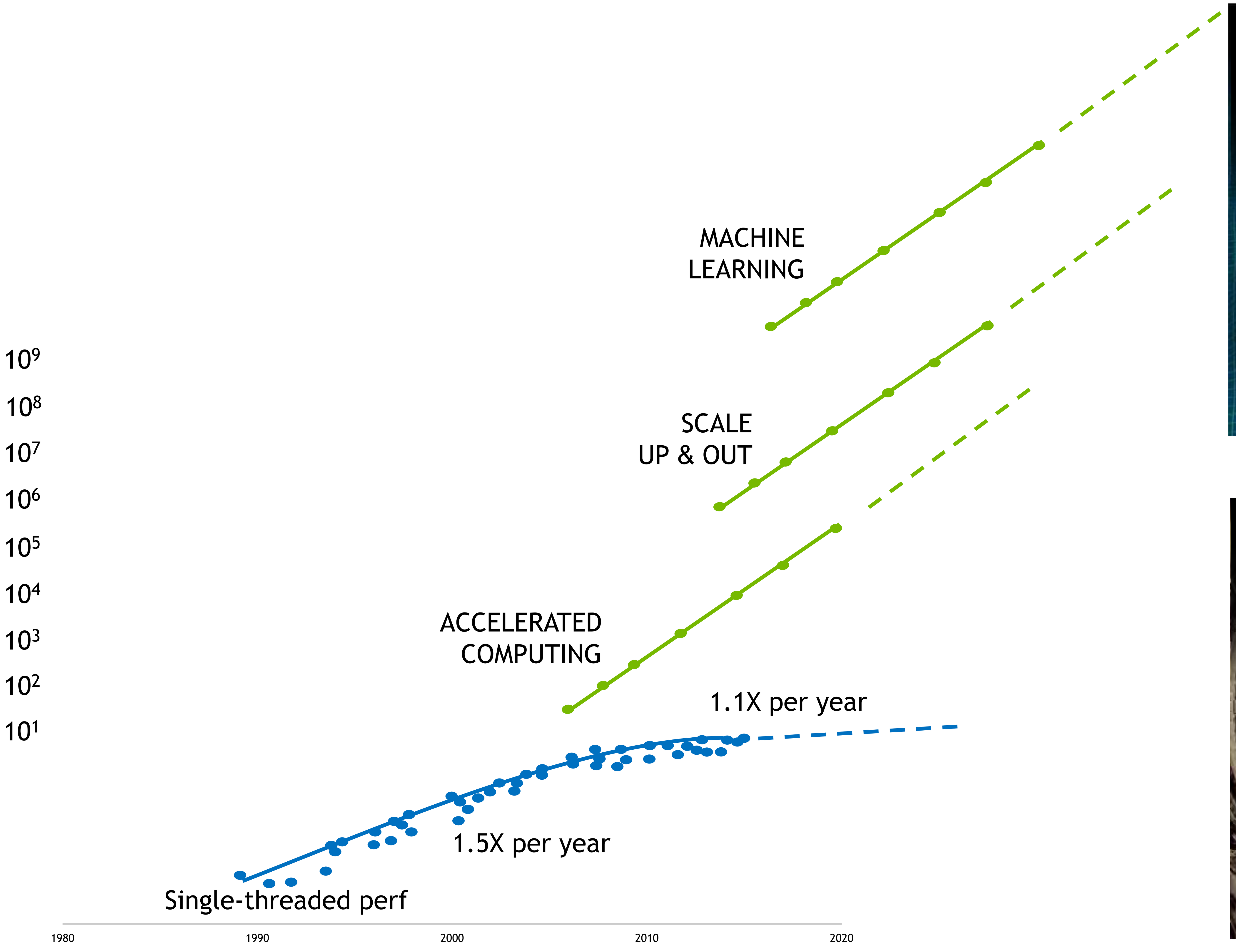
Frameworks Interoperability – ***Data Conversion Bottleneck***

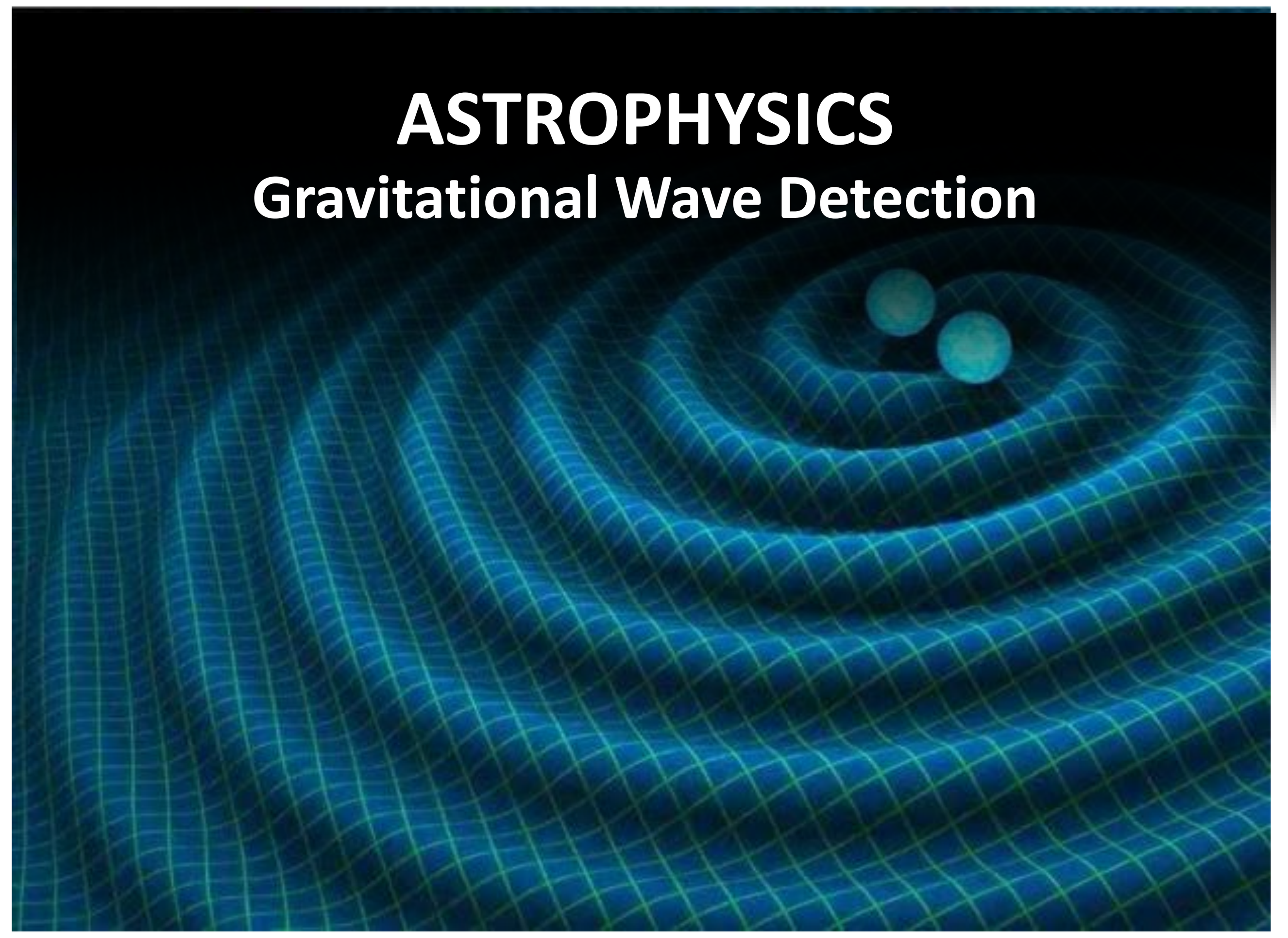
ZERO-COPY end-to-end pipeline – example jupyter notebook on Minerva

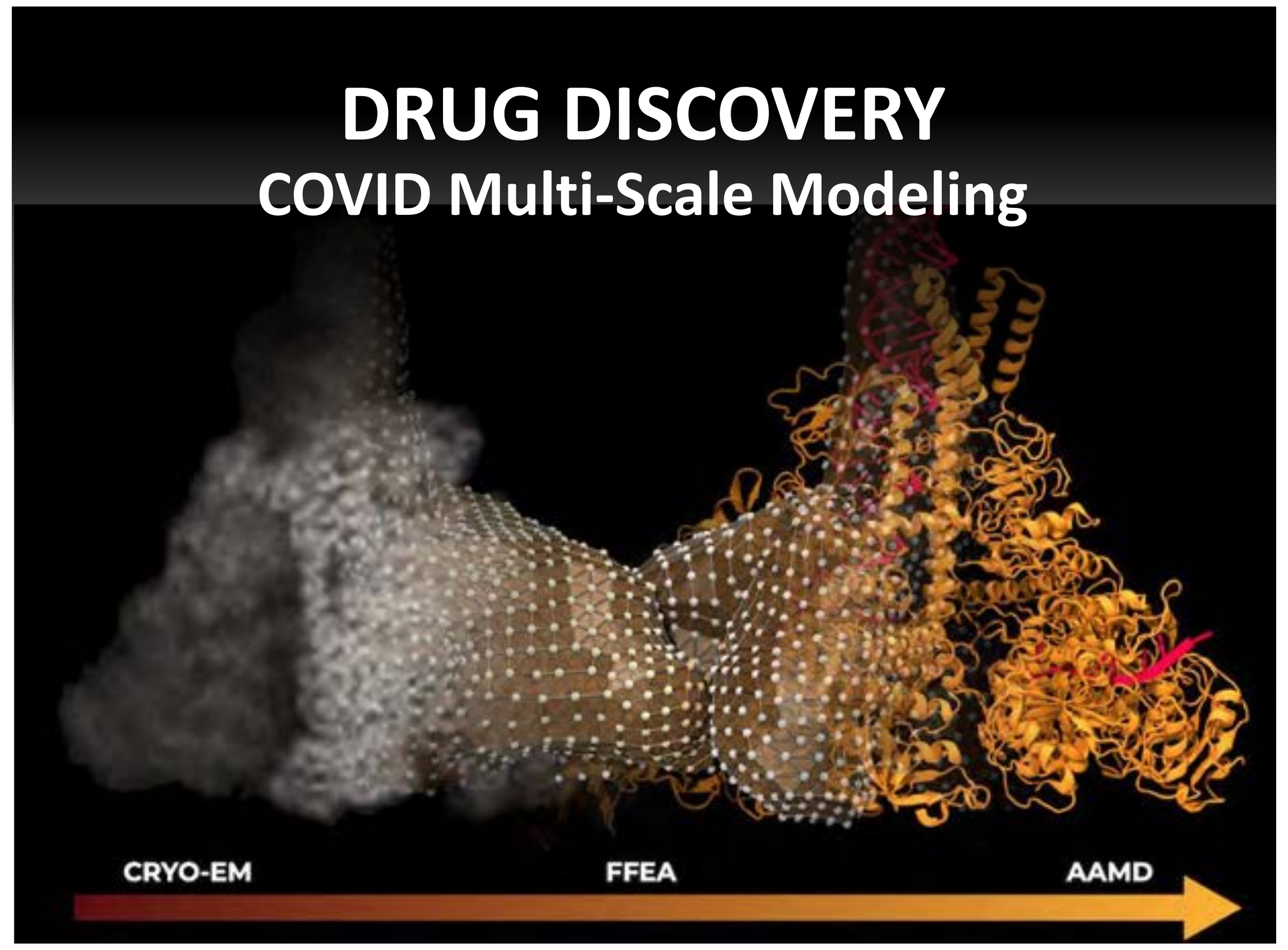
Overview of GPU Computing

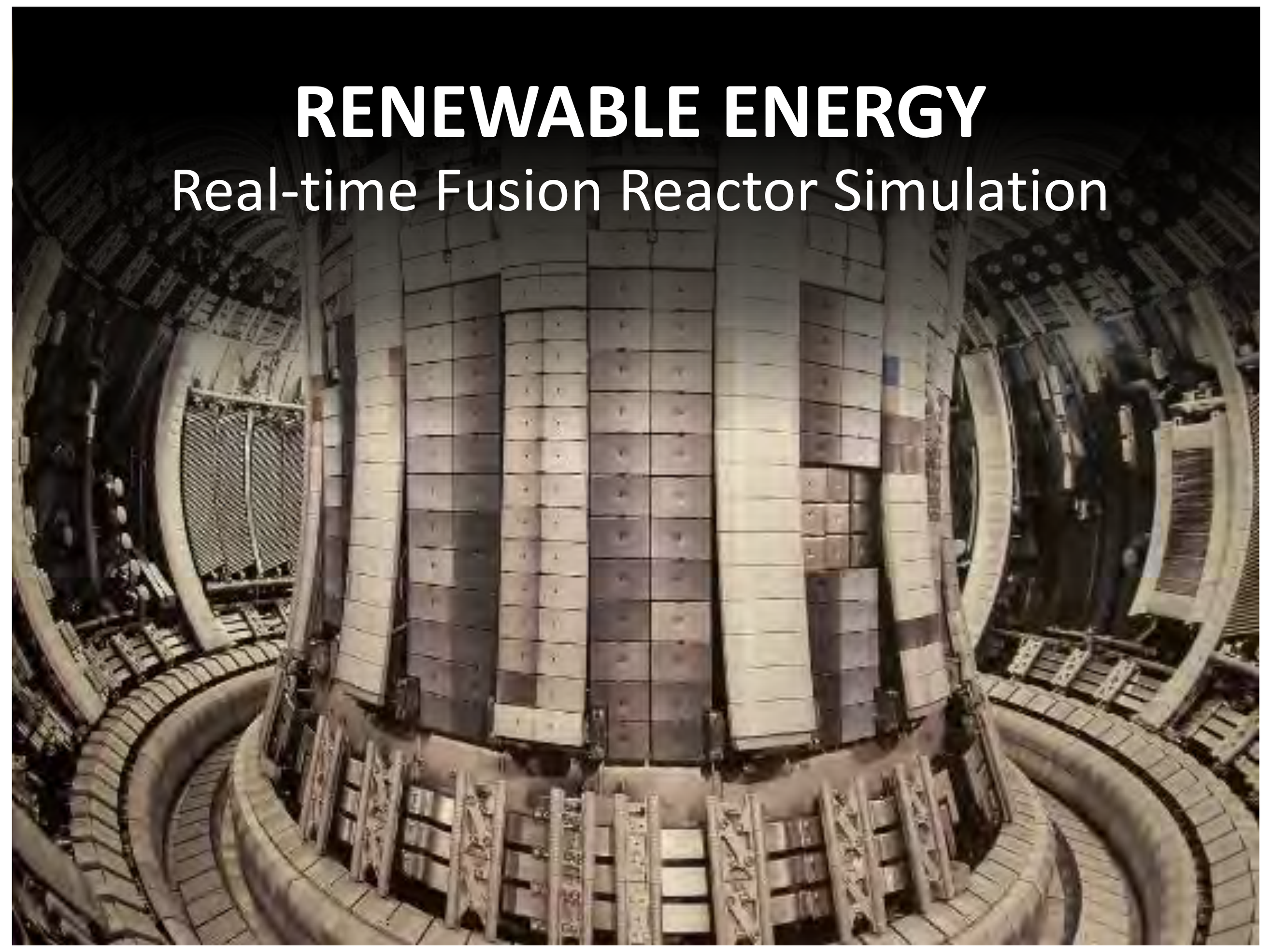
MILLION-X SPEEDUP FOR INNOVATION AND DISCOVERY

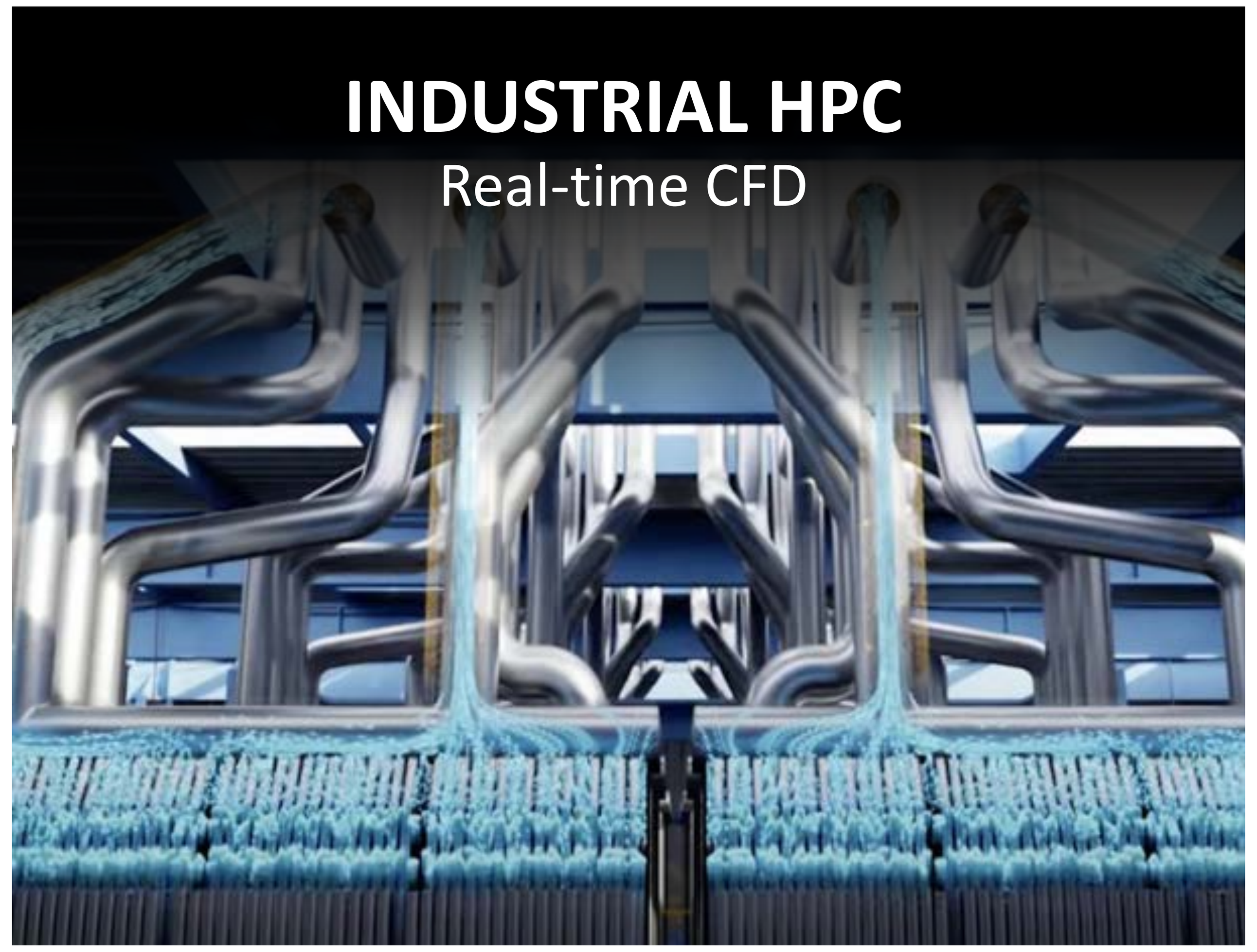
Combination of Accelerated Computing, Data Center Scale and AI











