RAPIDS

Distributed Multi-GPU Computing with Dask, CuPy and RAPIDS

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Outline

- Interoperability / Flexibility
- Acceleration (Scaling Up)
- Distribution (Scaling Out)

Clustering
Code Example

```
from sklearn.datasets import make_moons
import pandas

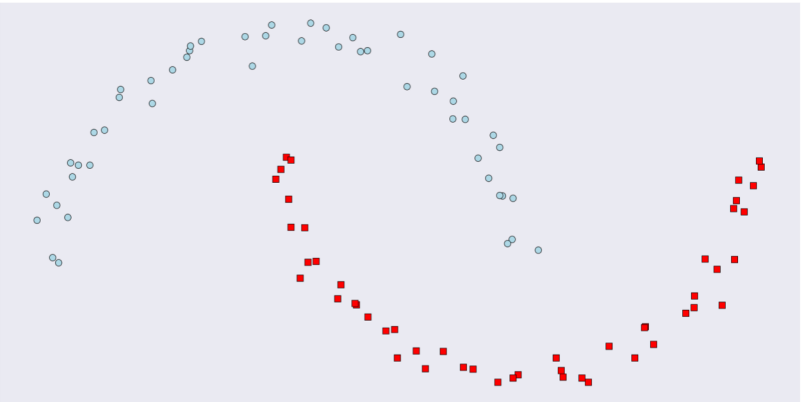
X, y = make_moons(n_samples=int(1e2),
                  noise=0.05, random_state=0)

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)

dbscan.fit(X)

y_hat = dbscan.predict(X)
```



