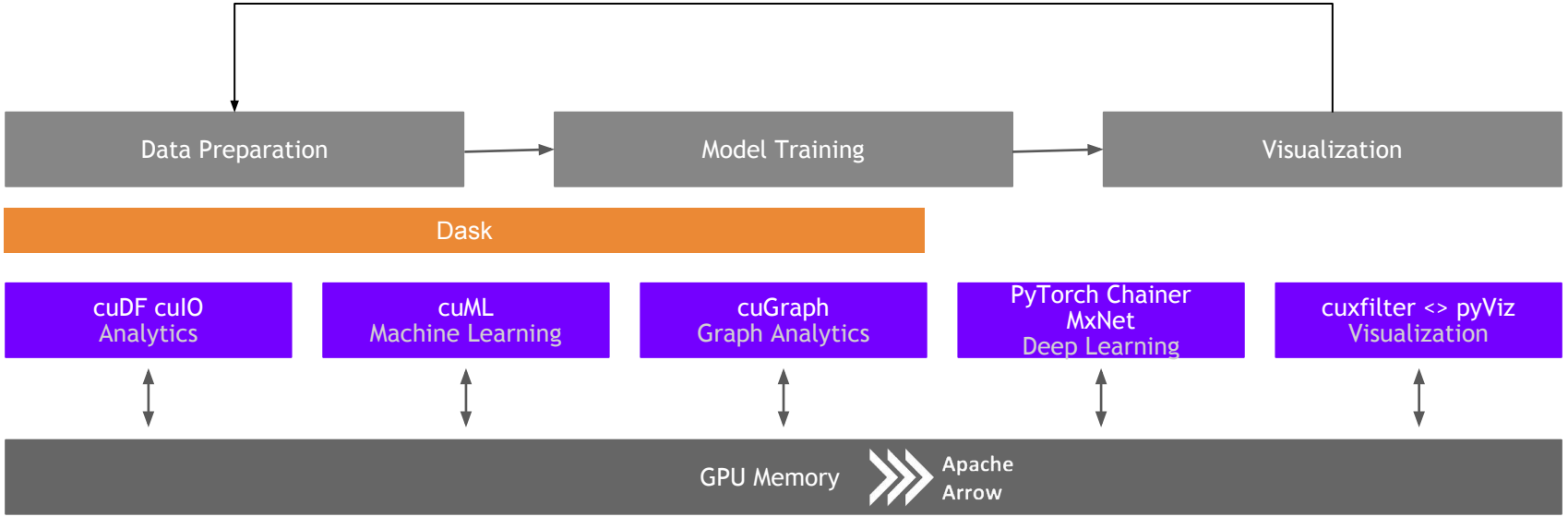
RAPIDS

The Platform Inside and Out

Nick Becker
RAPIDS Engineering

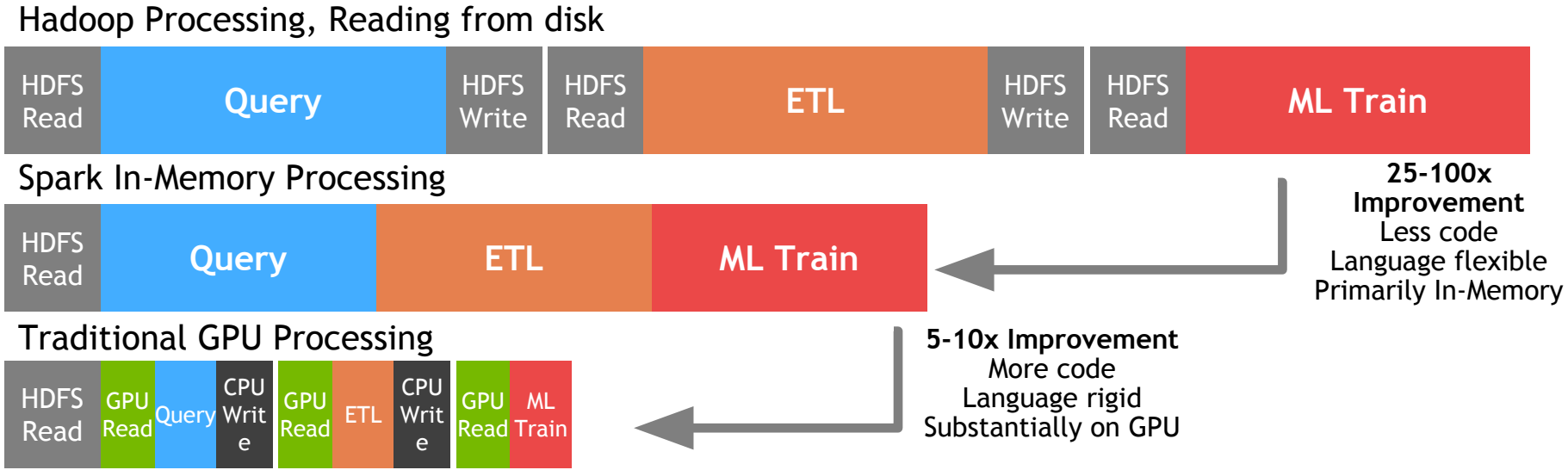
RAPIDS

End-to-End Accelerated GPU Data Science