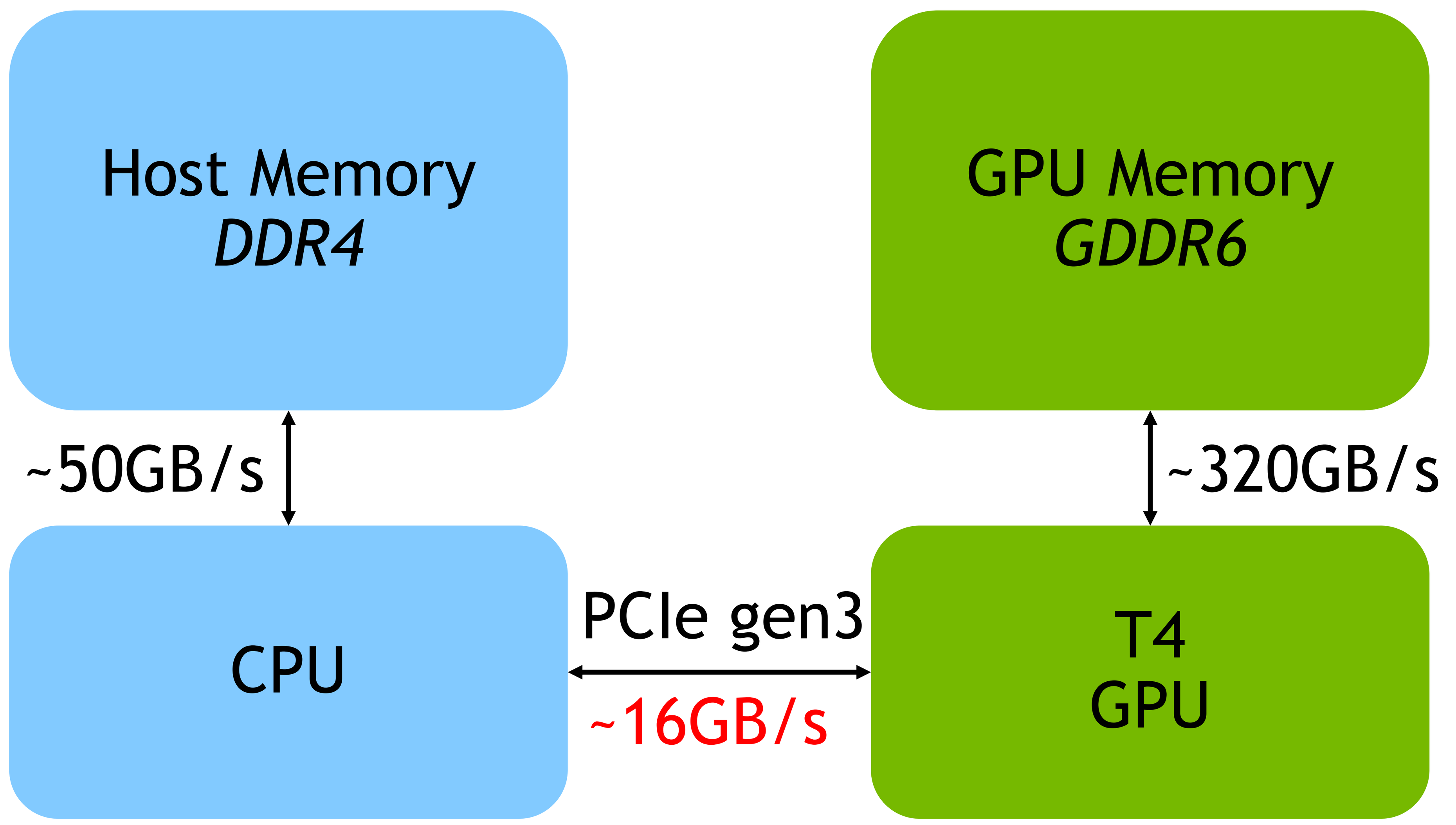
ACCELERATED COMPUTING WITH GPUS

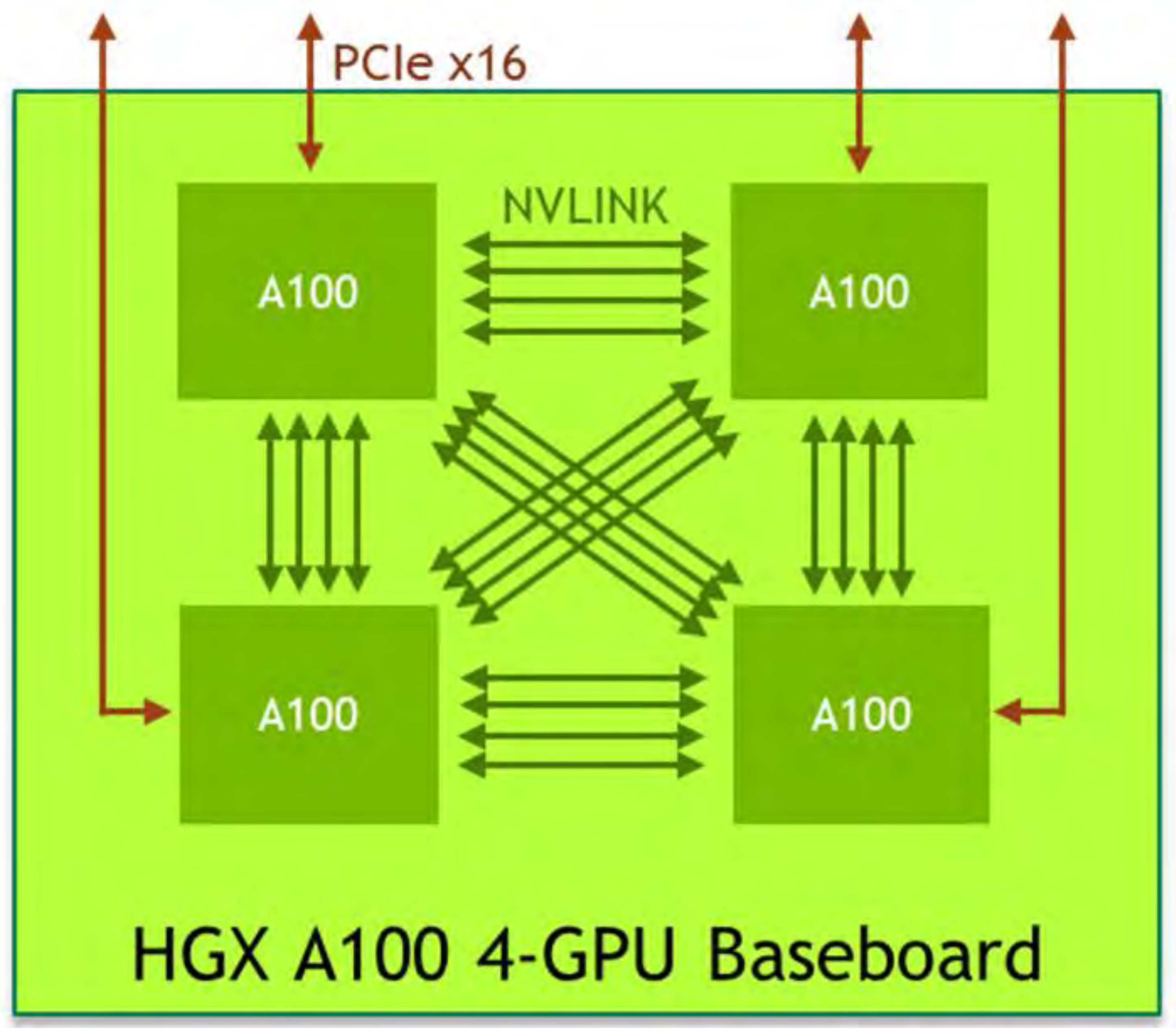
A FEW GENERAL TIPS FOR SUCCESSFUL GPU COMPUTING

- **Minimize data movement to and from the GPU**
  - What happens on the GPU, stays on the GPU!
  - PCI express is a bottleneck for data movement
  - Try NVLink for GPU peer-to-peer, 600 GB/s!

- **GPUs are parallel processing machines**
  - Leave serial operations to the CPU
  - Look for high arithmetic intensity, chunky loops, dense linear algebra
  - Experiment with reduced precision, mixed-precision iterative refinement
  - High memory bandwidth - Fast FFTs.

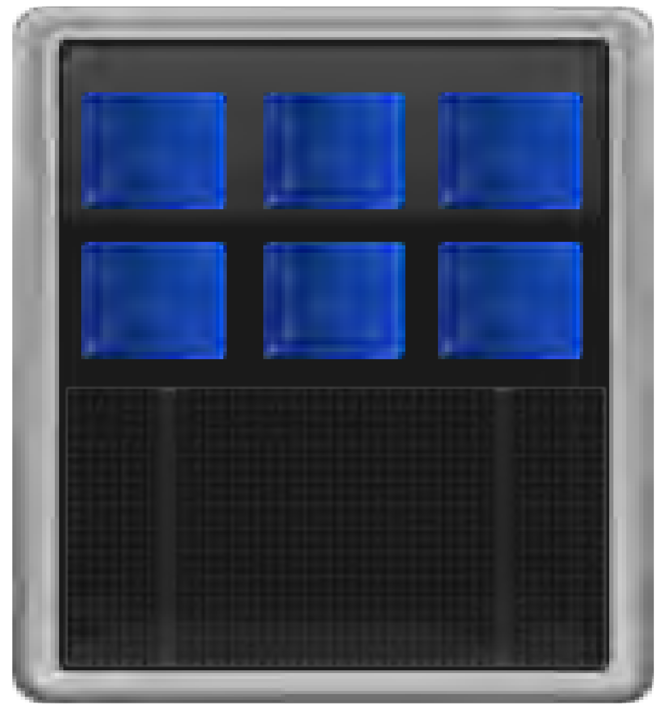
- **Stand on the Shoulders of Those Before You!**
  - There is a rich ecosystem of GPU-accelerated libraries
    https://developer.nvidia.com/gpu-accelerated-libraries
  - Profiling tools (Nsight) are compatible with Python GPU tools
    We care about performance - make a relevant test suite!
  - Many applications are already GPU-accelerated
  - https://www.nvidia.com/en-us/gpu-accelerated-applications/
  - https://ngc.nvidia.com/



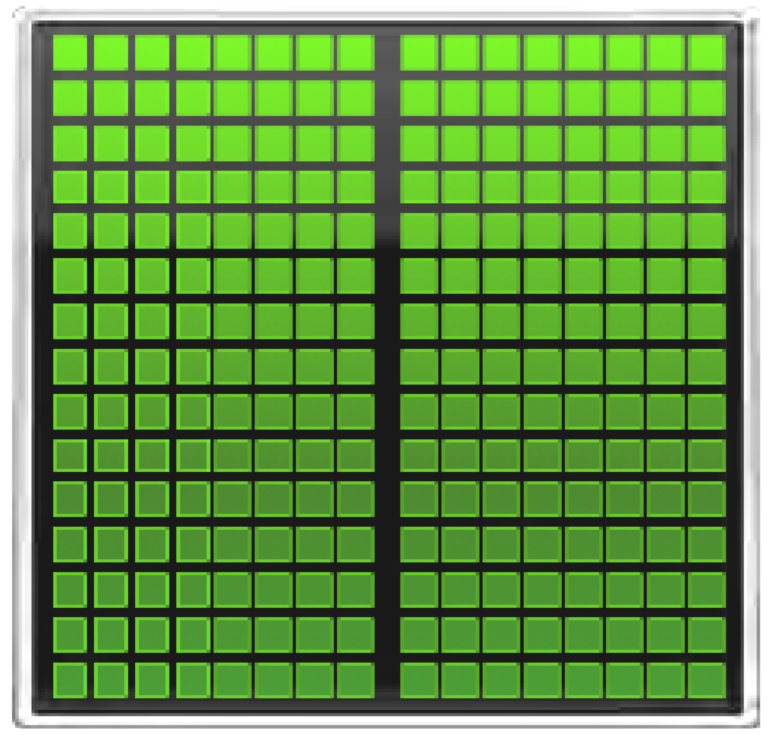


GPU-Accelerated Numerical Computing with *CuPy*

NUMERICAL COMPUTING IN PYTHON



- Mathematical focus
- Operates on arrays of data
  - *ndarray*, holds data of same type
- Many years of development
- Highly tuned for CPUs



- NumPy like interface
- Trivially port code to GPU
- Copy data to GPU
  - CuPy *ndarray*
- Data interoperability with DL frameworks, RAPIDS, and Numba
- Uses high tuned NVIDIA libraries
- Can write custom CUDA functions

CUPY

A NumPy like interface to GPU-acceleration ND-Array operations

BEFORE

```
import numpy as np

size = 4096
A = np.random.randn(size,size)

Q, R = np.lingalg.qr(A)
```

AFTER

```
import cupy as cp

size = 4096
A = cp.random.randn(size,size)

Q, R = cp.lingalg.qr(A)
```

NumPy

52x Speedup!

CuPy

CUNUMERIC

Automatic NumPy Acceleration and Scalability

cuNumeric

cuNumeric transparently accelerates and scales existing Numpy workloads

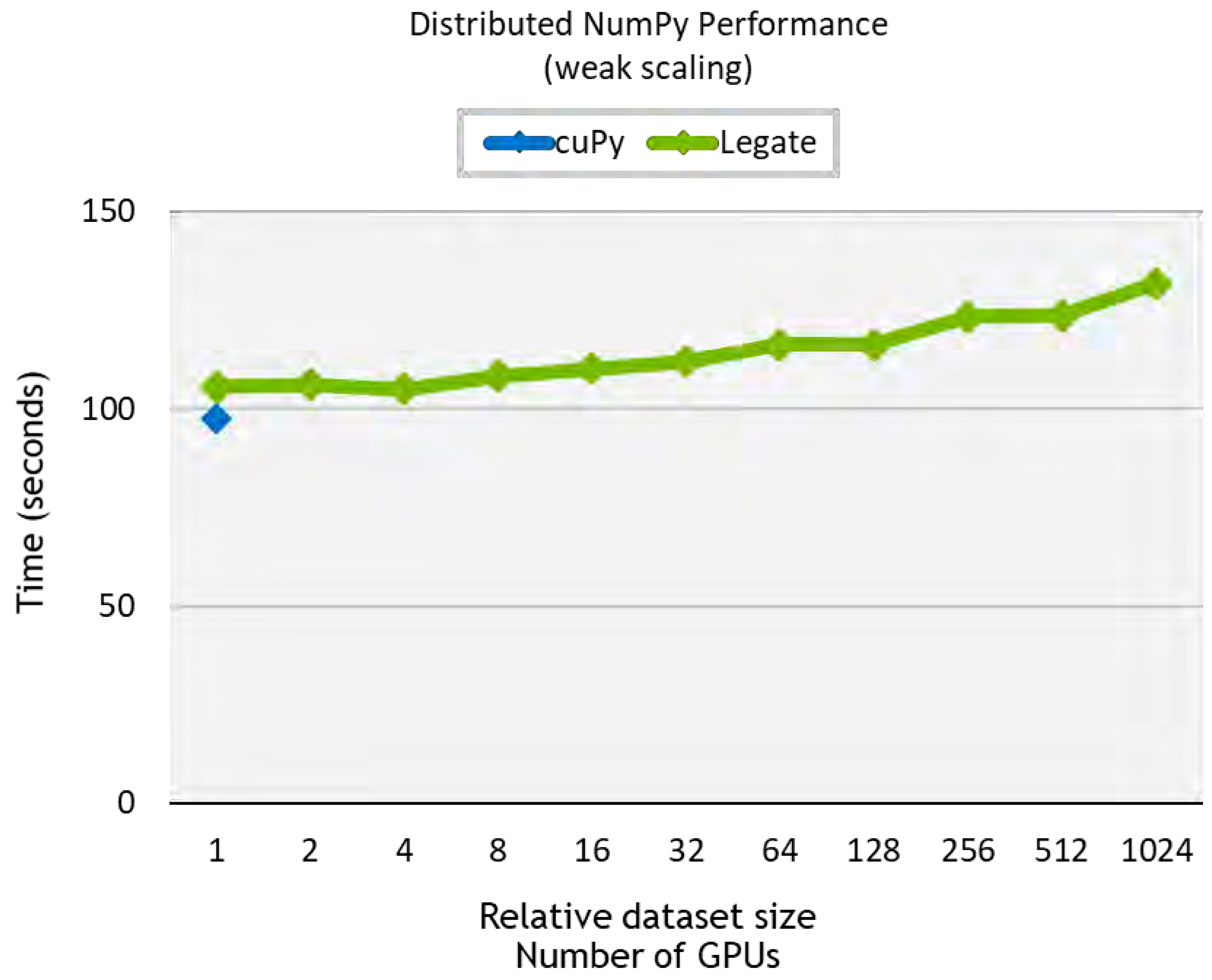
Program from the edge to the supercomputer in Python by changing 1 import line