GPU-Accelerated Clustering

Code Example

```
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]
                      for i in range(X.shape[1])})
```

```
from cuml              import DBSCAN
dbscan = DBSCAN(eps = 0.3, min_samples = 5)

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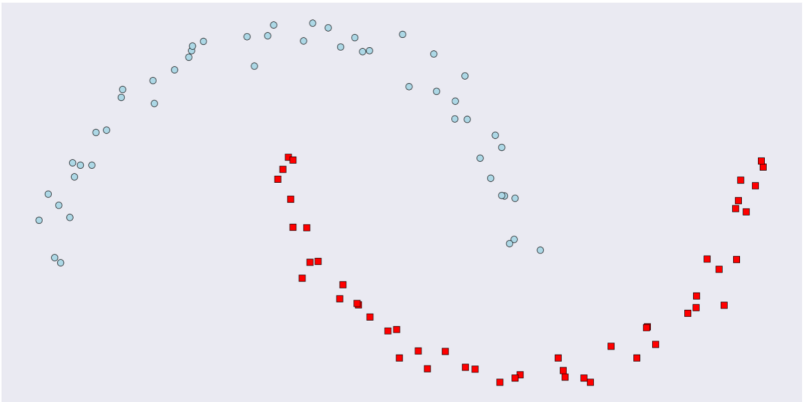


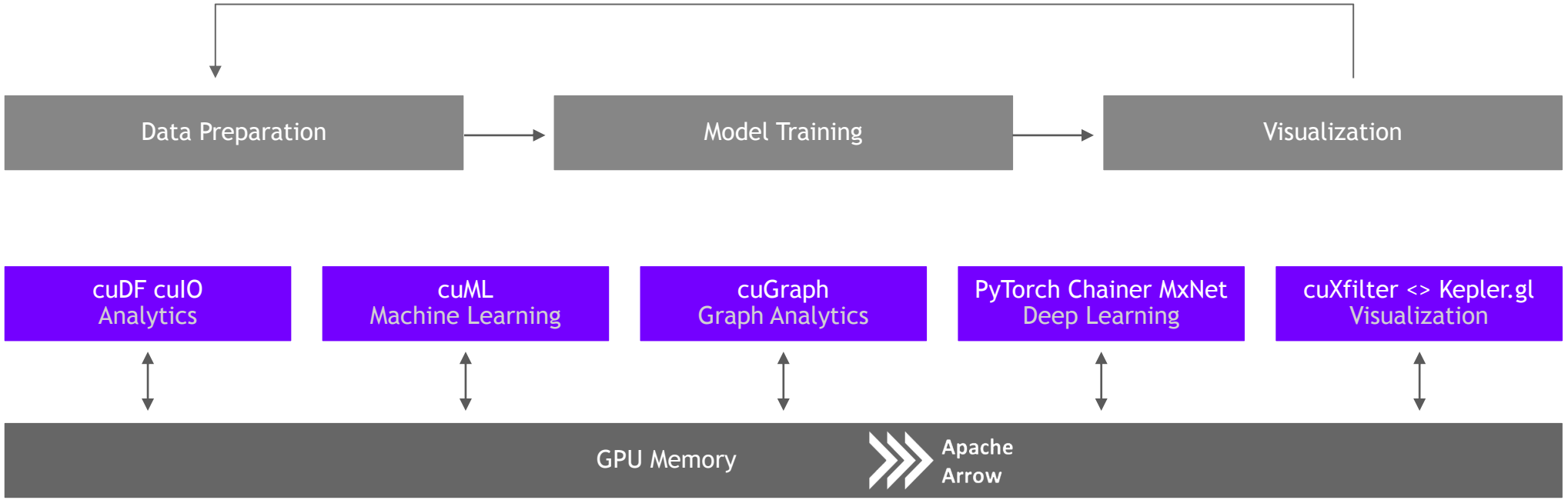
What is RAPIDS?

New GPU-Accelerated Data Science Pipeline

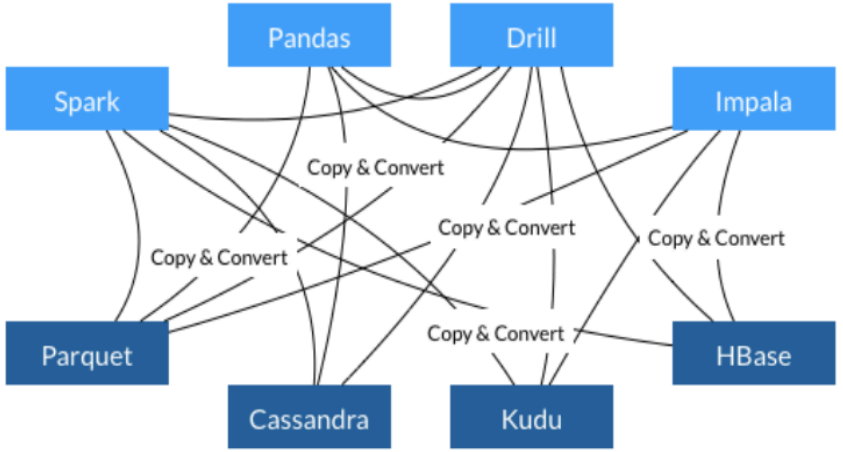
- Suite of open source, end-to-end data science tools
- Built on CUDA
- Unifying framework for GPU data science
- Pandas-like API for data preparation
- Scikit-learn-like API for machine learning

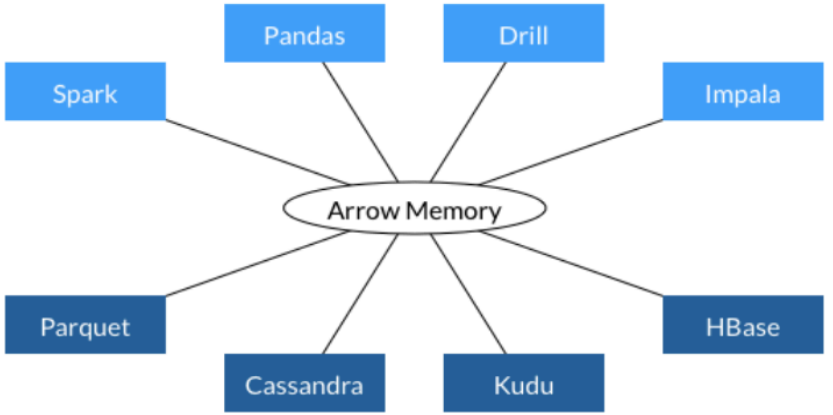
RAPIDS

End-to-End GPU-Accelerated Data Science



Learning from Apache Arrow





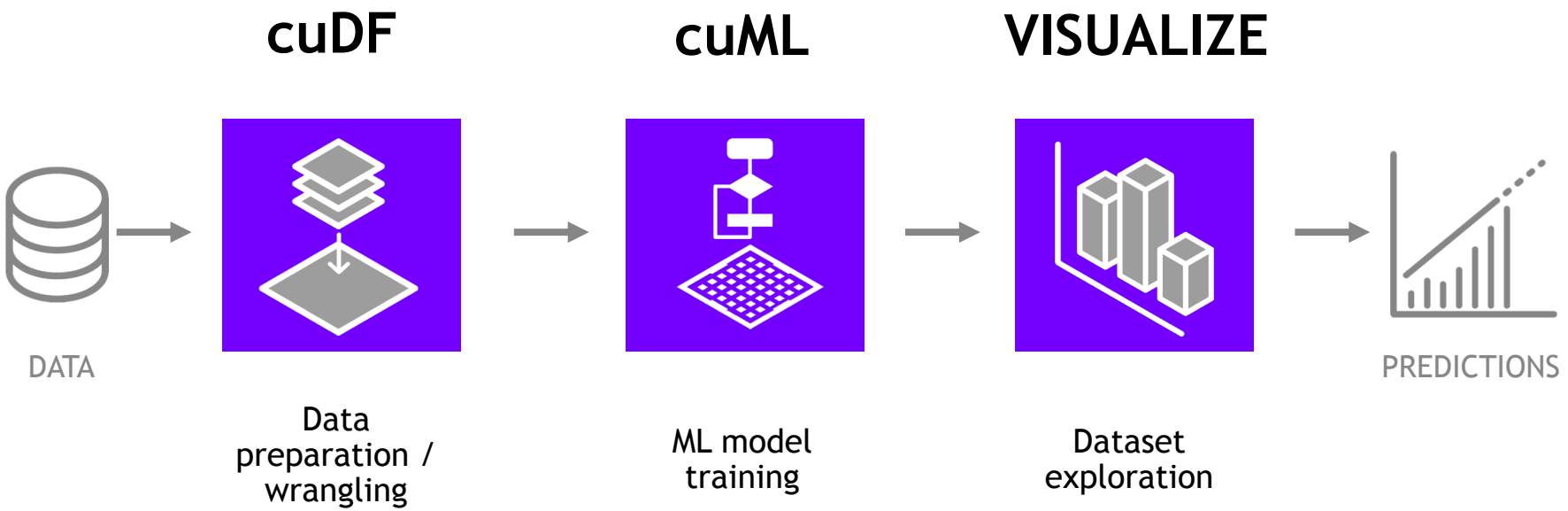
- Each system has its own internal memory format
- 70-80% computation wasted on serialization and deserialization
- Similar functionality implemented in multiple projects

- All systems utilize the same memory format
- No overhead for cross-system communication