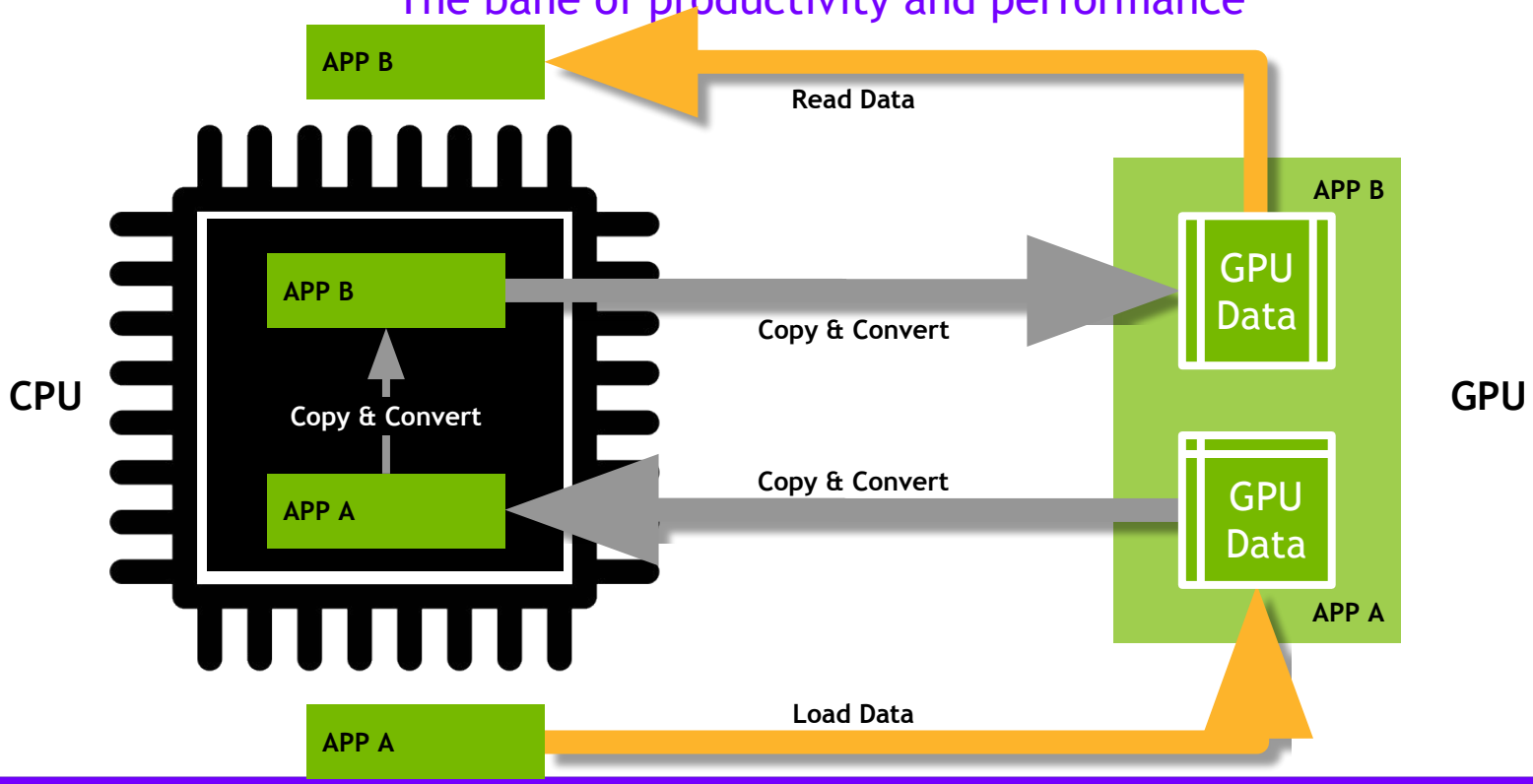
Data Processing Evolution

Faster data access, less data movement



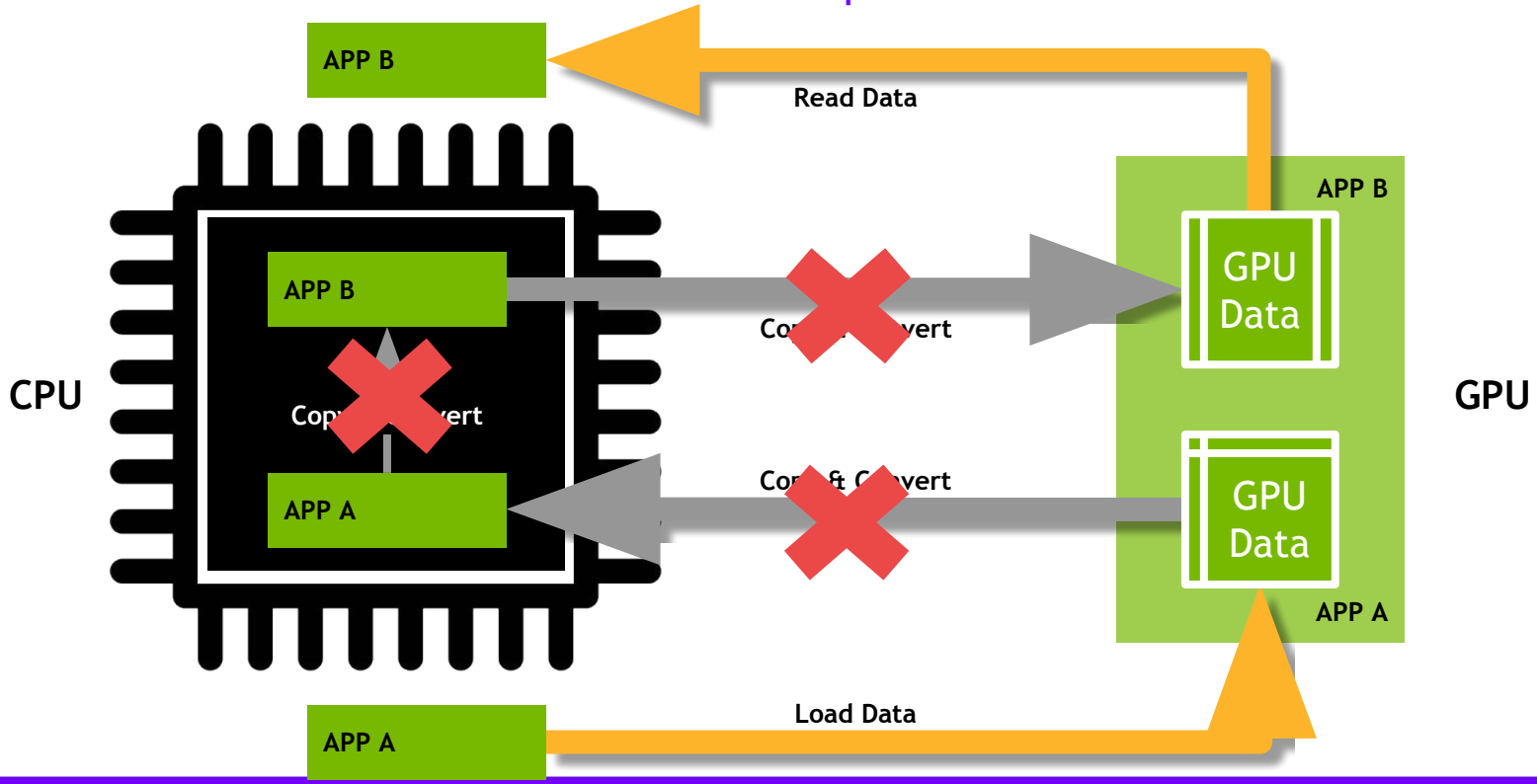
Data Movement and Transformation

The bane of productivity and performance