Pass data between Legate libraries without worrying about distribution or synchronization requirements

Learn more at the landing page

```
for _ in range(iter):
    un = u.copy()

    vn = v.copy()
    b = build_up_b(rho, dt, dx, dy, u, v)
    p = pressure_poisson_periodic(b, nit, p, dx, dy)

…
```

Extracted from "CFD Python" course at https://github.com/barbagroup/CFDPython
Barba, Lorena A., and Forsyth, Gilbert F. (2018). CFD Python: the 12 steps to Navier-Stokes equations. *Journal of Open Source Education*, **1**(9), 21, https://doi.org/10.21105/jose.00021



GPU-Accelerated Data Science with RAPIDS

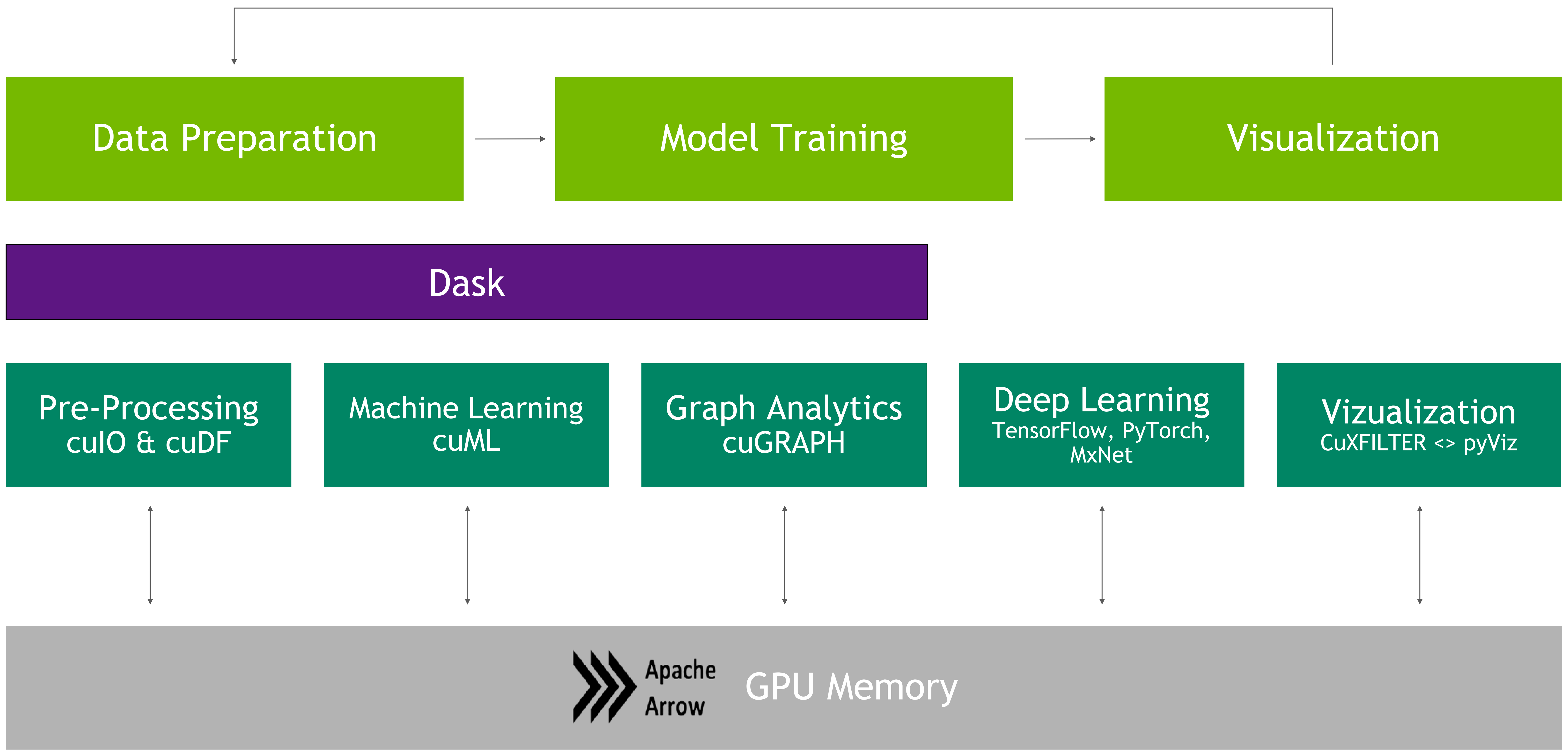
RAPIDS ACCELERATES POPULAR DATA SCIENCE TOOLS

Delivering enterprise-grade data science solutions in pure python

The RAPIDS suite of open source software libraries gives you the freedom to execute end-to-end data science and analytics pipelines entirely on GPUs.

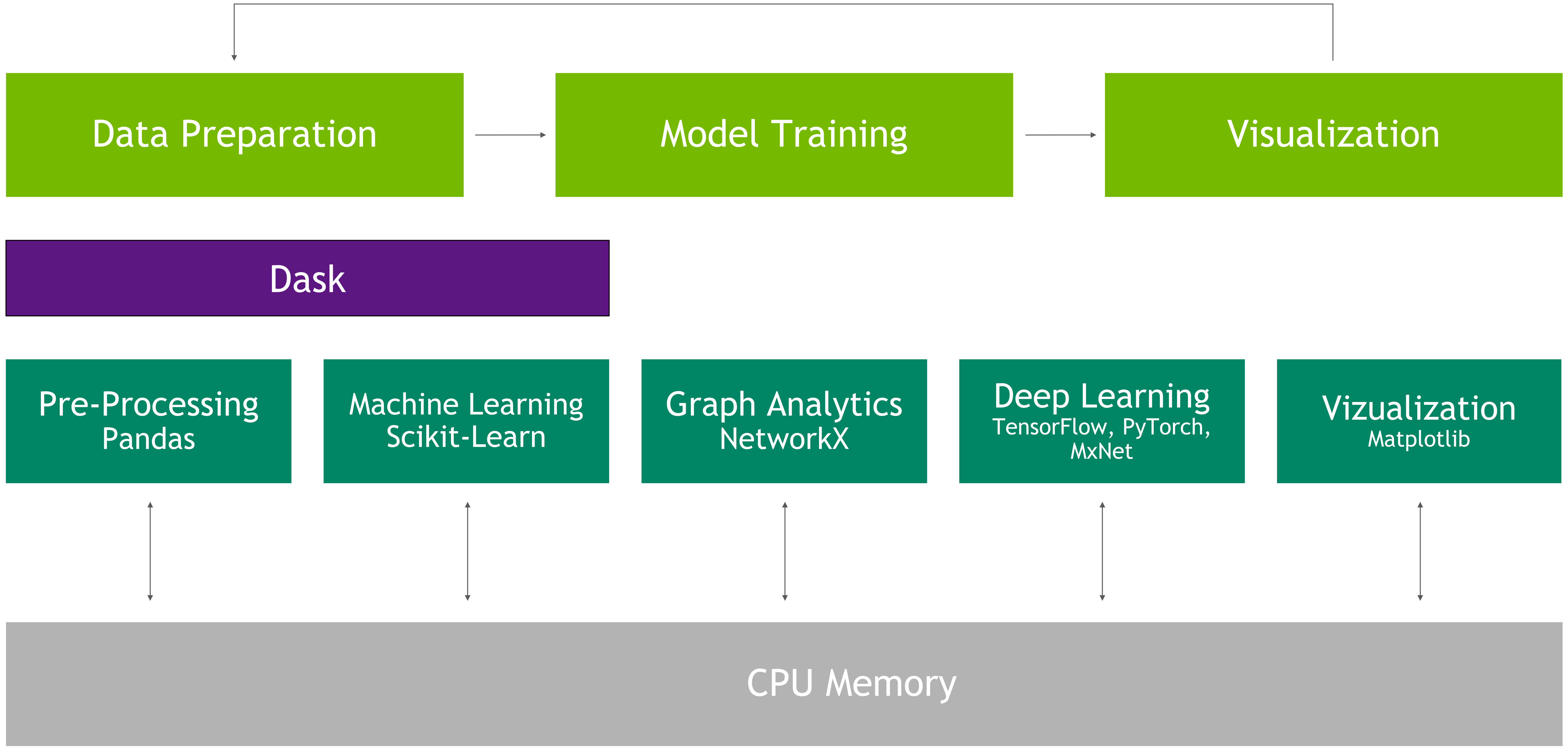
RAPIDS utilizes **NVIDIA CUDA** primitives for low-level compute optimization and exposes GPU parallelism and high-bandwidth memory speed through user-friendly Python interfaces like PyData.

With Dask, RAPIDS can scale out to multi-node, multi-GPU cluster to power through big data processes.

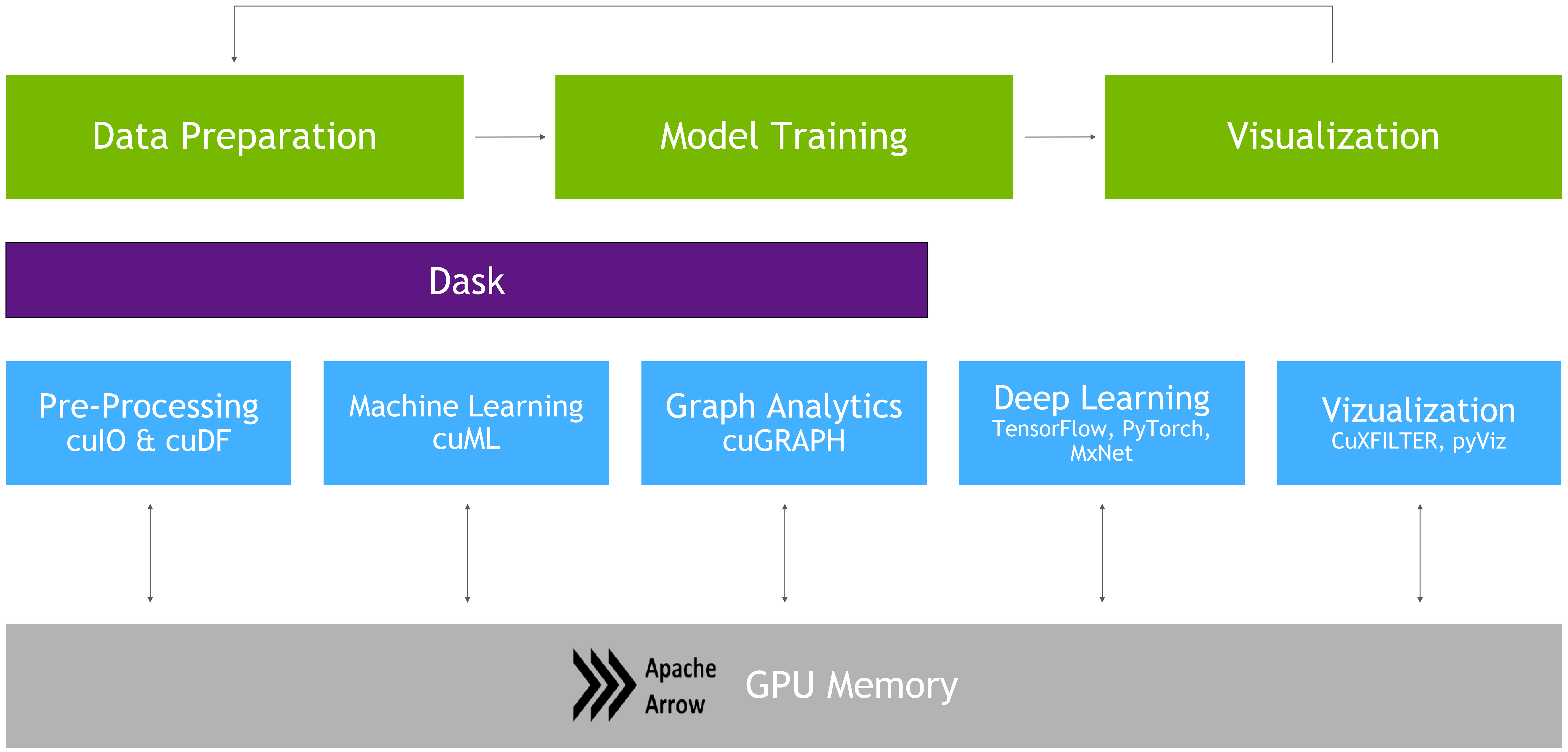


RAPIDS enables the Python stack with the power of NVIDIA GPUs

TRADITIONAL DATA SCIENCE APPLICATIONS



RAPIDS: GPU-ACCELERATED DATA SCIENCE
WITH API ALIGNMENT



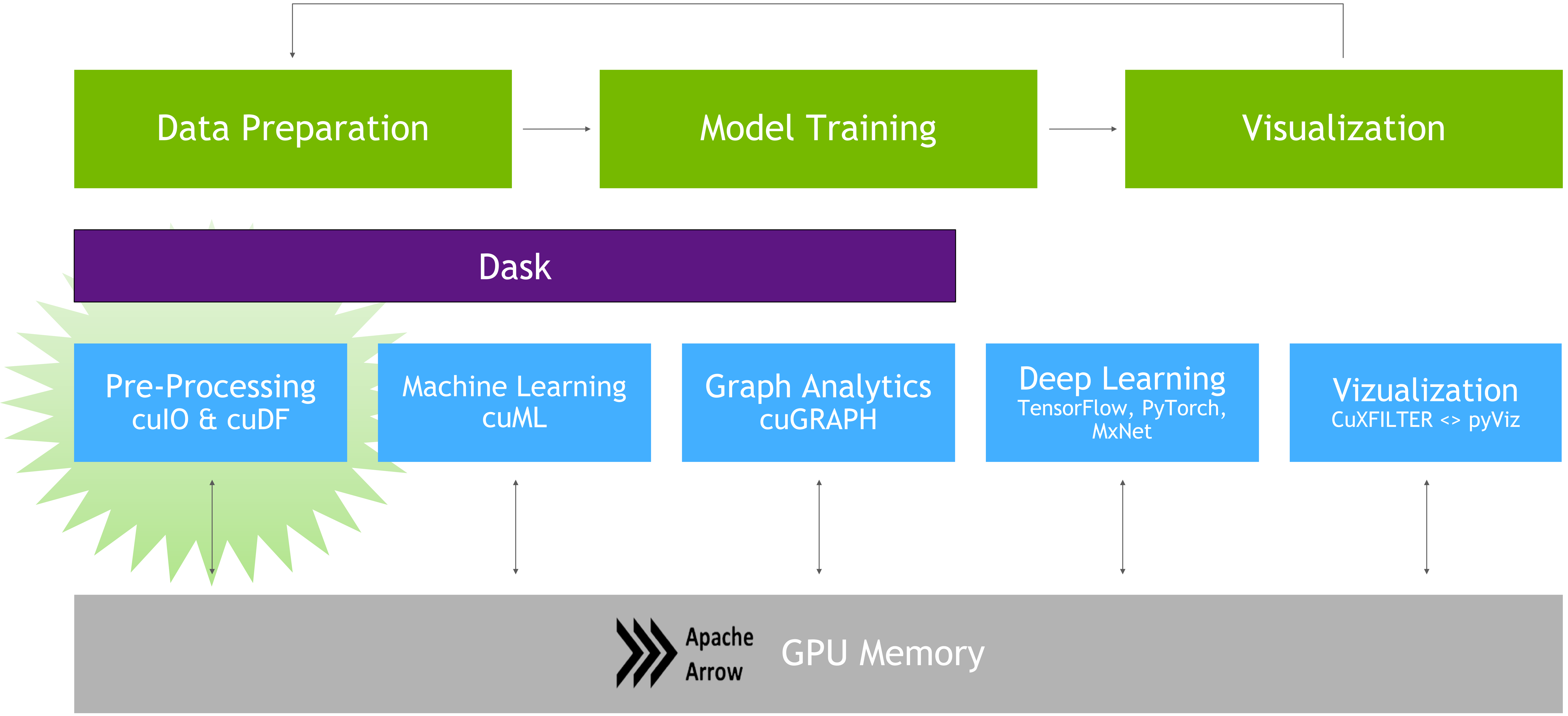
DATA SCIENCE API ALIGNMENT

Open source software that accelerates popular data science packages

Function	CPU	GPU/RAPIDS
Data handling	pandas	cuDF **
Machine learning	scikit-learn	cuML **
Graph analytics	NetworkX	cuGraph
Geospatial	GeoPandas/SciPy	cuSpatial
Signals	SciPy.signal	cuSignal
Image Processing	scikit-image	cuCIM

The RAPIDS and GPU-accelerated PyData stack bring GPGPU to data scientists at the Python layer providing familiar APIs without the steep curve of learning new programming language or paradigm

RAPIDS: GPU-ACCELERATED DATA SCIENCE *WITH API ALIGNMENT*



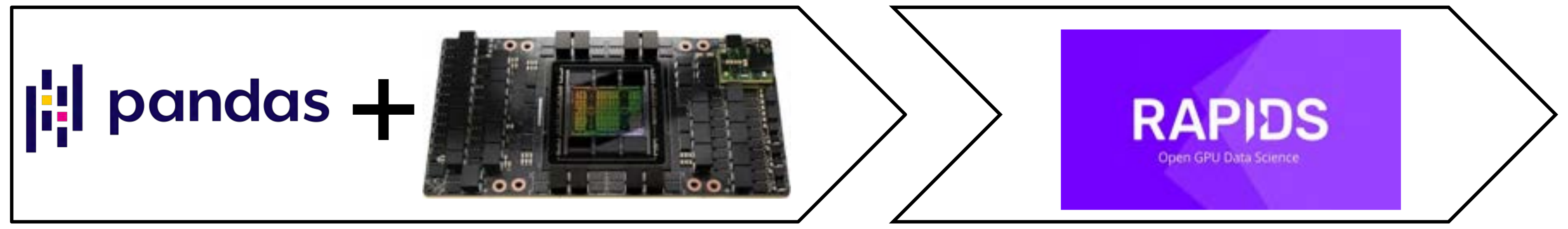
THE BURDEN OF DATA PROCESSING: EXTRACT, TRANSFORM, LOAD

*The Average Data Scientist Spends **90+%** of Their Time in ETL as Opposed to Training Models*

NVIDIA.