- Projects can share functionality (eg, Parquet-to-Arrow reader)

From Apache Arrow Home Page - https://arrow.apache.org/

Data Science Workflow with RAPIDS

Open Source, GPU-Accelerated ML Built on CUDA



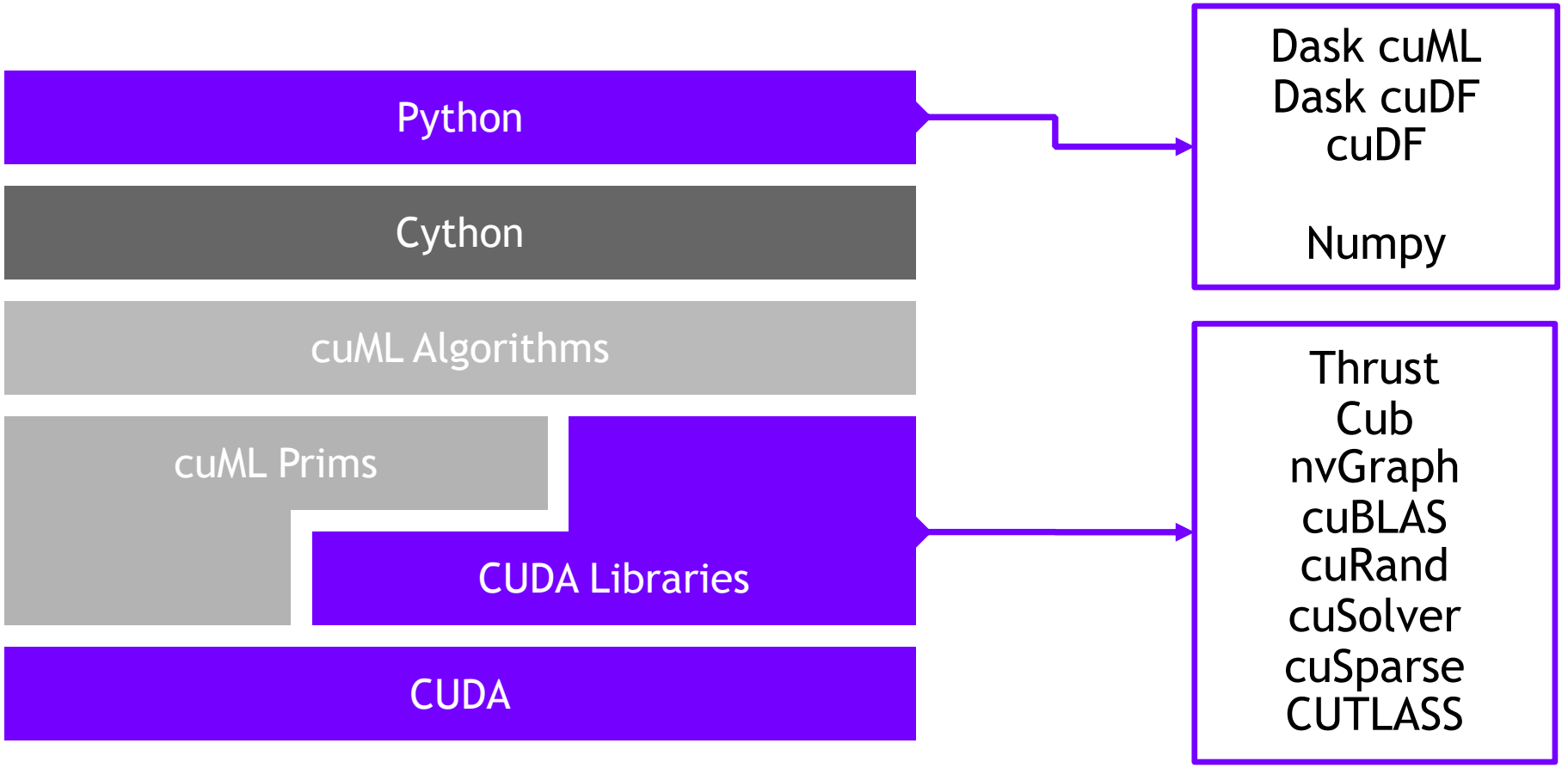
Ecosystem Partners

Community Contributors

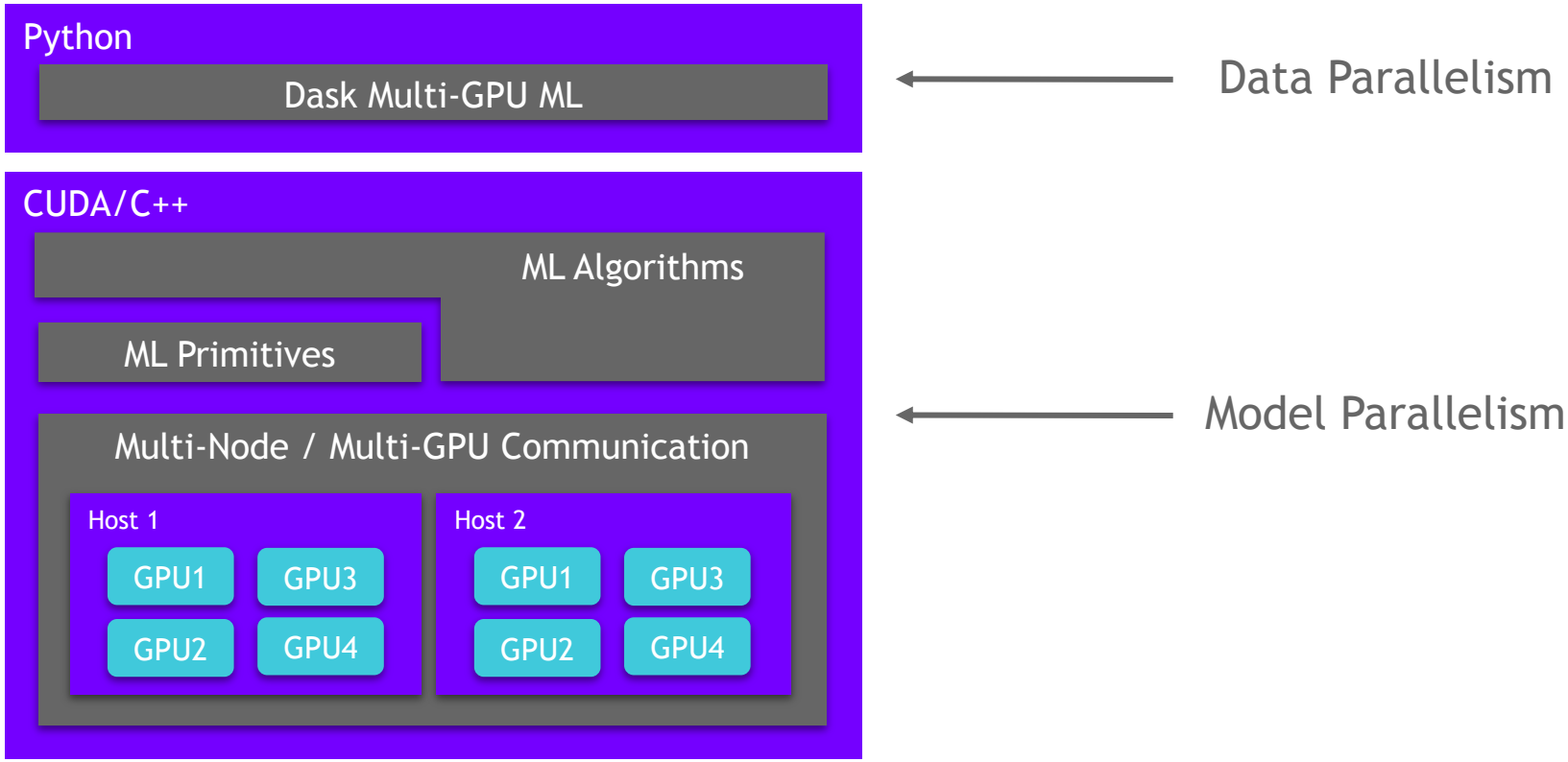
Ecosystem Partners

Walmart

ML Technology Stack



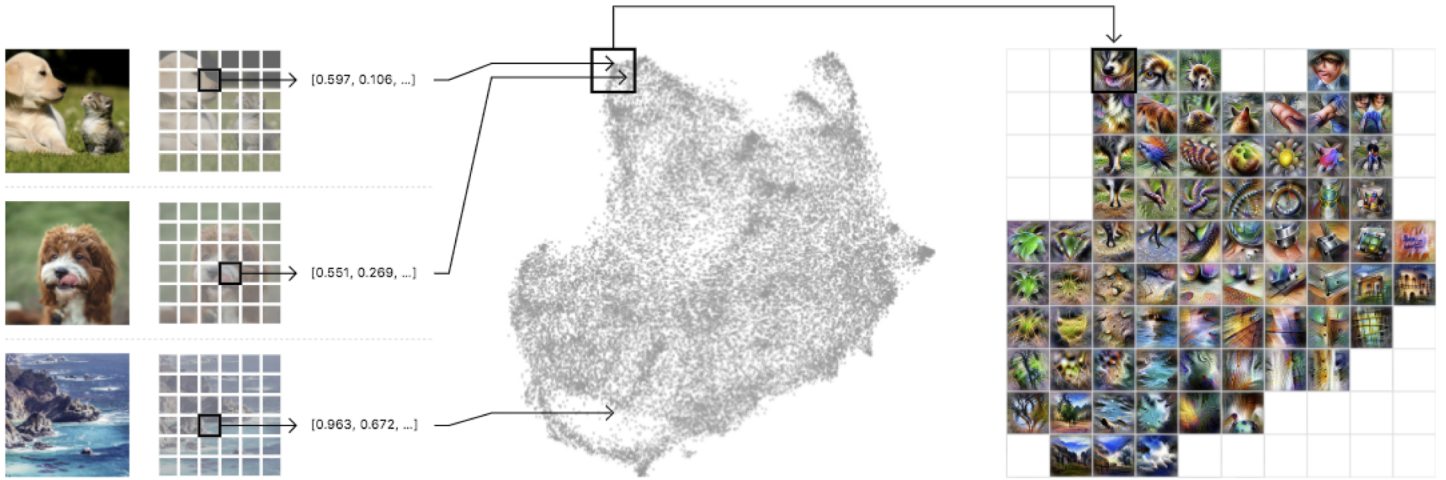
High-Level APIs



UMAP

Dimensionality reduction technique now on GPU

Uniform Manifold Approximation and Projection (UMAP) is a dimension reduction technique that can be used for visualization similarly to t-SNE, but also for general non-linear dimension reduction.



https://ai.googleblog.com/2019/03/exploring-neural-networks.html

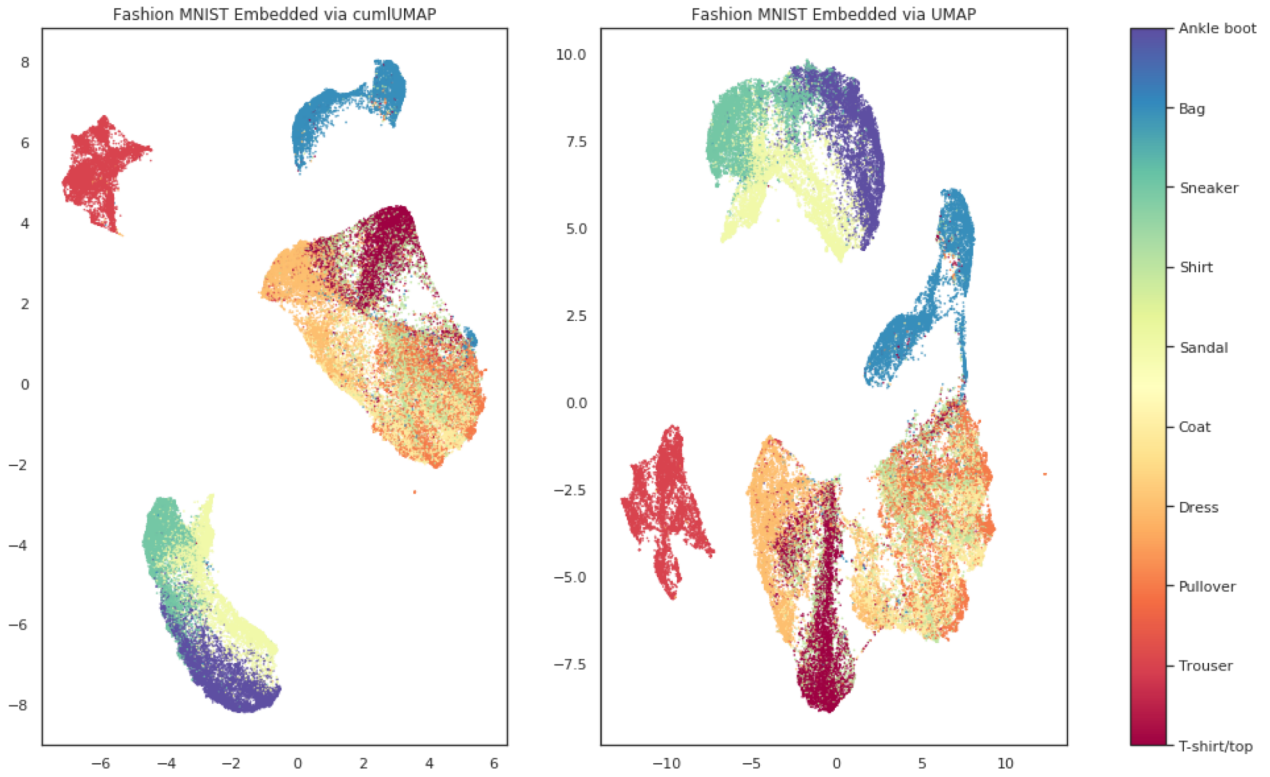
- **Fast**
- **General purpose** dimension reduction
- **Scales beyond** what most t-SNE packages can manage
- Often **preserves global structure** better than t-SNE
- Supports a **wide variety of distance functions**
- Supports **adding new points to an existing embedding** via the standard scikit-learn transform method
- **Supports supervised and semi-supervised** dimension reduction
- Has **solid theoretical foundations** in manifold learning

https://arxiv.org/pdf/1802.03426.pdf

UMAP

GPU vs CPU

GPU: 10.5 seconds



CPU: 100 seconds

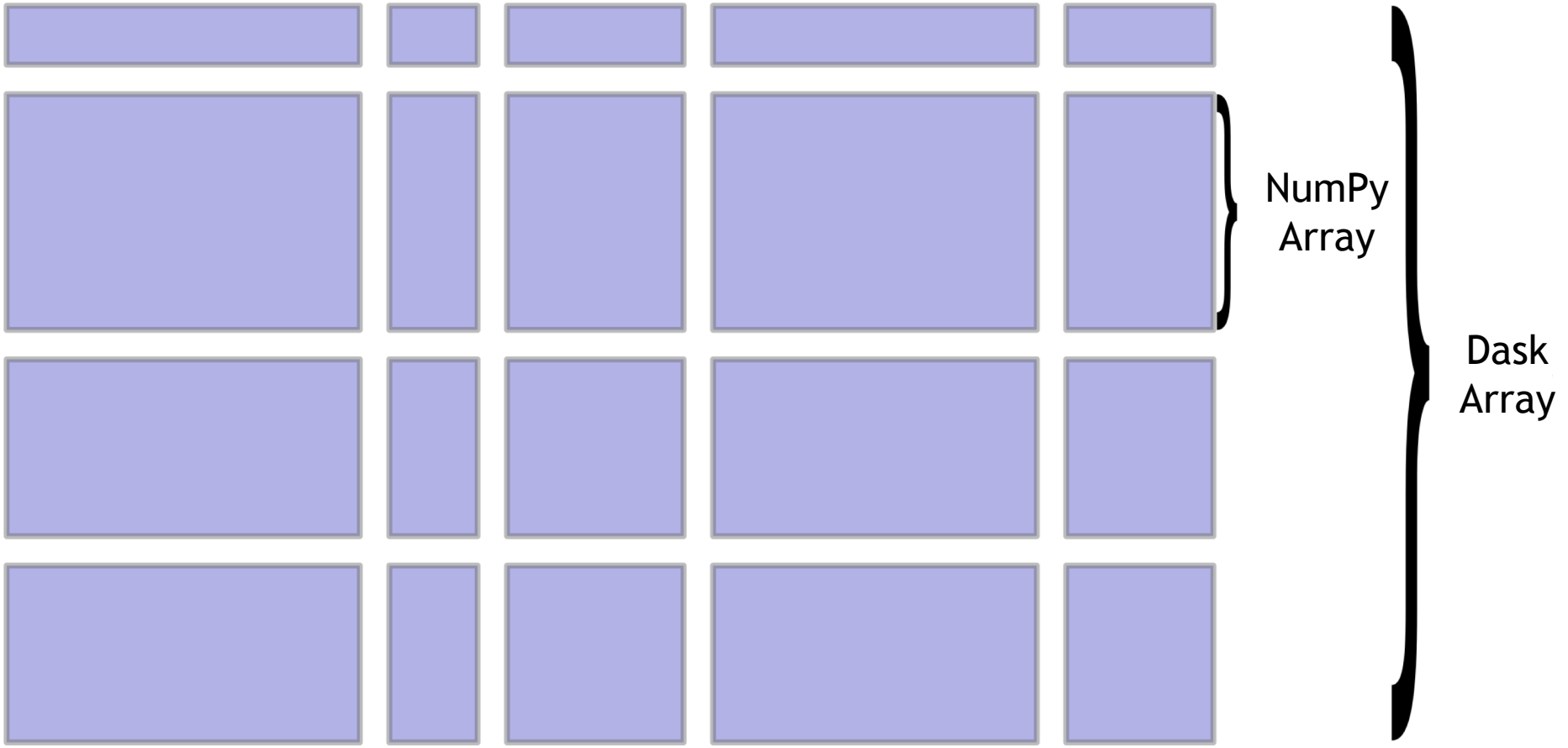
Dask

What is Dask and why does RAPIDS use it for scaling out?

- Distributed compute scheduler built to scale Python
- Scales workloads from laptops to supercomputer clusters
- Extremely modular: disjoint scheduling, compute, data transfer and out-of-core handling
- Multiple workers per node allow easier one-worker-per-GPU model

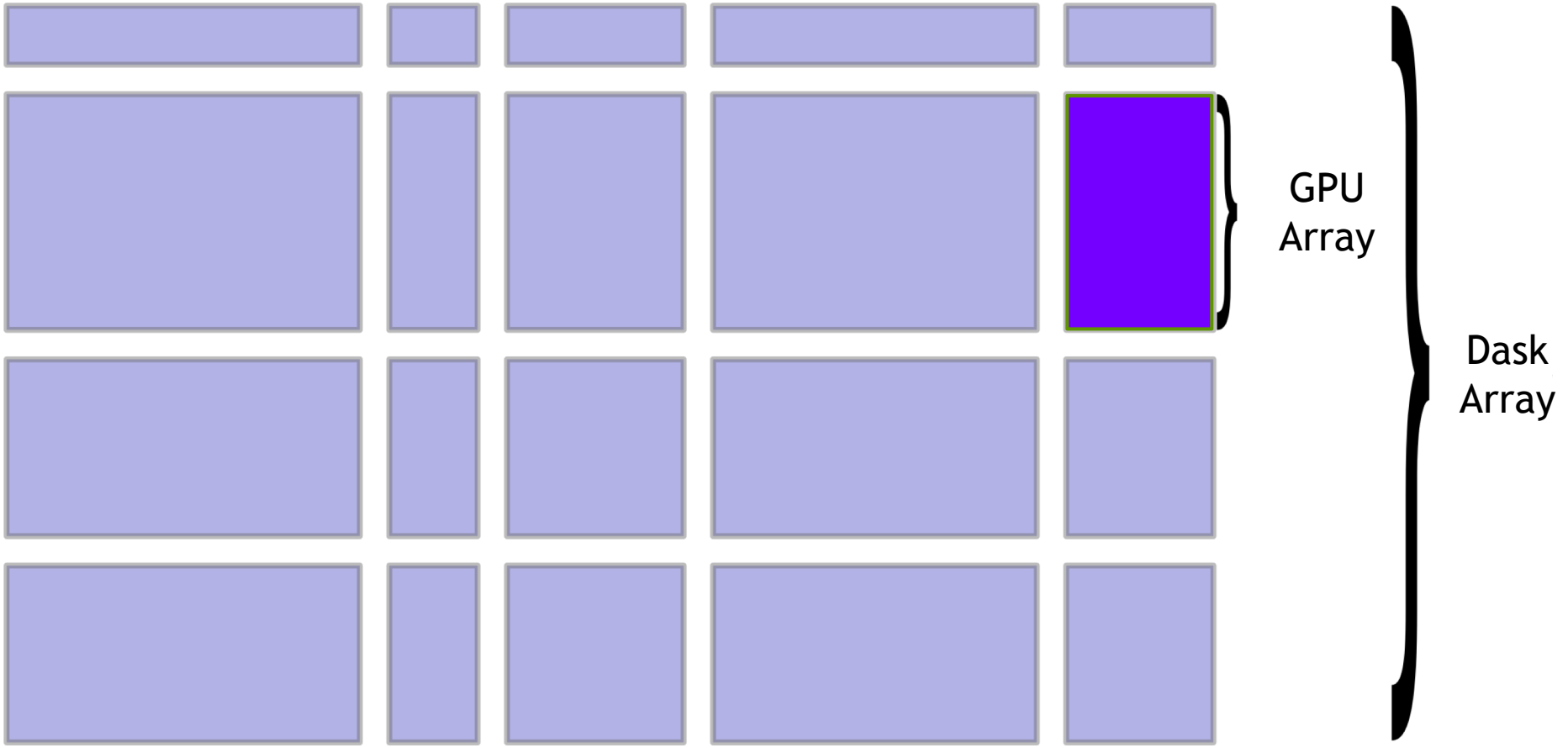
Distributing Dask

Distributed array from many arrays



Combine Dask with CuPy

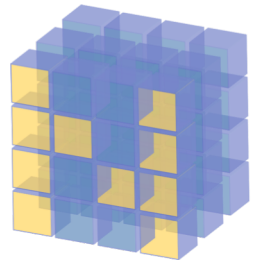
Distributed GPU array from many GPU arrays



NumPy Array Function (NEP-18)

Interoperability of NumPy-like Libraries

- Function dispatch mechanism
- Allows using NumPy as a high-level API
- NumPy-like arrays need only to implement `__array_function__`



NumPy

CuPy

DASK

Dask SVD Example

Interoperability of NumPy-like Libraries