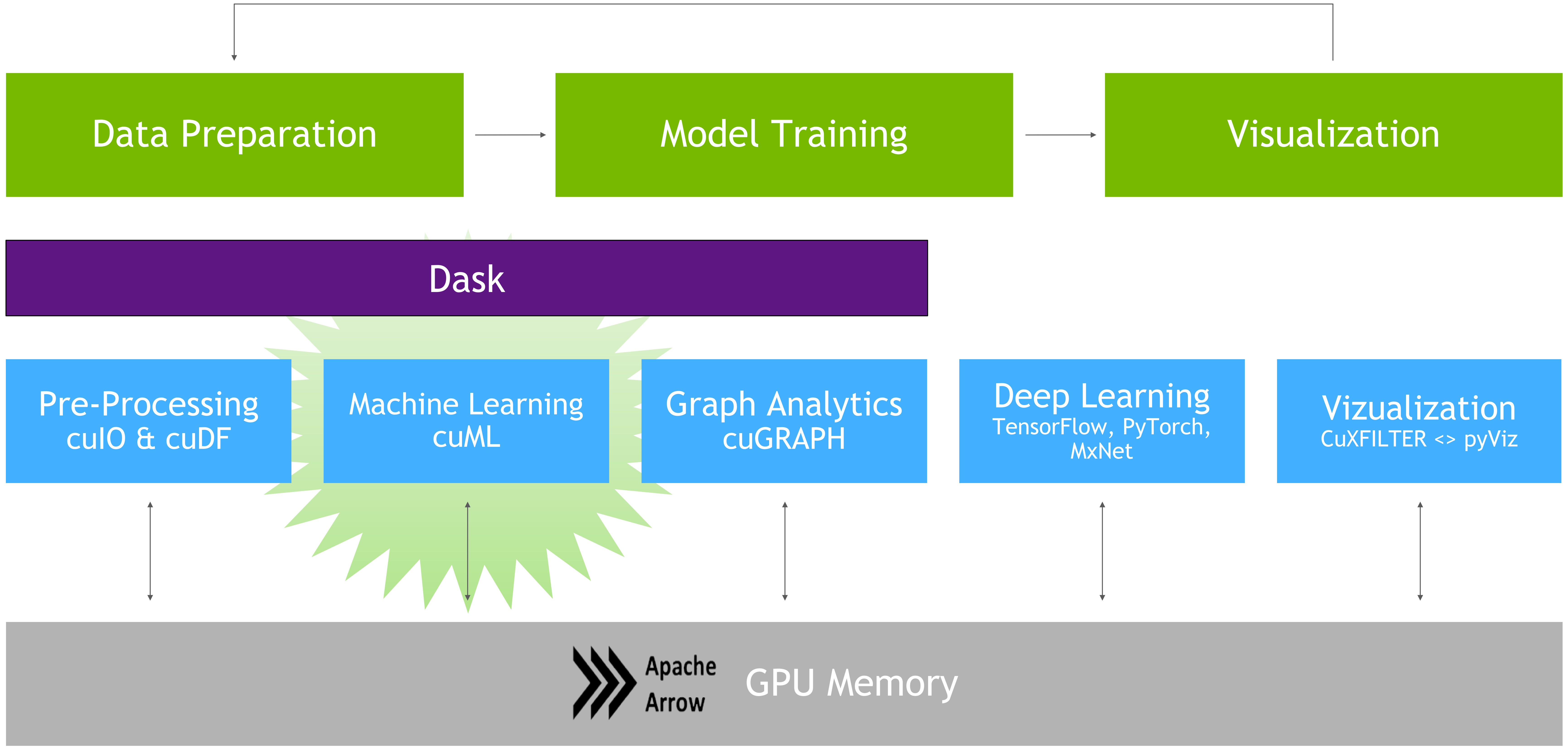
GPU-ACCELERATED PANDAS WITH CUDF

- Use RAPIDS CuDF to accelerate computationally expensive ETL operations
- Manipulate GPU DataFrames following the Pandas API
- Create GPU DataFrames from Numpy arrays, CuPy arrays, Pandas DataFrames, and PyArrow Tables
- Python interface to CUDA C++ library with additional functionality
- Available via pip and conda




```
import cudf as pd
import numpy as np
from time import time

import matplotlib.pyplot as plt
import seaborn as sns

%matplotlib inline

wine_set = pd.read_csv("data/winequality.csv")

wine_set.head(n=5)
wine_set.tail(n=5)
```

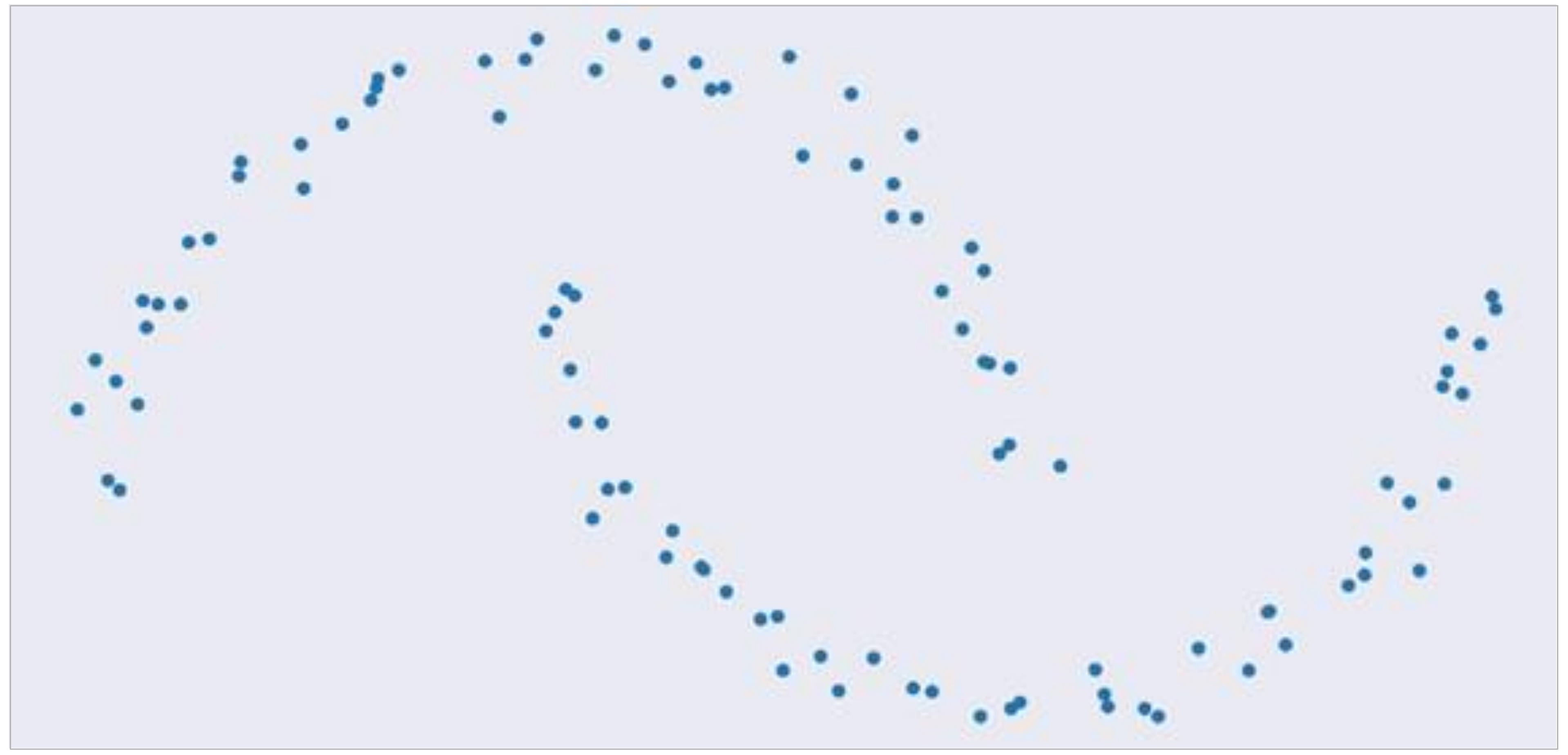
RAPIDS: GPU-ACCELERATED DATA SCIENCE
WITH API ALIGNMENT

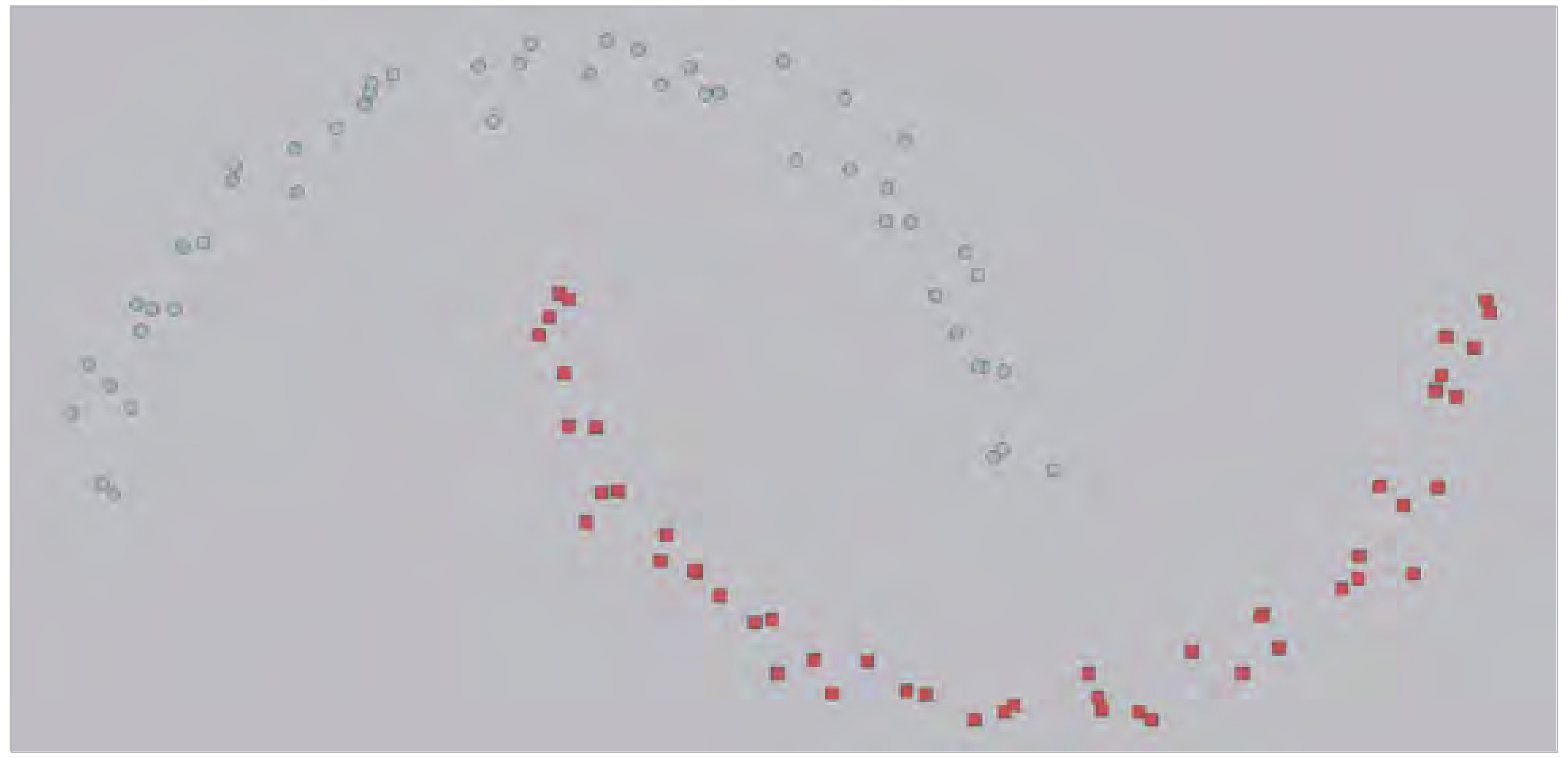


DATASET SIZES CONTINUE TO GROW

```
from sklearn.datasets import make_moons
import pandas

X, y = make_moons(n_samples=int(1e2),
                  noise=0.05, random_state=0)

X = pandas.DataFrame({'fea%d'%i: X[:, i]
             for i in range(X.shape[1])})
```

```
from sklearn.cluster import DBSCAN
dbscan = DBSCAN(eps = 0.3, min_samples = 5)

y_hat = dbscan.fit_predict(X)
```





DATASET SIZES CONTINUE TO GROW

```
from sklearn.datasets import make_moons
import cudf

X, y = make_moons(n_samples=int(1e2),
                  noise=0.05, random_state=0)

X = cudf.DataFrame({'fea%d'%i: X[:, i]
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```