```
In [1]: import dask, dask.array
   ...: import numpy


In [2]: x = numpy.random.random((1000000, 1000))
   ...: dx = dask.array.from_array(x, chunks=(10000, 1000), asarray=False)

In [3]: u, s, v = numpy.linalg.svd(dx)

In [4]: %%time
   ...: u, s, v = dask.compute(u, s, v)
CPU times: user 39min 4s, sys: 47min 31s, total: 1h 26min 35s
Wall time: 1min 21s
```

Dask+CuPy SVD Example

Interoperability of NumPy-like Libraries

```
In [1]: import dask, dask.array
   ...: import numpy
   ...: import cupy

In [2]: x =  cupy.random.random((1000000, 1000))
   ...: dx = dask.array.from_array(x, chunks=(10000, 1000), asarray=False)

In [3]: u, s, v = numpy.linalg.svd(dx)

In [4]: %%time
   ...: u, s, v = dask.compute(u, s, v)
CPU times: user 34.5 s, sys: 17.6 s, total: 52.1 s
Wall time: 41 s
```

NumPy Array Function (NEP-18)

Protocol Limitations

- Universal functions – `__array_ufunc__` already addresses those
- `numpy.array()` and `numpy.asarray()` – will require their own protocol
- Dispatch for methods of any kind – e.g., `numpy.random.RandomState()`

uarray

Alternative to `__array_function__`

- Generic multiple-dispatch mechanism
- Intended to address shortcomings of NEP-18
- https://uarray.readthedocs.io/

uarray

CuPy Example

```
In [1]: import uarray as ua
   ...: import unumpy as np
   ...: import unumpy.cupy_backend as cupy_backend


In [2]: with ua.set_backend(cupy_backend):
   ...:     a = np.ones((2, 2))
   ...:     print(np.sum(a))
   ...:     print(type(a))
   ...:     print(type(np.sum(a)))
4.0
<class 'cupy.core.core.ndarray’>
<class 'cupy.core.core.ndarray'>
```

uarray

Dask+CuPy Example

```
In [1]: import uarray as ua
   ...: import unumpy as np
   ...: import unumpy.cupy_backend as cupy_backend
   ...: import unumpy.dask_backend as dask_backend

In [2]: with ua.set_backend(cupy_backend), ua.set_backend(dask_backend):
   ...:     a = np.ones((2, 2))
   ...:     print(np.sum(a).compute())
   ...:     print(type(a))
   ...:     print(type(np.sum(a).compute()))
4.0
<class 'dask.array.core.Array'>
<class 'numpy.float64'>          # currently
<class 'cupy.core.core.ndarray'> # expected - Dask will need to support
                                   uarray for this to work!
```

Python CUDA Array Interface

Interoperability for Python GPU Array Libraries

- GPU array standard
- Allows sharing GPU array between different libraries
- Native ingest and export of `__cuda_array_interface__` compatible objects via Numba device arrays in cuDF
- Numba, CuPy, and PyTorch are the first libraries to adopt the interface:
  - https://numba.pydata.org/numba-doc/dev/cuda/cuda_array_interface.html
  - https://github.com/cupy/cupy/releases/tag/v5.0.0b4
  - https://github.com/pytorch/pytorch/pull/11984

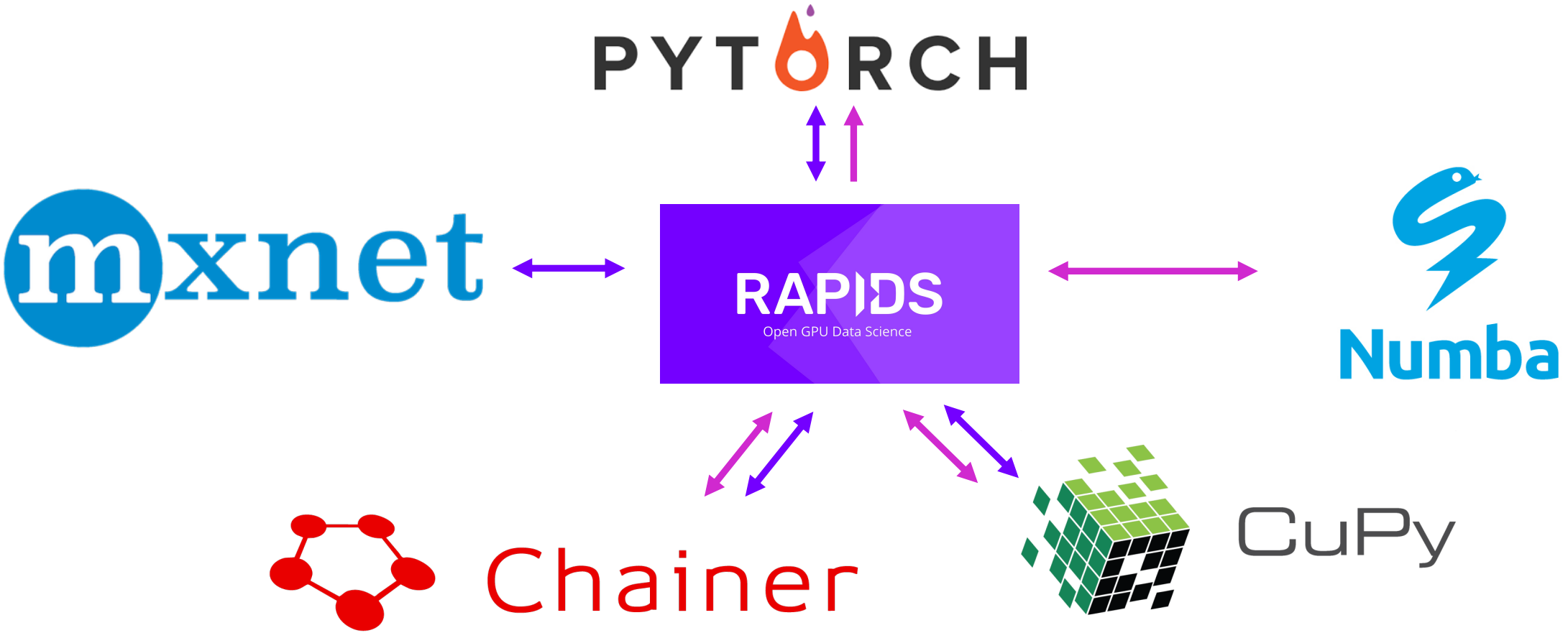
Numba

CuPy

PYTORCH

Interoperability for the Win

DLPack and __cuda_array_interface__



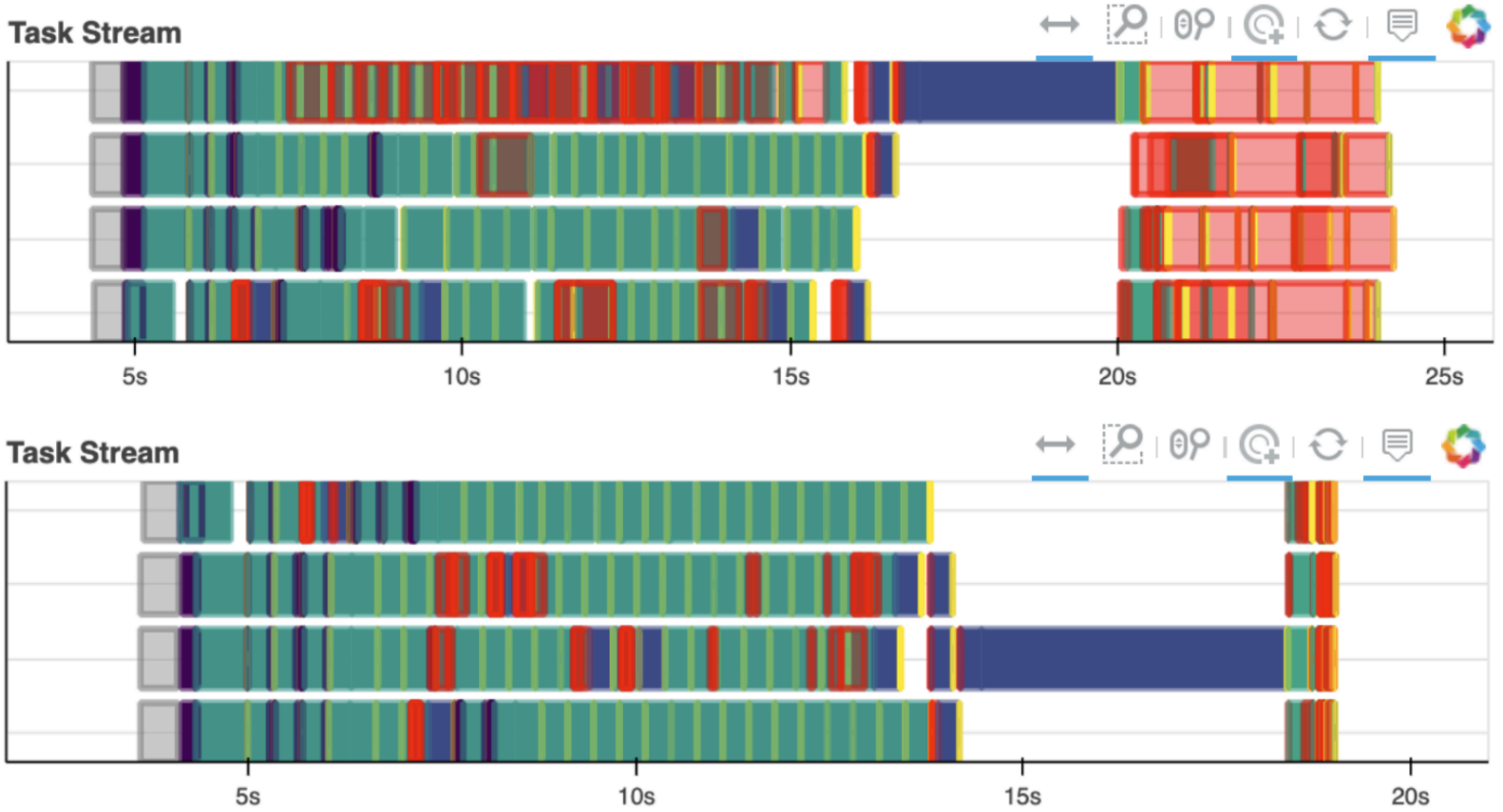
Challenges: Communication

OpenUCX

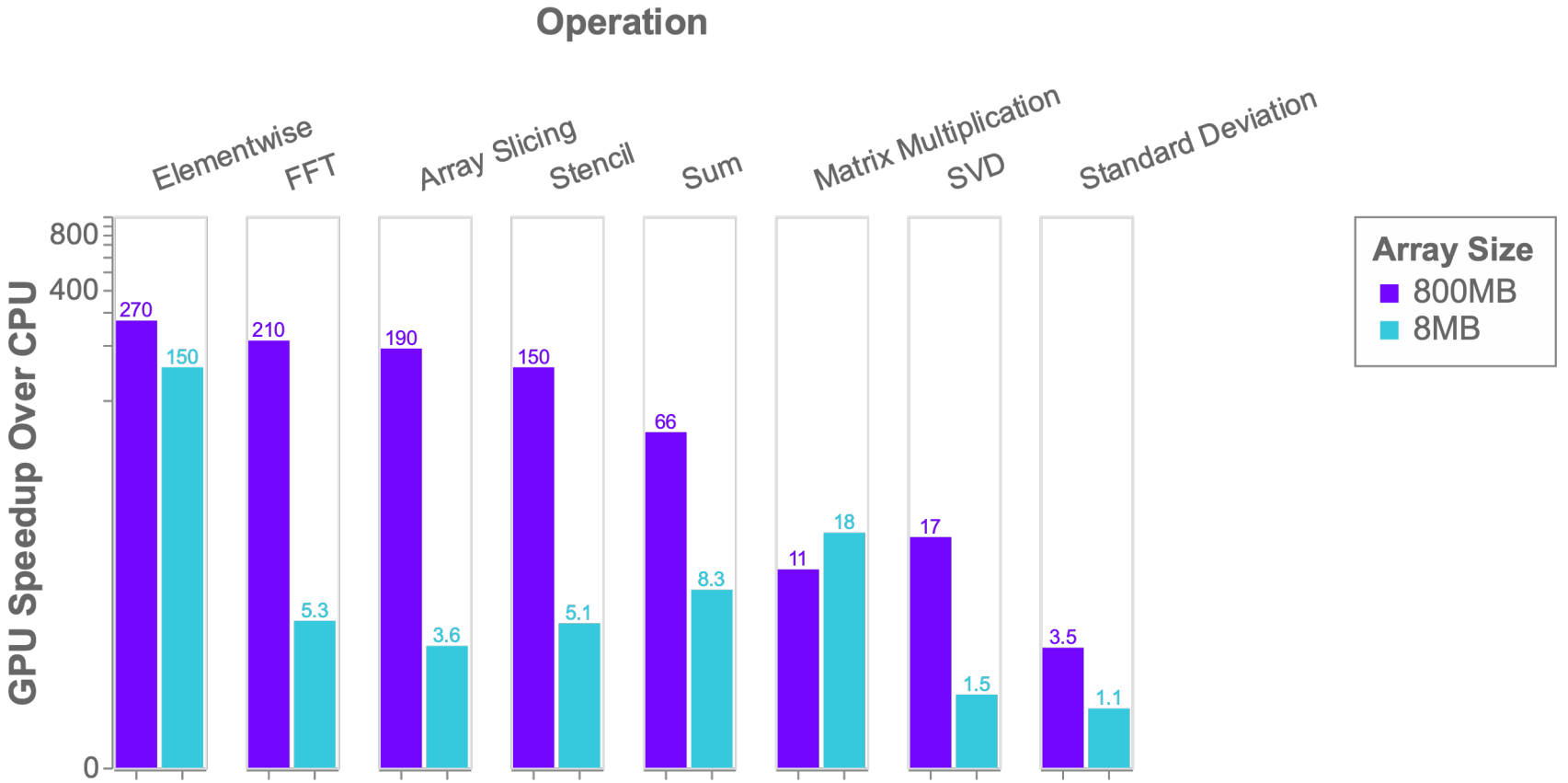
- TCP sockets are slow!
- UCX provides uniform access to transports (TCP, InfiniBand, shared memory, NVLink)
- Python bindings for UCX (ucx-py) in the works https://github.com/rapidsai/ucx-py
- Will provide best communication performance, to Dask according to available hardware on nodes/cluster

Challenges: Communication

OpenUCX Performance – Before and After

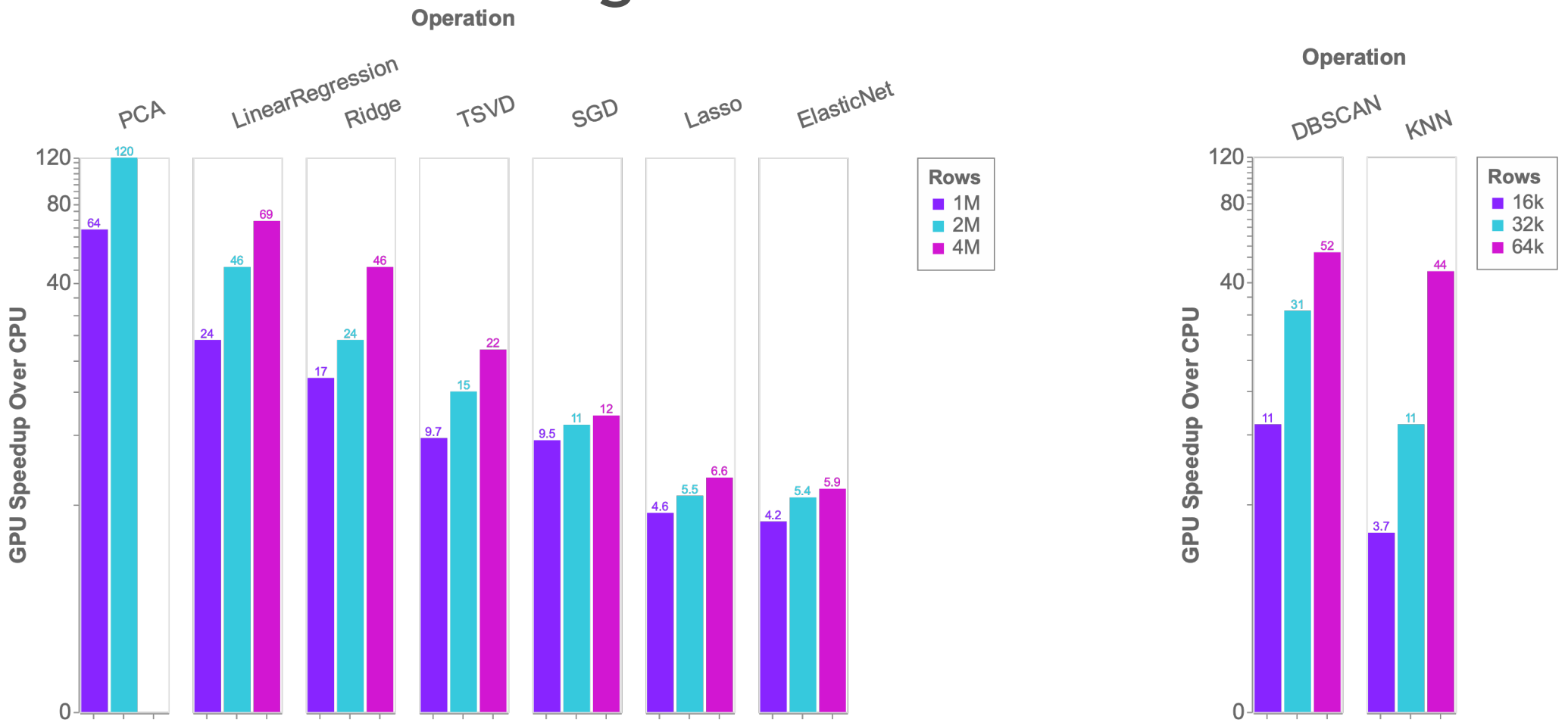