```
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```
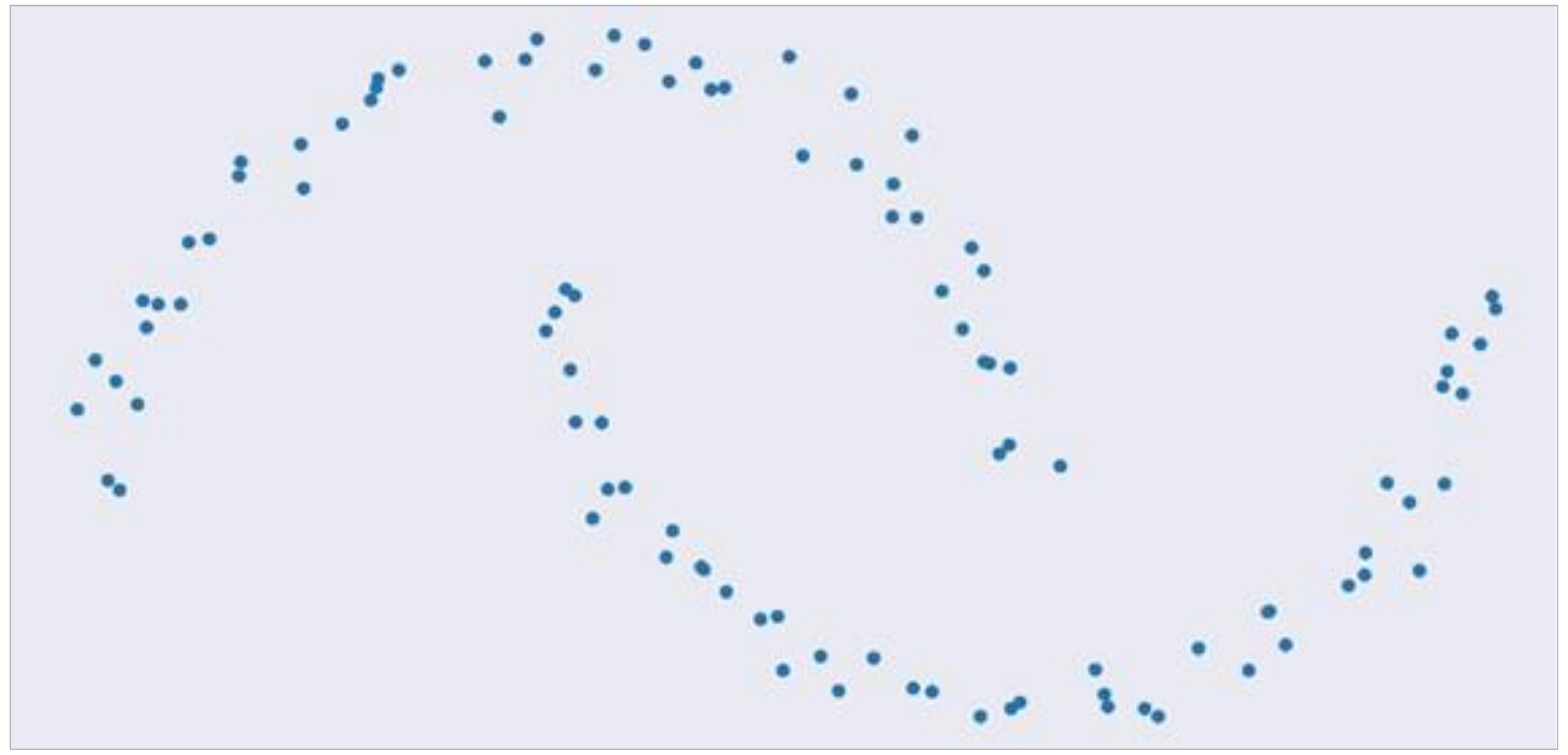
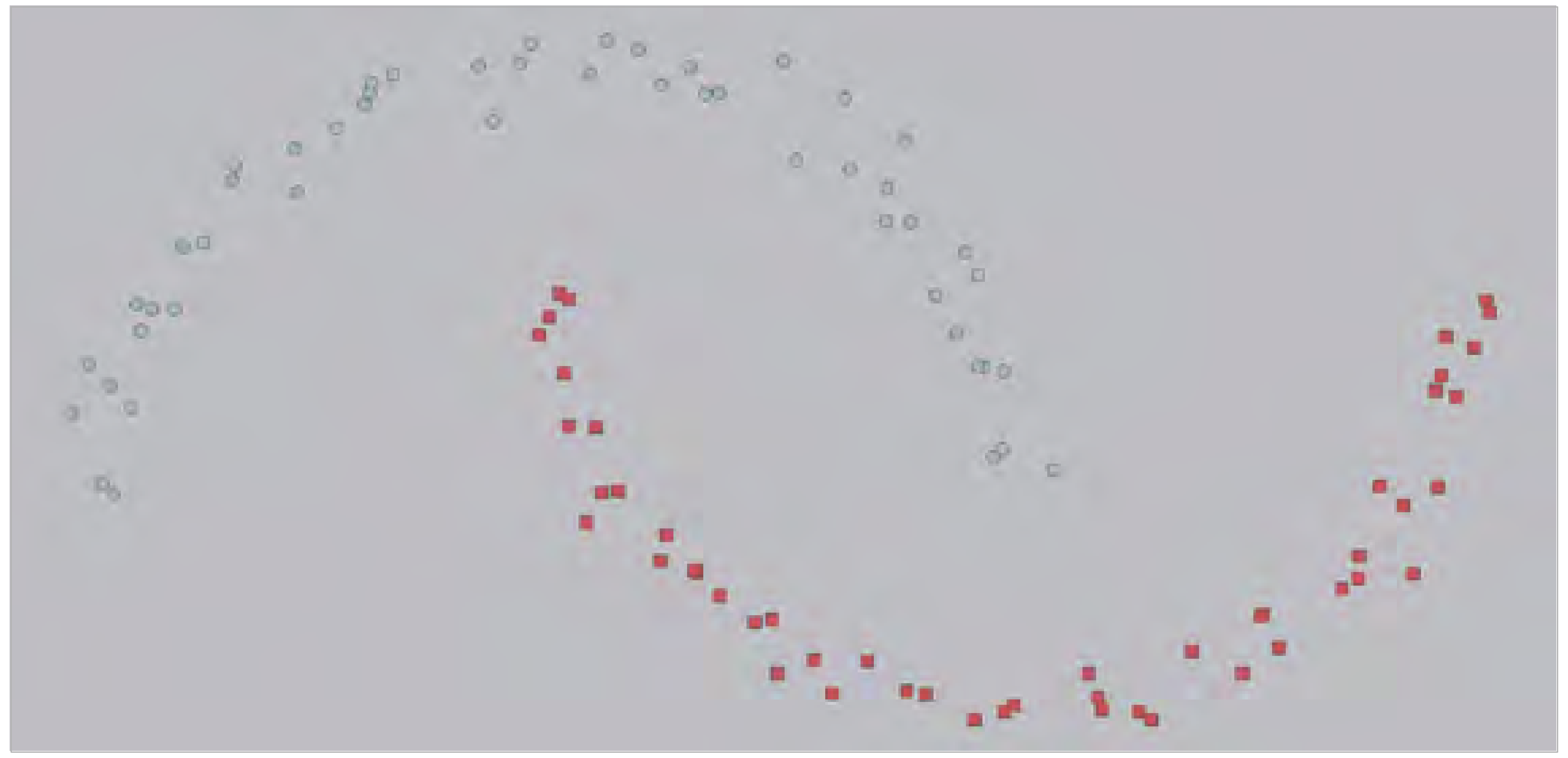
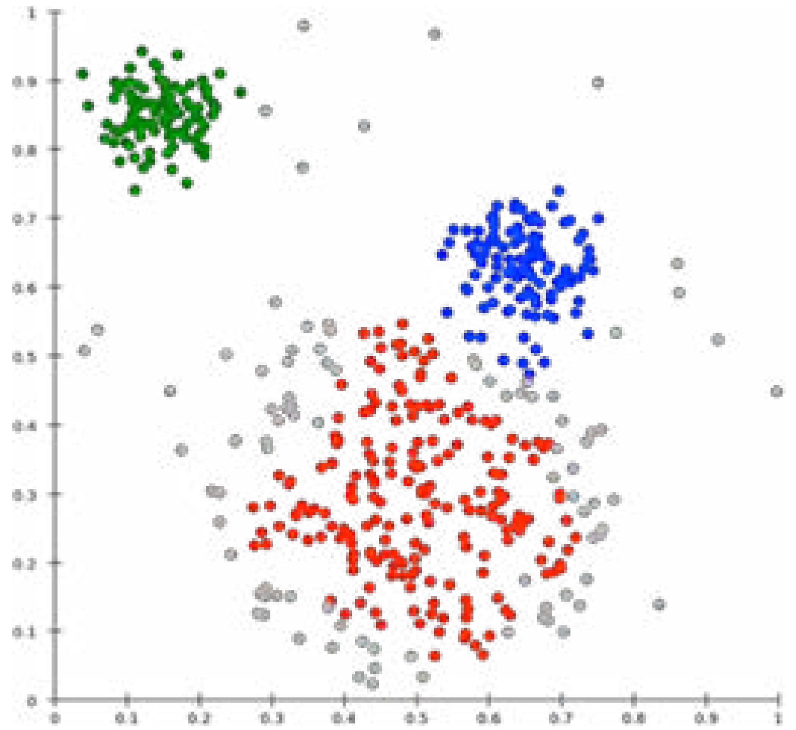





CUML ALGORITHMS

Classification / Regression

Decision Trees / **Random Forests**
Linear/Lasso/Ridge/**LARS**/ElasticNet Regression
Logistic Regression
K-Nearest Neighbors (**exact or approximate**)
Support Vector Machine Classification and Regression
Naive Bayes



Inference

Random Forest / GBDT Inference (FIL)

Preprocessing

Text vectorization (TF-IDF / Count)
Target Encoding
Cross-validation / splitting

Clustering Decomposition Dimensionality Reduction

K-Means
DBSCAN
Spectral Clustering
Principal Components (including iPCA)
Singular Value Decomposition
UMAP
Spectral Embedding T-SNE

Time Series

Holt-Winters
Seasonal ARIMA / Auto ARIMA

Hyper-parameter Tuning

Cross Validation

More to come!

MONAI Core

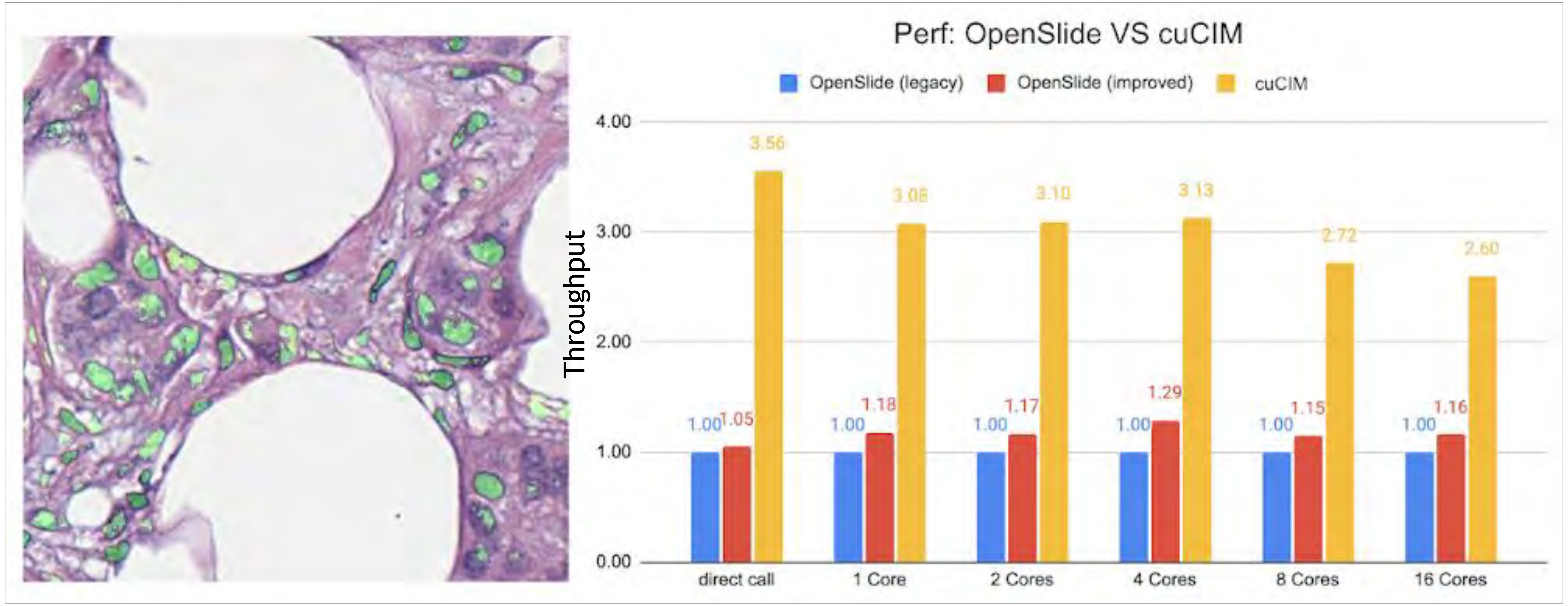
1. Medical imaging specifi

2. Superior performance

3. Friendly community

Optimize data loading

cuCIM - Whole Slide Imaging (digital pathology)



cuCIM - a library within [RAPIDS]()

MONAI Core

1. Medical imaging specif

2. Superior performance

3. Friendly community

Optimize GPU utilization

Do transforms on GPU

cuCIM -> common transforms in digital pathology

```
from monai.transforms import (
    Activations,
    AsDiscrete,
    CastToType,
    CastToTyped,
    Compose,
    CuCIM,
    GridSplitd,
    Lambdad,
    RandCuCIM,
    RandFlipd,
    RandRotate90d,
    RandZoomd,
    ScaleIntensityRanged,
    ToCupy,
    ToNumpyd,
    TorchVisiond,
    ToTensor,
    ToTensord,
)
```

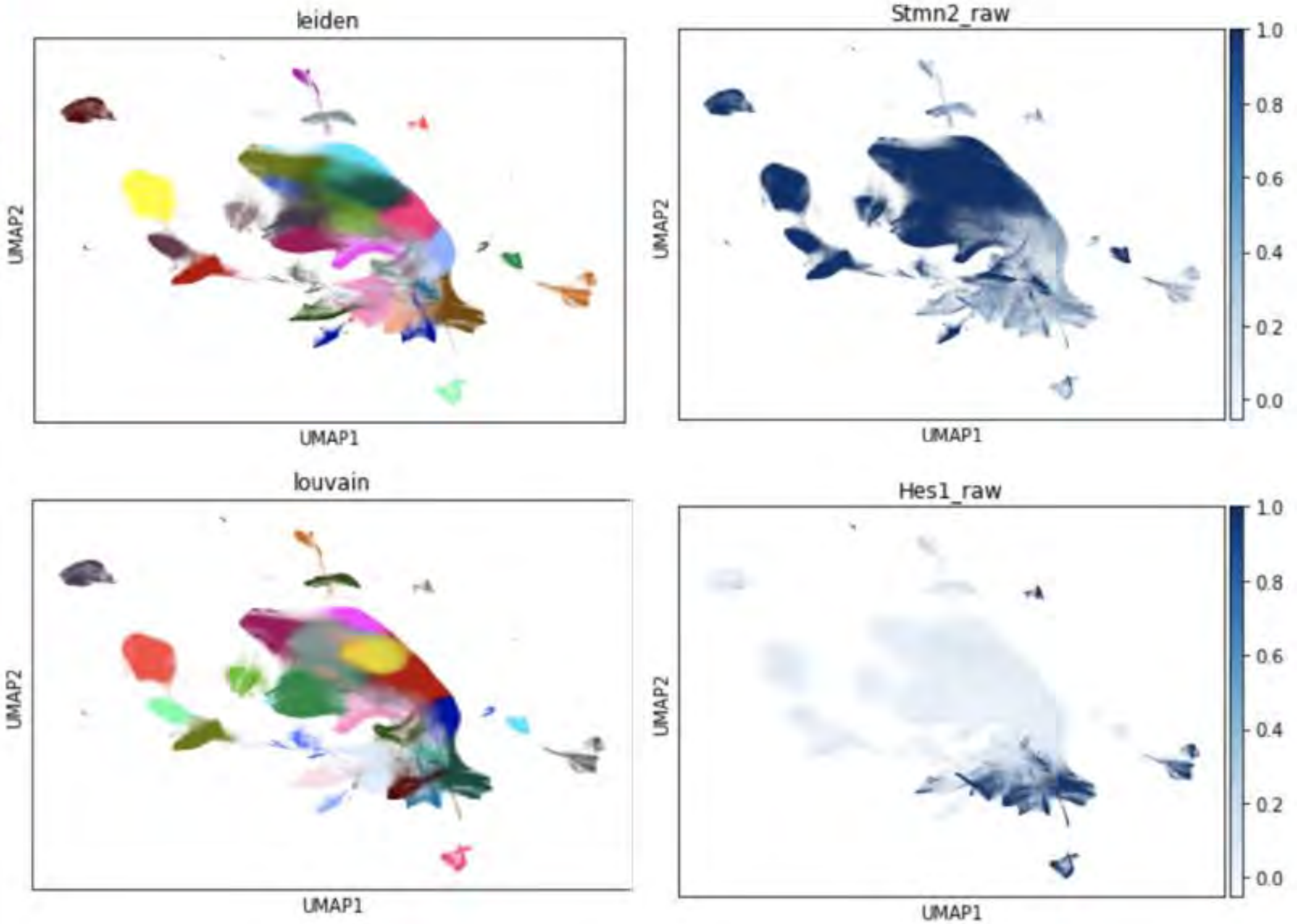
MONAI Core pathology tutorials

SINGLE-CELL RNA-SEQ ANALYSIS USING RAPIDS

GPU ANALYSIS OF 1 MILLION CELLS

From 3.5 hours to 8 minutes

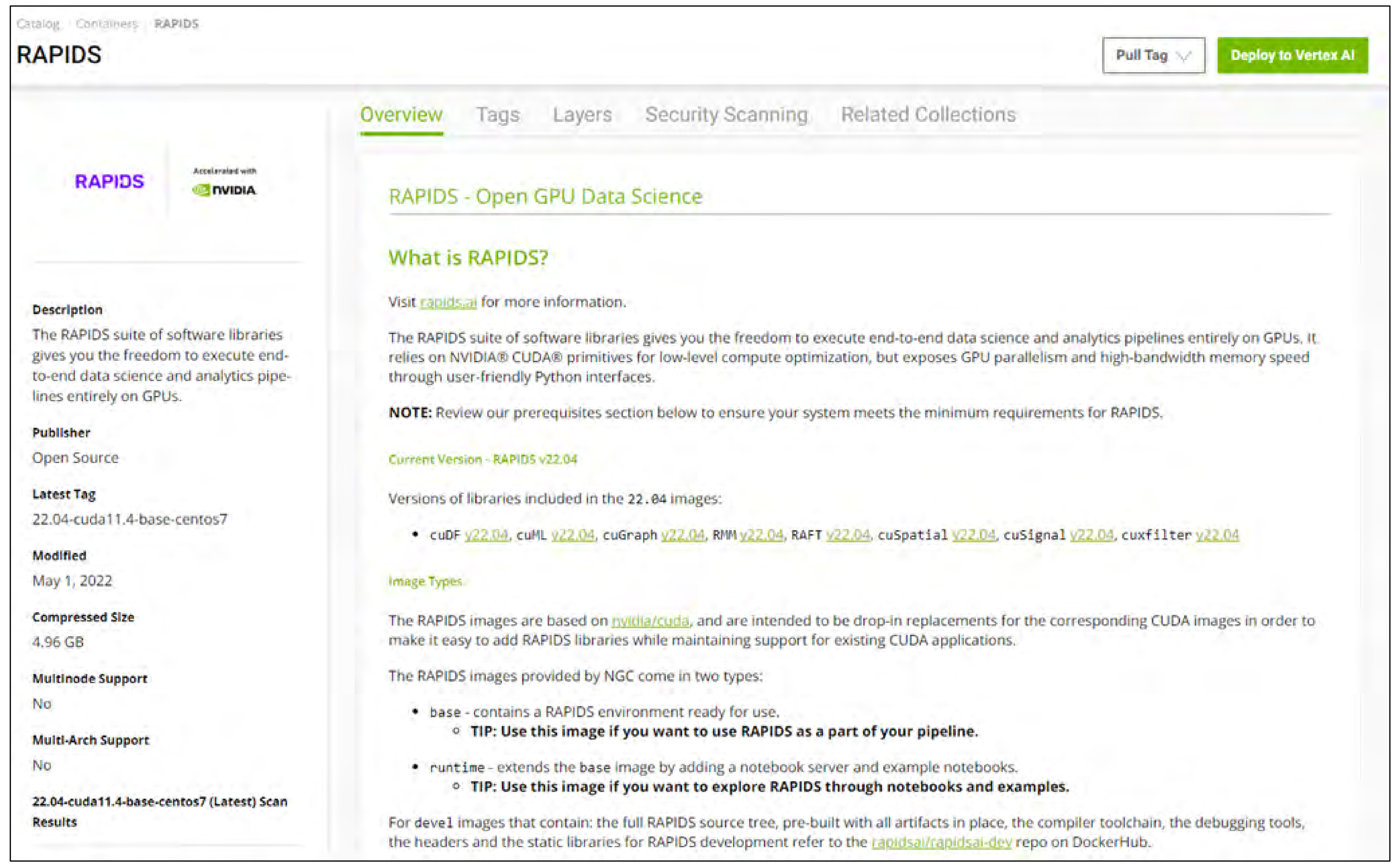
	CPU Runtime n1-highmem-32 32 vCPUs	GPU runtime a2-highgpu-1g Tesla A100 40GB GPU	GPU acceleration
Preprocessing	28m35s	3m21s	9x
PCA	29.2s	11.4s	2.6x
t-SNE	1hr23m10s	28s	178x
KNN	3m5s	46s	4x
UMAP	21m47s	13.4s	98x
k-means clustering	2m6s	1.9s	66x
Louvain clustering	15m5s	1.9s	476x
Leiden clustering	51m1s	1.4s	2186x
End-to-end runtime	3hr31m48s	8m22s	25x
End-to-end cost	$6.682	$0.553	