Benchmark: single-GPU CuPy vs NumPy

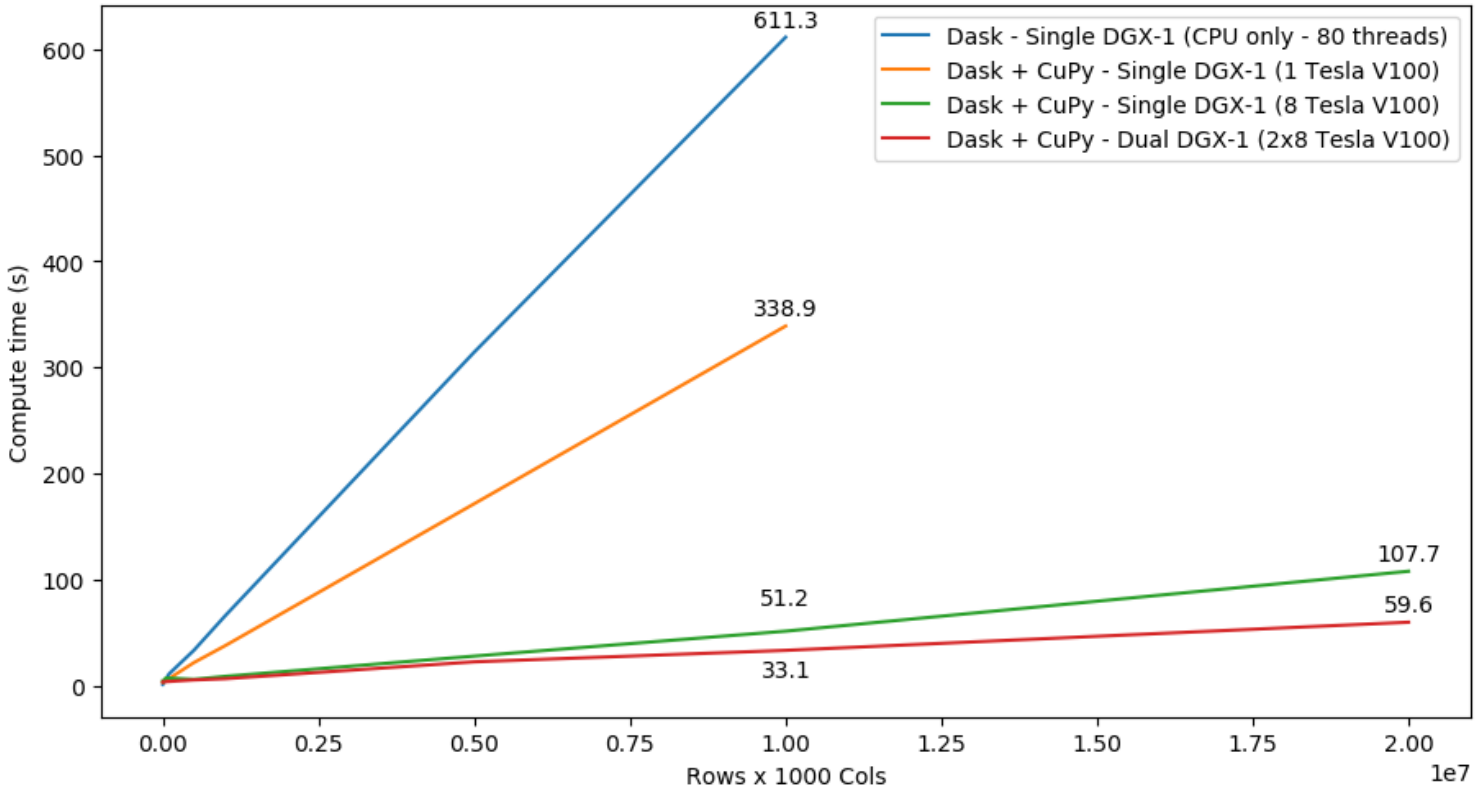


More details: https://blog.dask.org/2019/06/27/single-gpu-cupy-benchmarks

Benchmarks: single-GPU cuML vs scikit-learn



SVD Benchmark



Scale up with RAPIDS

Scale Up / Accelerate

RAPIDS and Others

Accelerated on single GPU

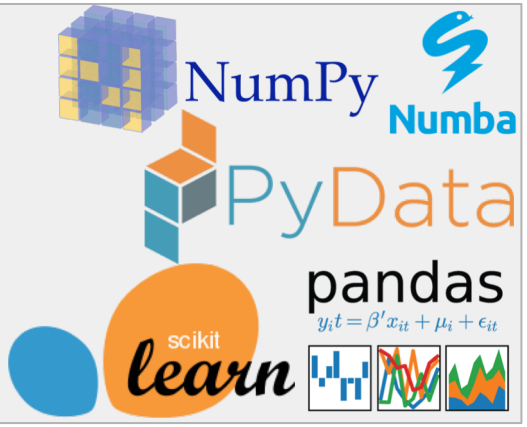
NumPy -> CuPy/PyTorch/..
Pandas -> cuDF
Scikit-Learn -> cuML
Numba -> Numba

RAPIDS

PyData

NumPy, Pandas, Scikit-Learn,
Numba and many more

Single CPU core
In-memory data



Scale up and out with RAPIDS and Dask

Scale Up / Accelerate

RAPIDS and Others

Accelerated on single GPU

NumPy -> CuPy/PyTorch/..
Pandas -> cuDF
Scikit-Learn -> cuML
Numba -> Numba

RAPIDS

Dask + RAPIDS

Multi-GPU
On single Node (DGX)
Or across a cluster

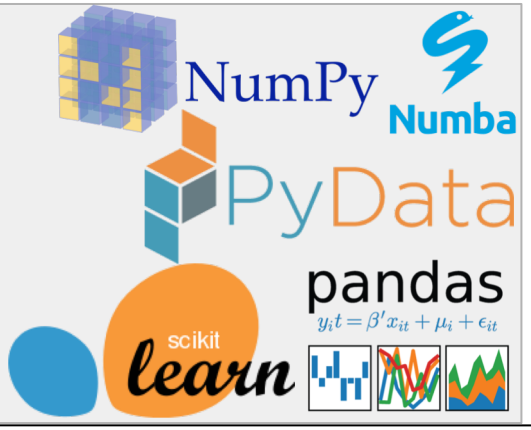
RAPIDS

DASK

PyData

NumPy, Pandas, Scikit-Learn, Numba and many more

Single CPU core
In-memory data



Dask

Multi-core and Distributed PyData

NumPy -> Dask Array
Pandas -> Dask DataFrame
Scikit-Learn -> Dask-ML
… -> Dask Futures

DASK

Scale out / Parallelize

Road to 1.0

October 2018 - RAPIDS 0.1

cuML	Single-GPU	Multi-GPU	Multi-Node-Multi-GPU
Gradient Boosted Decision Trees (GBDT)			
GLM			
Logistic Regression			
Random Forest (regression)			
K-Means			
K-NN			
DBSCAN			
UMAP			
ARIMA			
Kalman Filter			
Holts-Winters			
Principal Components			
Singular Value Decomposition			

Road to 1.0

June 2019 - RAPIDS 0.8

cuML	Single-GPU	Multi-GPU	Multi-Node-Multi-GPU
Gradient Boosted Decision Trees (GBDT)	■	■	■
GLM	■	■	
Logistic Regression	■		
Random Forest (regression)	■	■	■