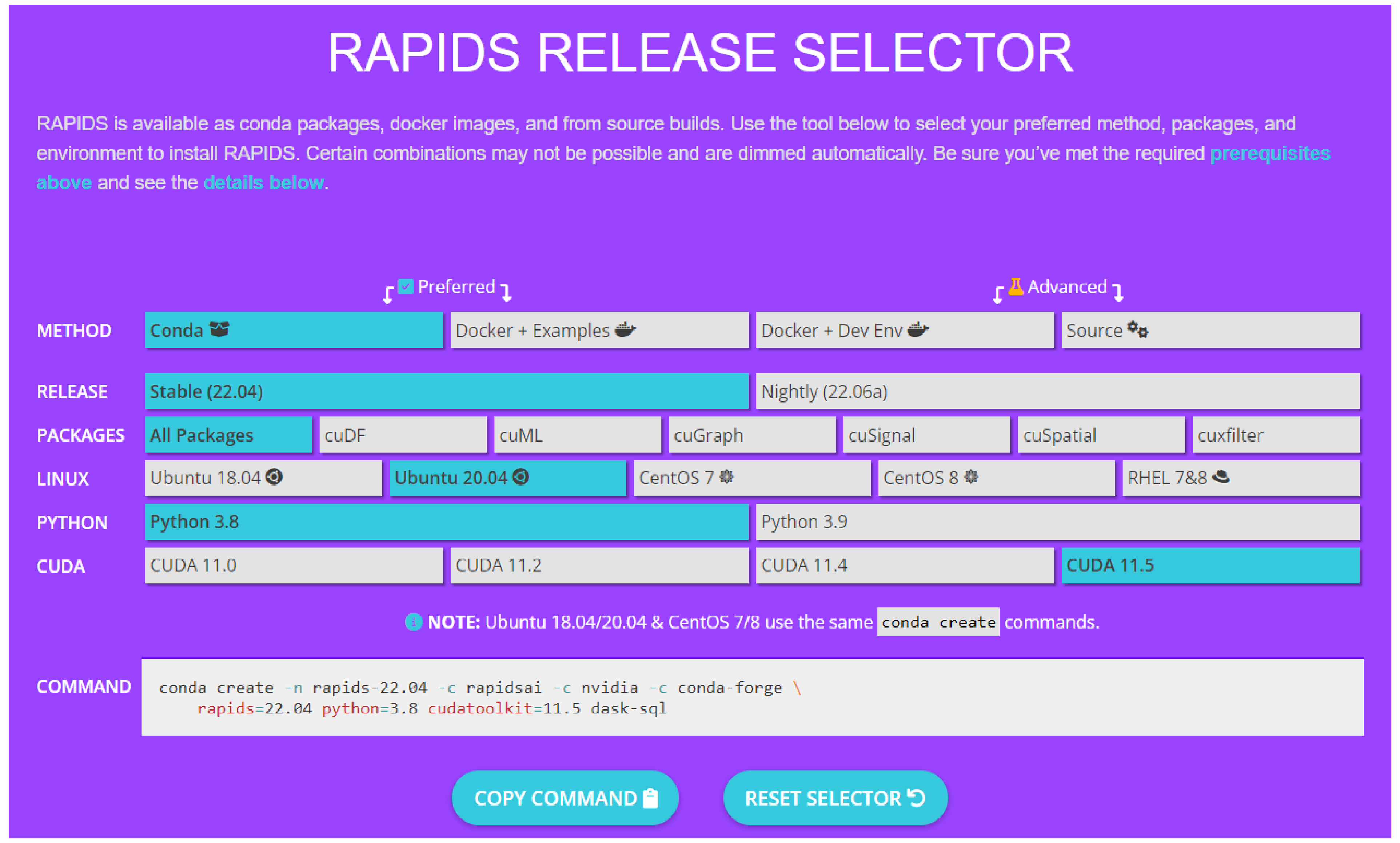
GTC session - [Deep Learning and Accelerated Computing for Single-Cell Genomic Data [S32511]]
Tutorial jupyter notebooks - https://github.com/NVIDIA-Genomics-Research/rapids-single-cell-examples

INSTALLATION

NVIDIA NGC
RAPIDS Container
https://ngc.nvidia.com



RAPIDS Release Selector
(conda, container, source)
https://rapids.ai



Available on Minerva!
Prebuilt RAPIDS modules

Custom GPU Kernels with ***Numba***

WHAT IS NUMBA? WHEN DO WE USE IT?

Lower-level CUDA kernel development without leaving Python

Just-in-time compiler

Numba is a JIT compiler for Python functions that you specify. Numba targets both CPU and GPU.

Opt-in

Numba only compiles functions you specify. You don't need to compile the full program

PyData ecosystem

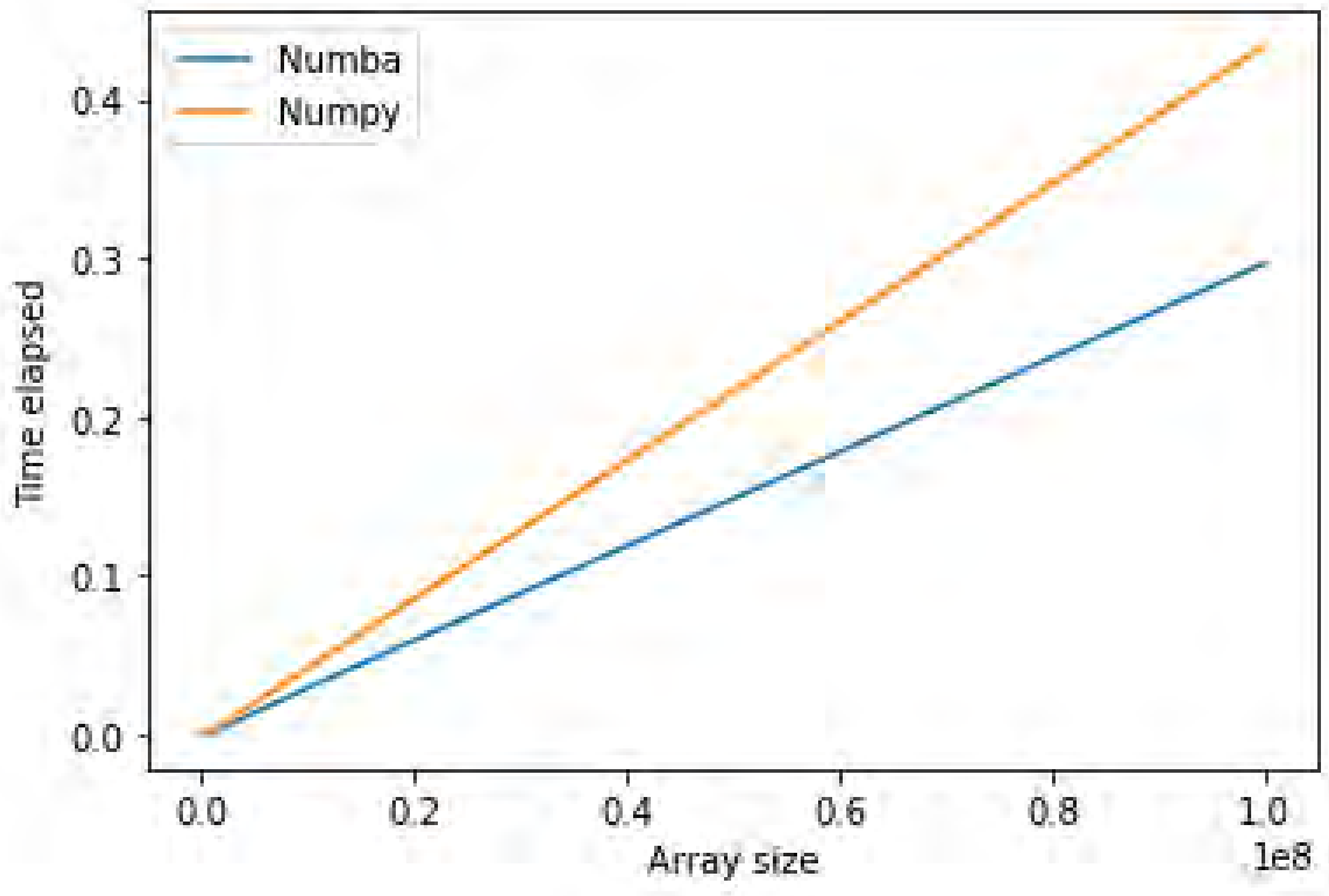
While not all functions in python can be compiled with Numba, the PyData ecosystem is well covered.

Numba provides the Python programmer a simple way to write customizable GPU accelerated code without needing CUDA C/C++

NUMBA VECTORIZE

NumPy ufuncs operate on data in element-by-element order, and Numba vectorize allows us to accelerate those types of operations

```
from numba import vectorize
import numpy as np
import time

@vectorize
def rel_diff(x, y):
    return 2 * (x - y) / (x + y)
```




```
size_list = [1000, 10000, 100000, 1000000, 10000000,
100000000]

numpy_times = []
numba_times = []

for size in size_list:
    x=np.random.randn(size).astype(np.float32) + 1
    y=np.random.randn(size).astype(np.float32) + 1.1

    # Run baseline Numpy implementation
    2 * (x - y) / (x + y)

    # Run our vectorized Numba function
    rel_diff(x, y)
```

With this "vectorized" Numba function we see improved performance as we increase our input size, making this solution ideal for large problem sizes.

NUMBA CUDA

Lower-level CUDA kernel development without leaving Python

BEFORE

```
import numba

@jit()
def vector_add(arr1, arr2):

    arr_size = arr1.shape[0]
    result = np.empty(size=(arr_size))

    for i in prange(arr_size):
        result[i] = arr1[i] + arr2[i]

    return result
```

AFTER

```
import numba

@cuda.jit()
def vector_add(arr1, arr2, result):

    startx = cuda.grid(1)
    stridex = cuda.gridsize(1)

    arr_size = arr1.shape[0]

    for i in range(startx, arr_size, stridex):
        result[i] = arr1[i] + arr2[i]
```

- Initialize data or copy data to GPU
- Lower-level support for custom CUDA kernels without C/C++
- JIT compiled kernels for fast execution
- Move data between DL frameworks, RAPIDS, and Numba

Numba

NVIDIA

SUMMARY

Function	CPU	GPU/RAPIDS
Data handling	pandas	cuDF
Machine learning	scikit-learn	cuML
Function	**CPU**	**GPU**
Numerical Computing	NumPy	CuPy
JIT Kernels	Numba	Numba

NVIDIA DEEP LEARNING INSTITUTE

Self-paced courses

Instructor-led workshops

RAPIDS

FUNDAMENTALS ★ NEW

Accelerating End-to-End Data Science Workflows

6 hours | $90 | Rapids, cuDF, cuML, cuGraph, Apache Arrow

Certificate Available

View Course ›

Numba

FUNDAMENTALS ★ POPULAR

Fundamentals of Accelerated Computing with CUDA Python

8 hours | $90 | CUDA , Python, Numba, NumPy

Certificate Available

View Course ›

SESSIONS AT PREVIOUS GTC

SEARCH ON NVIDIA ON DEMAND

If you found this content useful, please consider tuning into these sessions too:

- GPU-accelerated Feature Extraction and Image Similarity in Pure Python [S41661]
- Enabling Python User-Defined Functions in Accelerated Applications with Numba [S41056]
- No More Porting: Coding for GPUs with Standard C++, Fortran, and Python [S41496]
- Shifting through the Gears of GPU Programming: Understanding Performance and Portability Trade-offs [S41620]
- Evaluating Your Options for Accelerated Numerical Computing in Pure Python

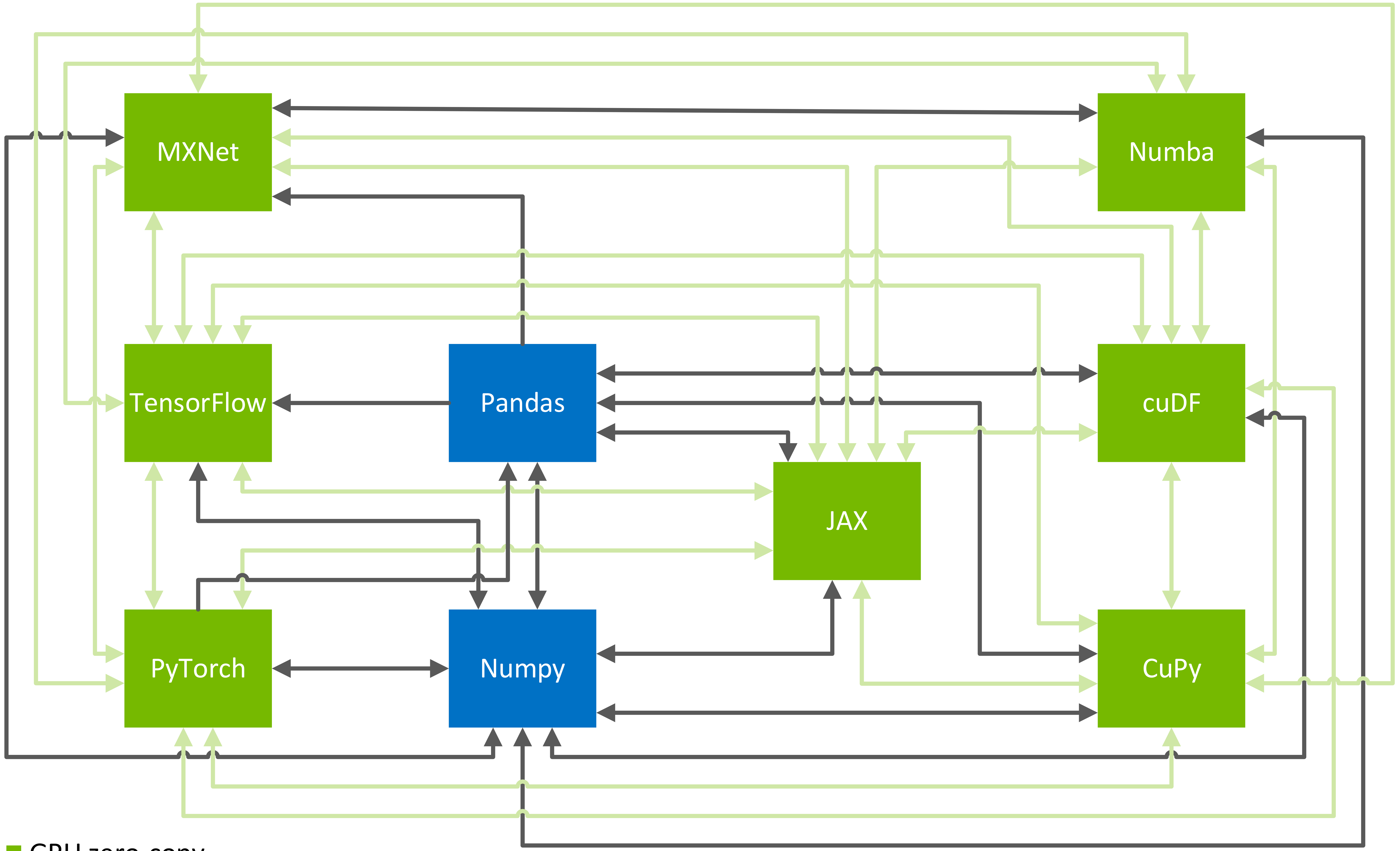
ML FRAMEWORKS INTEROPERABILITY

FRAMEWORK INTEROPERABILITY

When a single framework is not enough

MIX AND MATCH WORKFLOWS

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



GPU zero-copy
Copy & convert

MITIGATE DATA CONVERSION BOTTLENECK

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.fromDlpack(src.to_dlpack())

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.utils.dlpack.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

DLPACK & CUDA ARRAY INTERFACE

	DLPack		NumPy Array Interface	CUDA Array Interface
	CPU	GPU	CPU	GPU
Pandas	✗	n/a	✓	n/a
NumPy	✗	n/a	✓	n/a
cuDF	n/a	✓	n/a	✓
CuPy	n/a	✓	n/a	✓
JAX	✓	✓	✓	✓
Numba	✗	✗	✓	✓
TensorFlow	✓	✓	✓	✗
PyTorch	✓	✓	✓	✓
MXNet	✓	✓	✓	✗

CUDA Array Interface adopted by:

- Numba
- CuPy
- PyTorch
- PyArrow
- mpi4py
- ArrayViews
- JAX
- PyCUDA
- DALI
- RAPIDS
  - cuDF
  - cuML
  - cuSignal
  - RMM

Summary

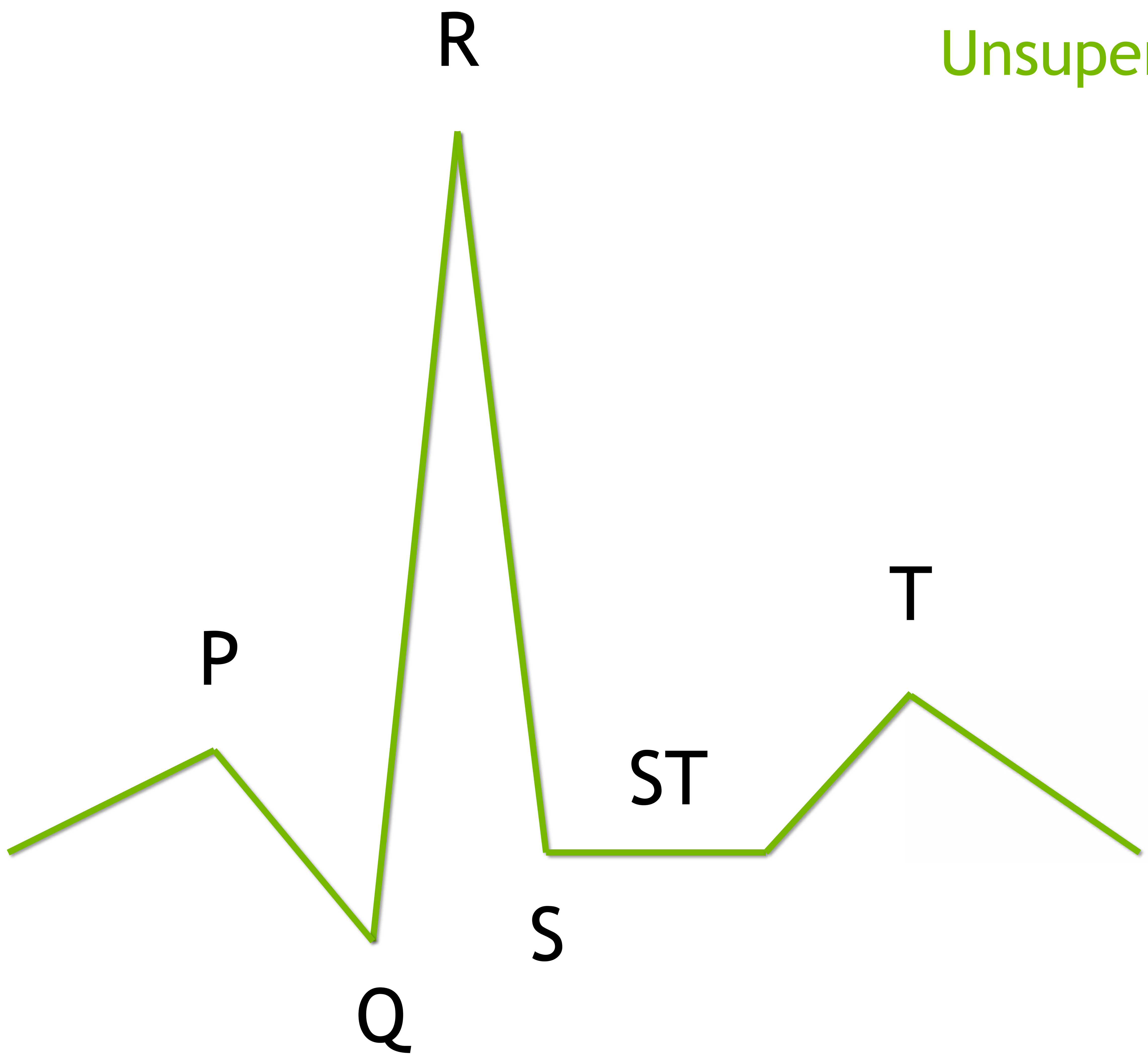
Complex workloads make use of multiple libraries.

Interoperability via DLPack and CUDA Array Interface (CAI).

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

ZERO-COPY END-TO-END PIPELINE

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 the latent space & generated heartbeats.

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

END-TO-END PIPELINE

Parse ECG from CSV

RAPIDS cuDF → CuPy → Numba → PyTorch → RAPIDS cuxfilter

```
data
1.38630000000000088e+00
1.73490000000000109e+00
2.18650000000000110e+00
2.74719999999999864e+00
3.75190000000000013e+00
5.02310000000000342e+00
6.47850000000000369e+00
8.00259999999999270e+00
9.49210000000000648e+00
1.08254000000000013e+01
1.18676999999999925e+01
1.24868000000000057e+01
1.25873000000000082e+01
1.21428999999999914e+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)
```