K-Means	■	■	
K-NN	■	■	
DBSCAN	■		
UMAP	■		
ARIMA			
Kalman Filter	■		
Holts-Winters			
Principal Components	■		
Singular Value Decomposition	■	■	

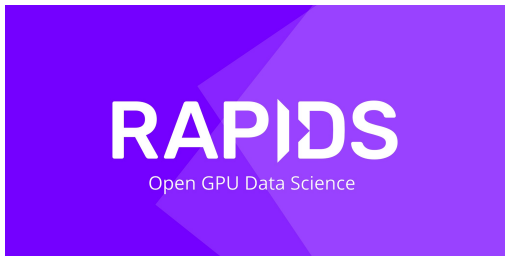
Road to 1.0

Q4 - 2019 - RAPIDS 0.12?

cuML	Single-GPU	Multi-GPU	Multi-Node-Multi-GPU
Gradient Boosted Decision Trees (GBDT)			
GLM			
Logistic Regression			
Random Forest (regression)			
K-Means			
K-NN			
DBSCAN			
UMAP			
ARIMA			
Kalman Filter			
Holts-Winters			
Principal Components			
Singular Value Decomposition			

Road to 1.0

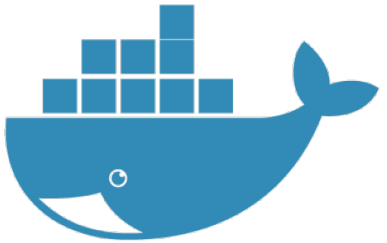
Focused on robust functionality, deployment, and user experience



Integration with every major cloud provider
Both containers and cloud specific machine instances
Support for Enterprise and HPC Orchestration Layers

RAPIDS

How do I get the software?



- https://github.com/rapidsai
- https://anaconda.org/rapidsai/

- https://ngc.nvidia.com/registry/nvidia-rapidsai-rapidsai
- https://hub.docker.com/r/rapidsai/rapidsai/

Additional Reading Material

- Python, Performance and GPUs (Matthew Rocklin): https://towardsdatascience.com/python-performance-and-gpus-1be860ffd58d?ncid=so-twi-n2-96487&linkId=100000006881312
- NEP-18: A Dispatch Mechanism for NumPy's high level array functions (Stephan Hoyer, et al.): https://www.numpy.org/neps/nep-0018-array-function-protocol.html
- uarray update: API changes, overhead and comparison to __array_function__ (Hameer Abbasi): https://labs.quansight.org/blog/2019/07/uarray-update-api-changes-overhead-and-comparison-to-__array_function__/

THANK YOU

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