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

RAPIDS

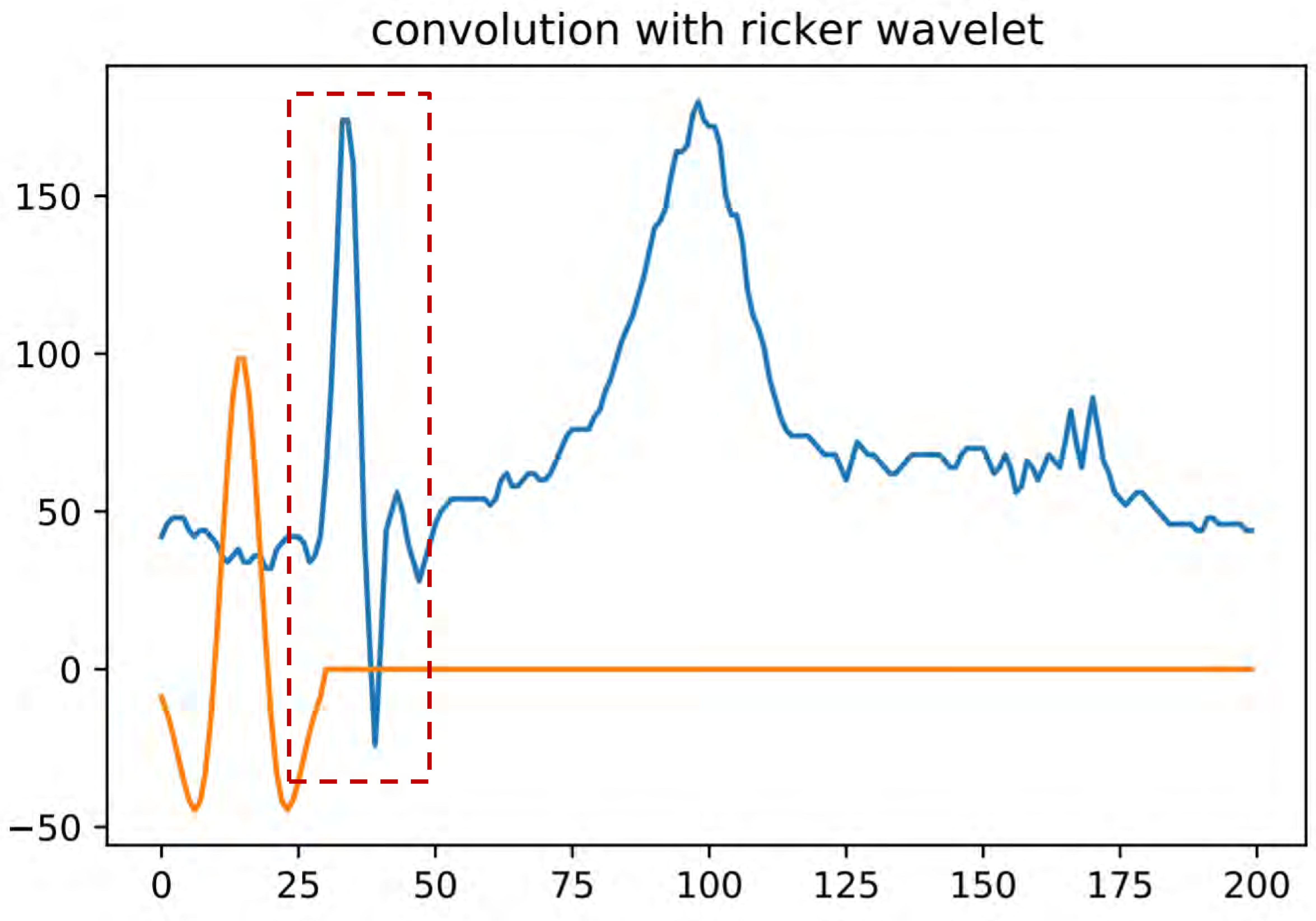
GPU

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

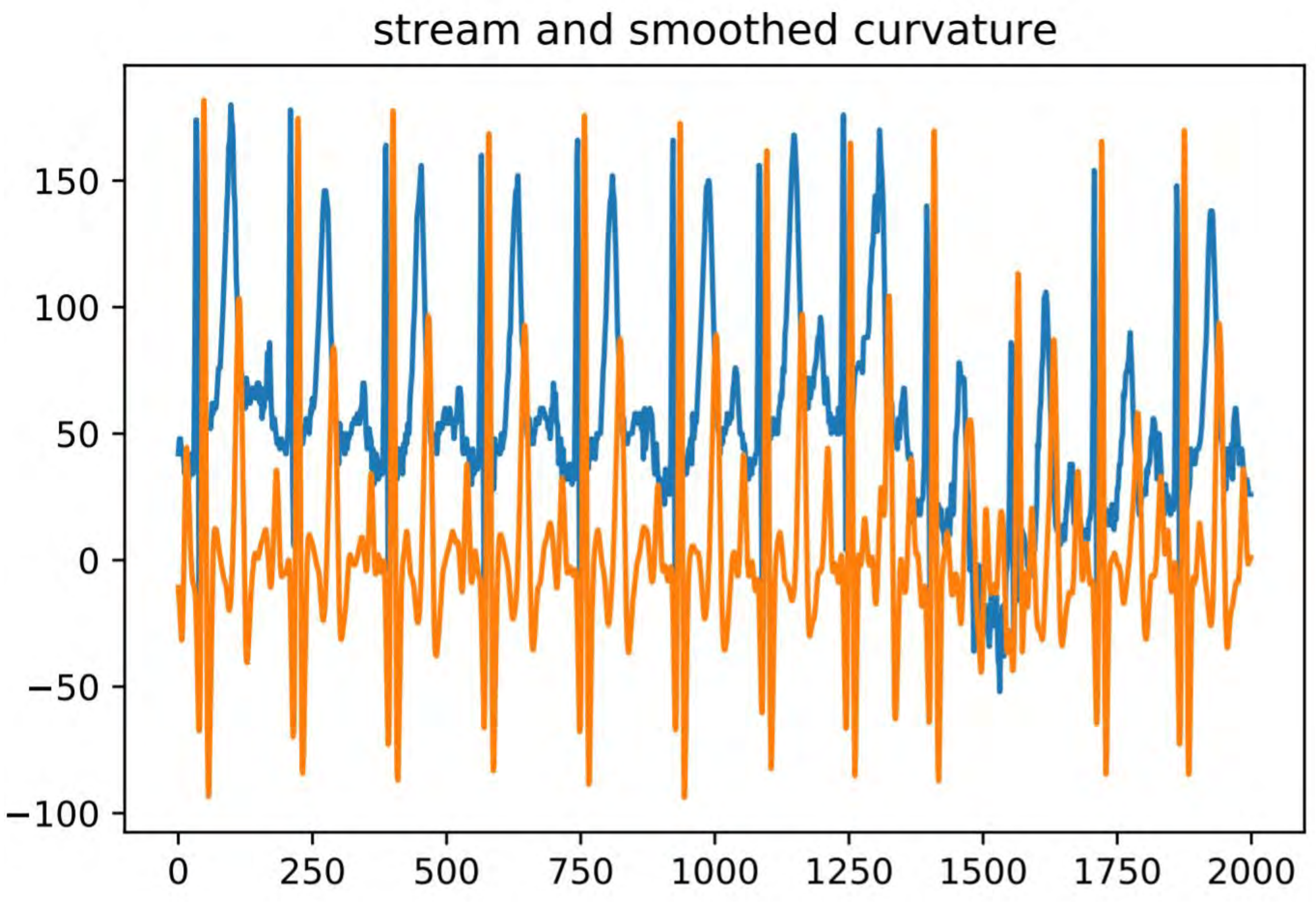
END-TO-END PIPELINE

Band-Pass Filter

RAPIDS cuDF → CuPy → Numba → PyTorch → RAPIDS cuxfilter



FFT based convolution

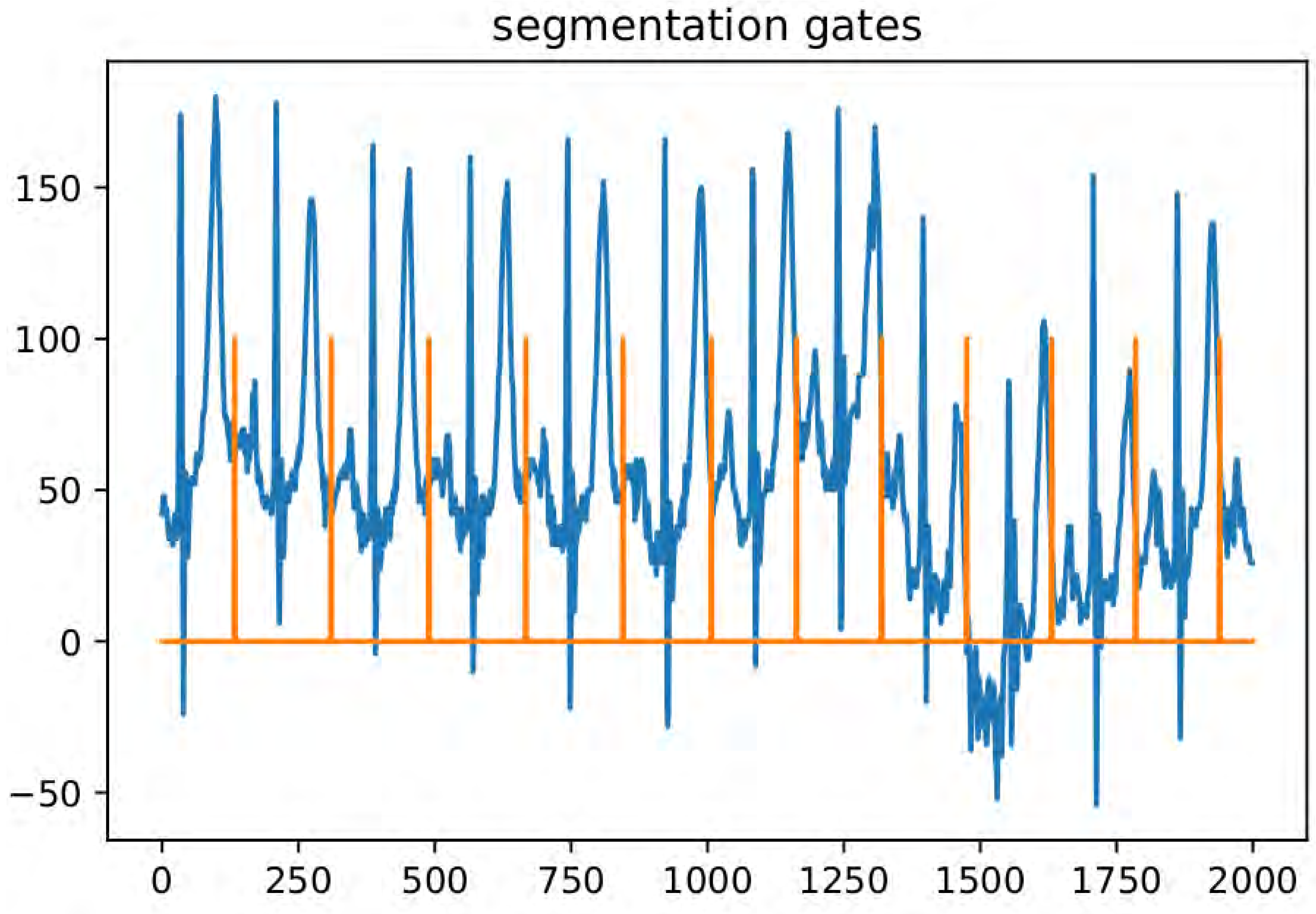


QRS Complex Detection

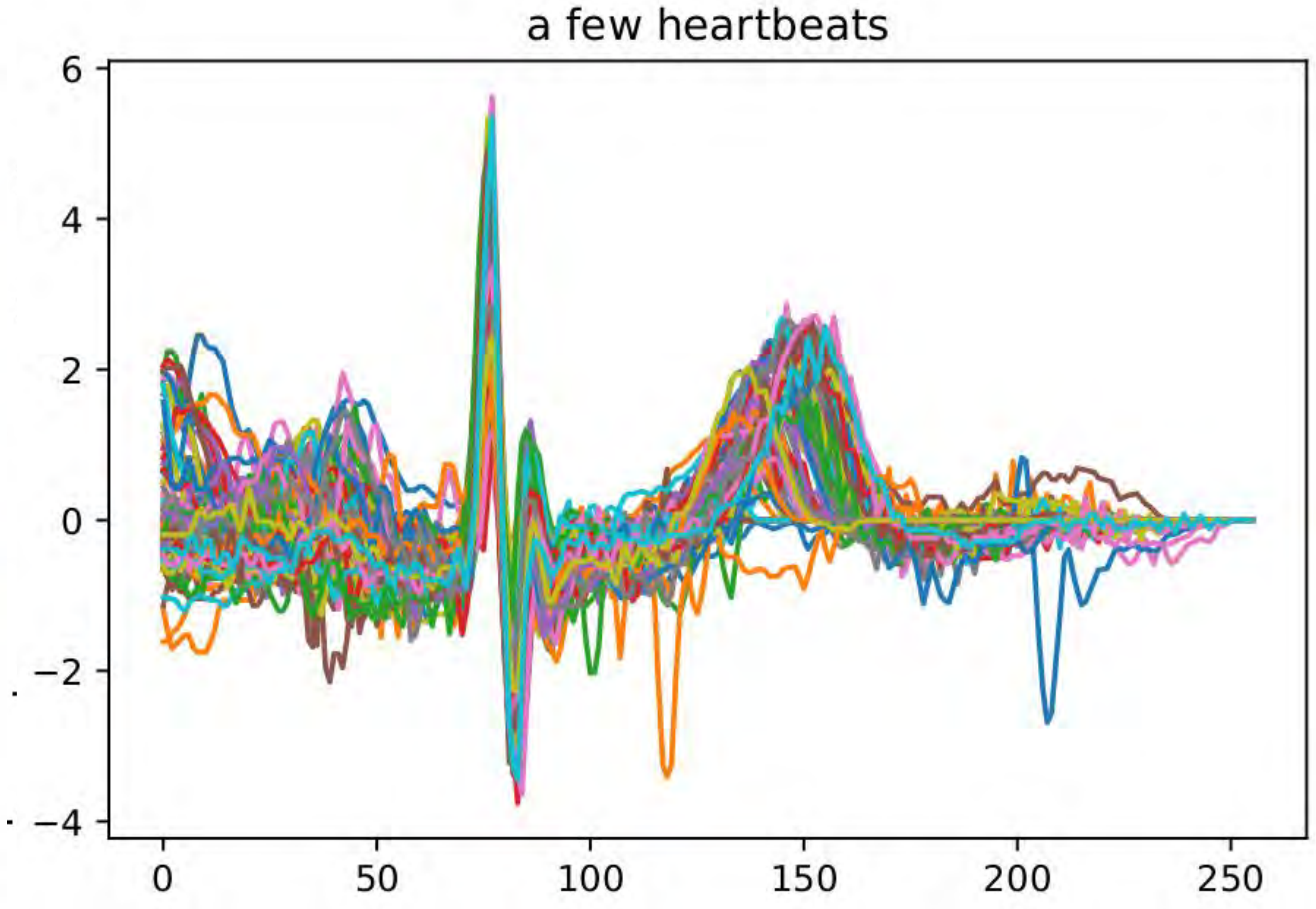
END-TO-END PIPELINE

Non-trivial Preprocessing

RAPIDS cuDF → CuPy → Numba → PyTorch → RAPIDS cuxfilter



1D non-max suppression

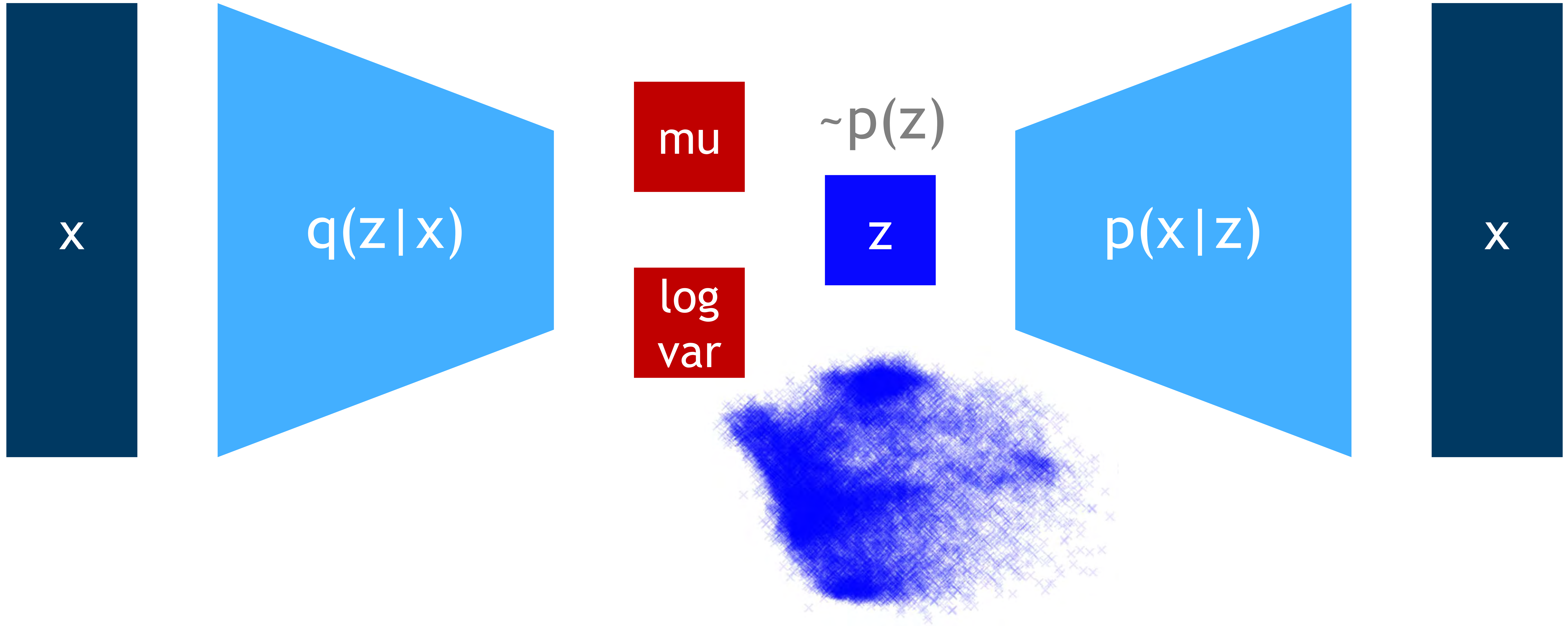


normalization and embedding

END-TO-END PIPELINE

Variational Autoencoder (VAE)

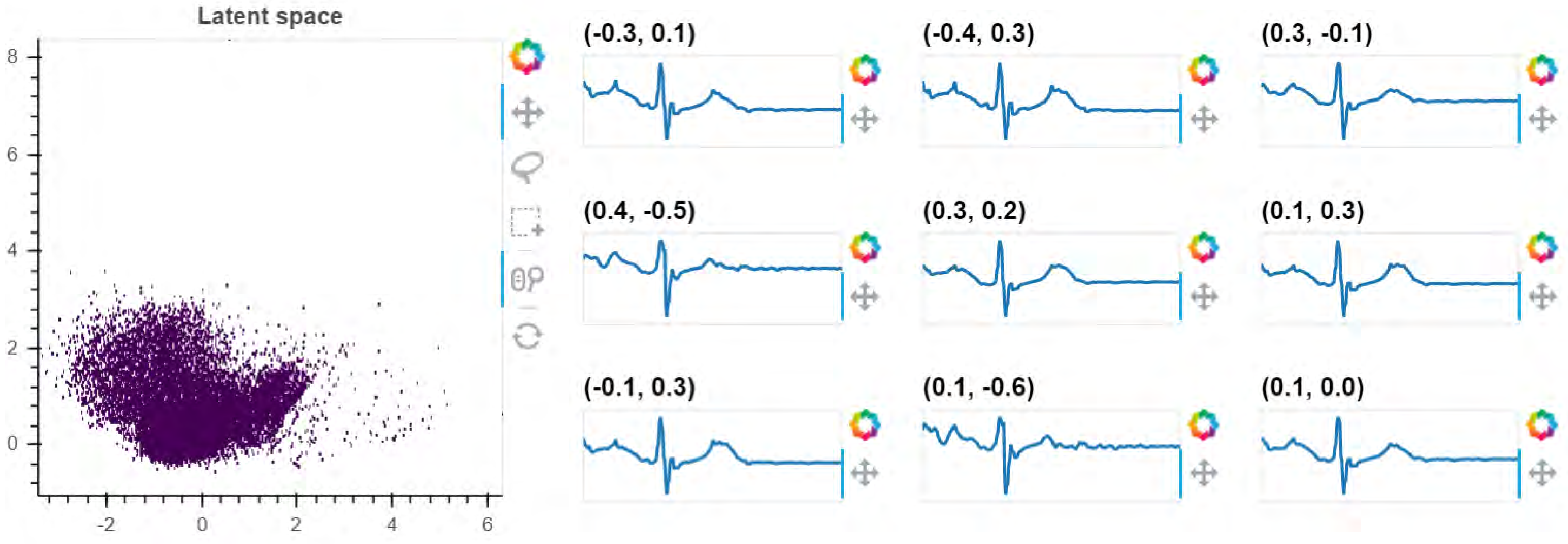
RAPIDS cuDF → CuPy → Numba → PyTorch → RAPIDS cuxfilter



END-TO-END PIPELINE

Visualization

RAPIDS cuDF → CuPy → Numba → PyTorch → RAPIDS cuxfilter



MIX AND MATCH WORKFLOWS

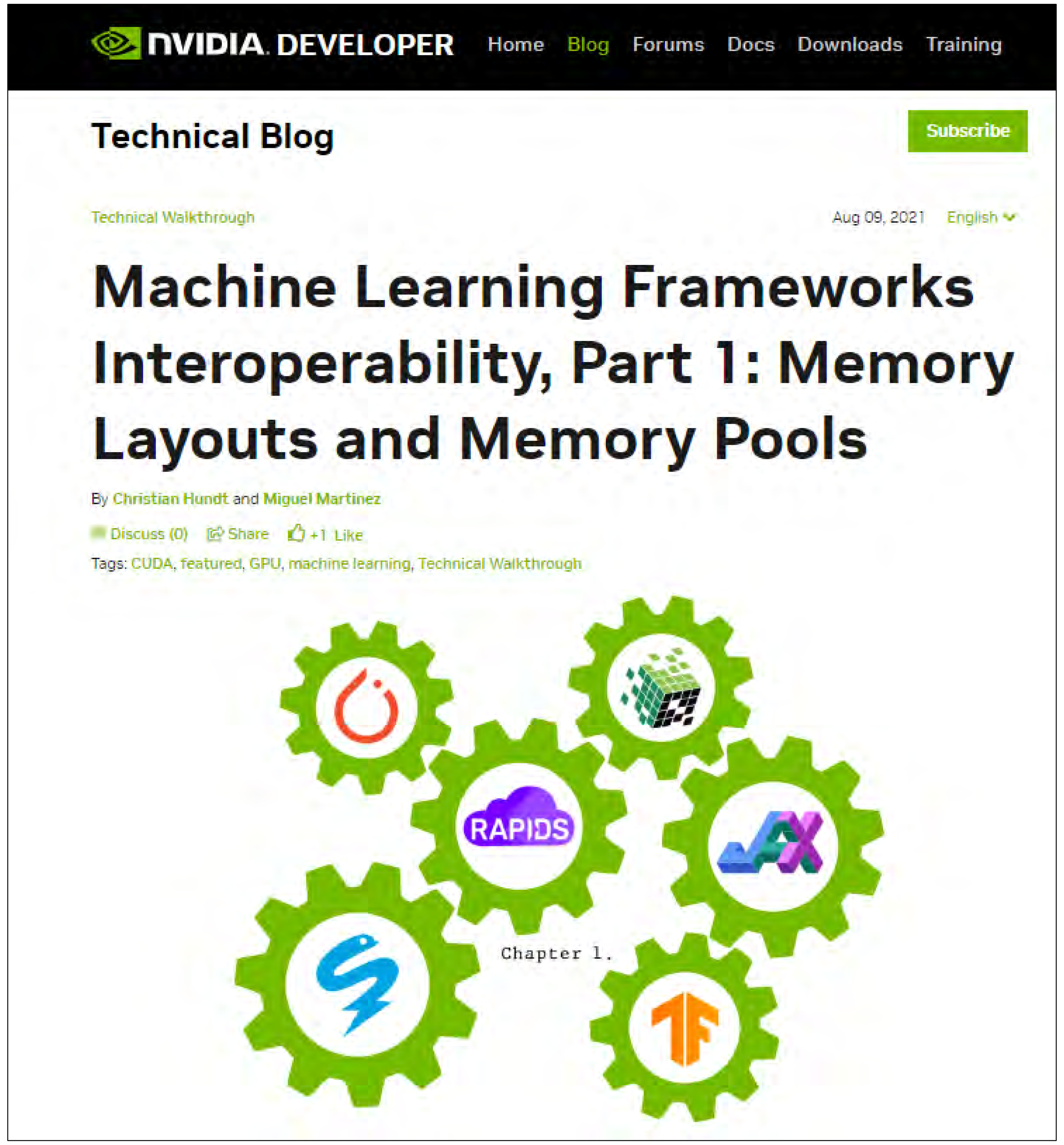
Endless possibilities!

RAPIDS cuDF → CuPy → Numba → PyTorch → RAPIDS cuxfilter

RAPIDS cuDF	JAX	Numba	TensorFlow	RAPIDS cuxfilter
Pandas	CuPy	PyCuda	PyTorch	Bokeh
RAPIDS cuDF	Numpy	Numba	MXNet	Plotly Dash
Pandas	Numpy	Numba	Chainer	Datashader

And many others!

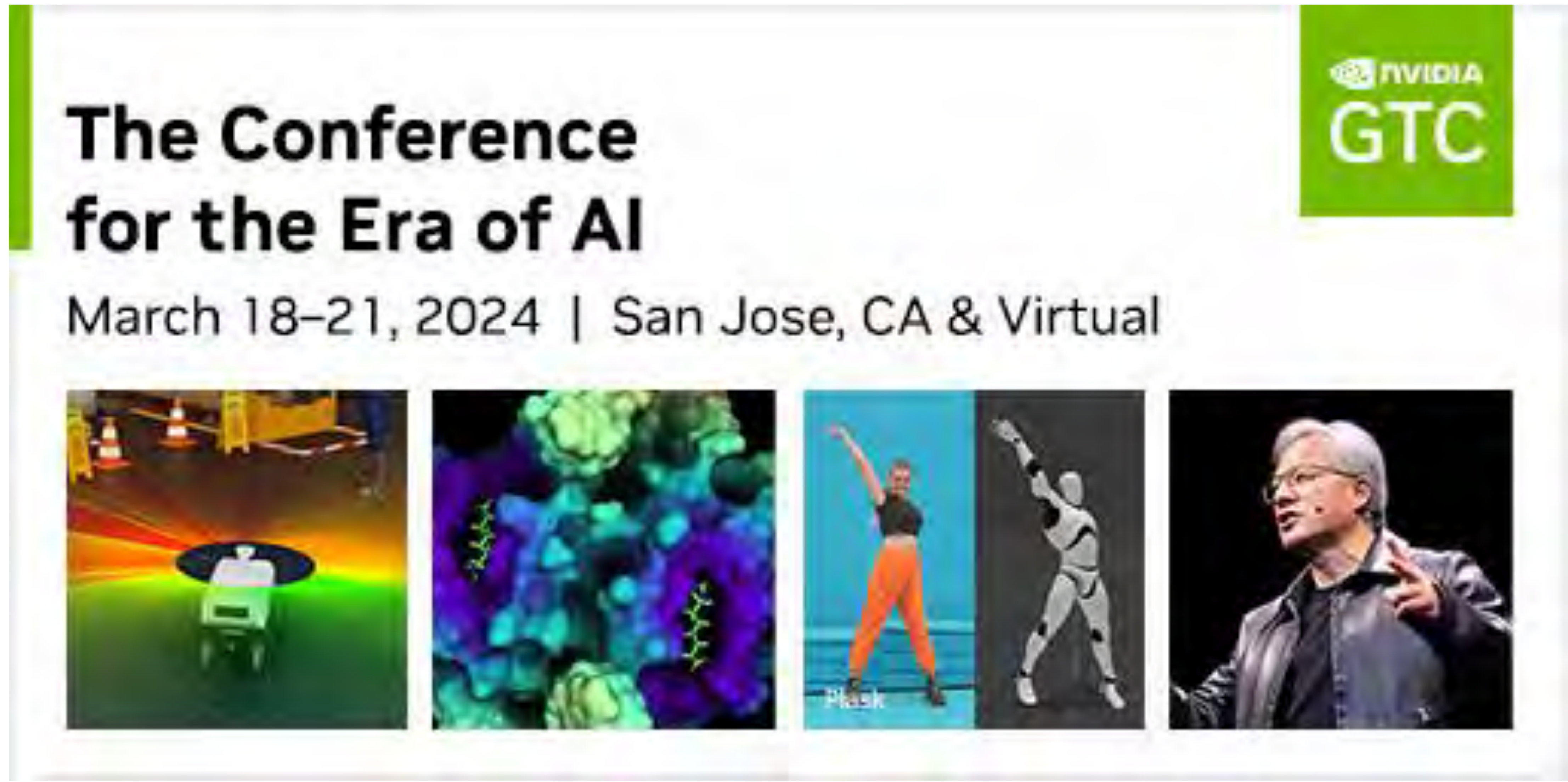
ADDITIONAL RESOURCE



[Tech blog & GTC session]()

GTC SESSIONS ON DATA SCIENCE

NVIDIA On Demand - Latest Data Science playlist



Q & A

HUIWEN JU - HJU@NVIDIA.COM - SOLUTIONS ARCHITECT, HIGHER EDUCATION & RESEARCH

4/17/2024 @ MOUNT SINAI