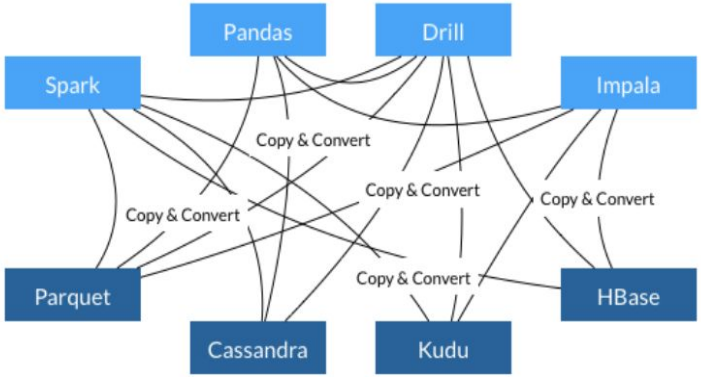


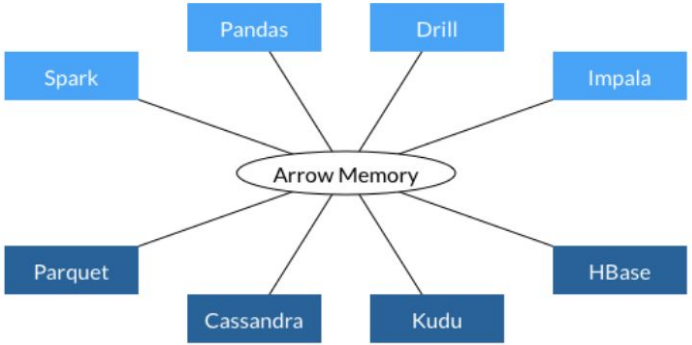
Data Movement and Transformation

What if we could keep data on the GPU?



Learning from Apache Arrow





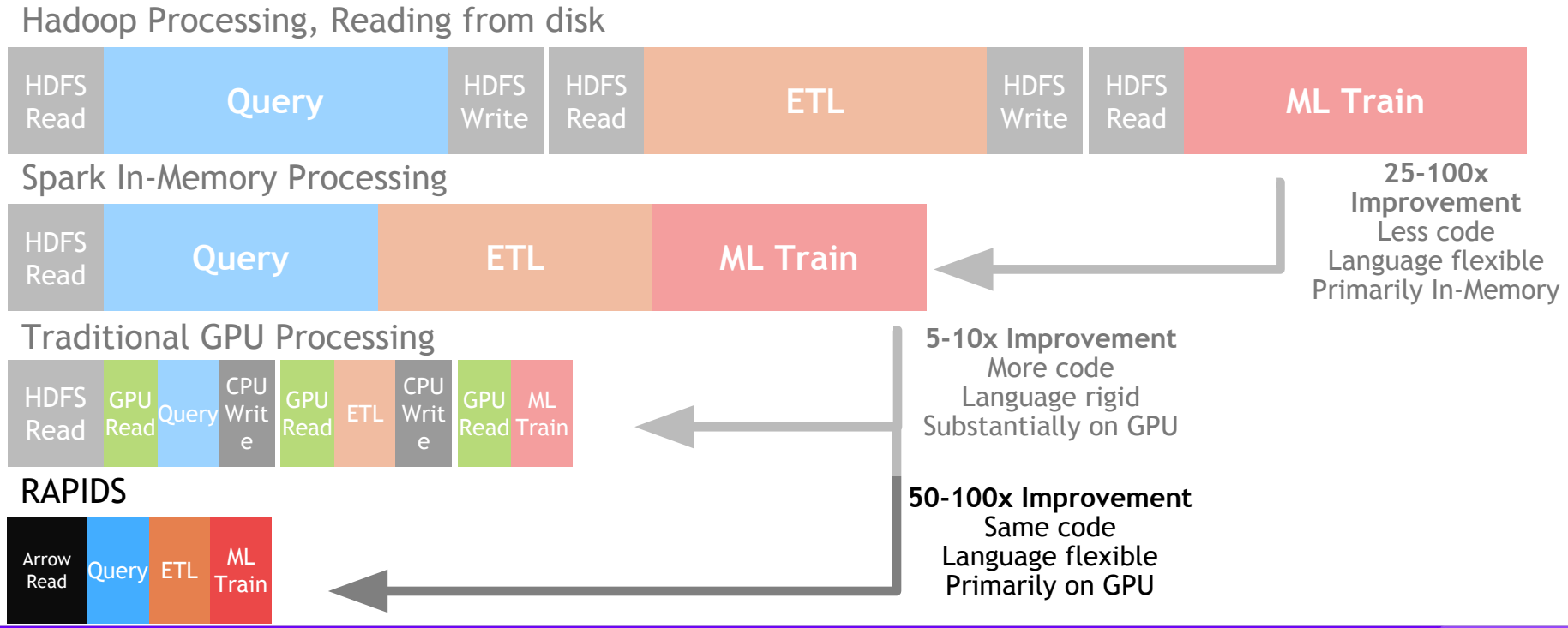
- Each system has its own internal memory format
- 70-80% computation wasted on serialization and deserialization
- Similar functionality implemented in multiple projects

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

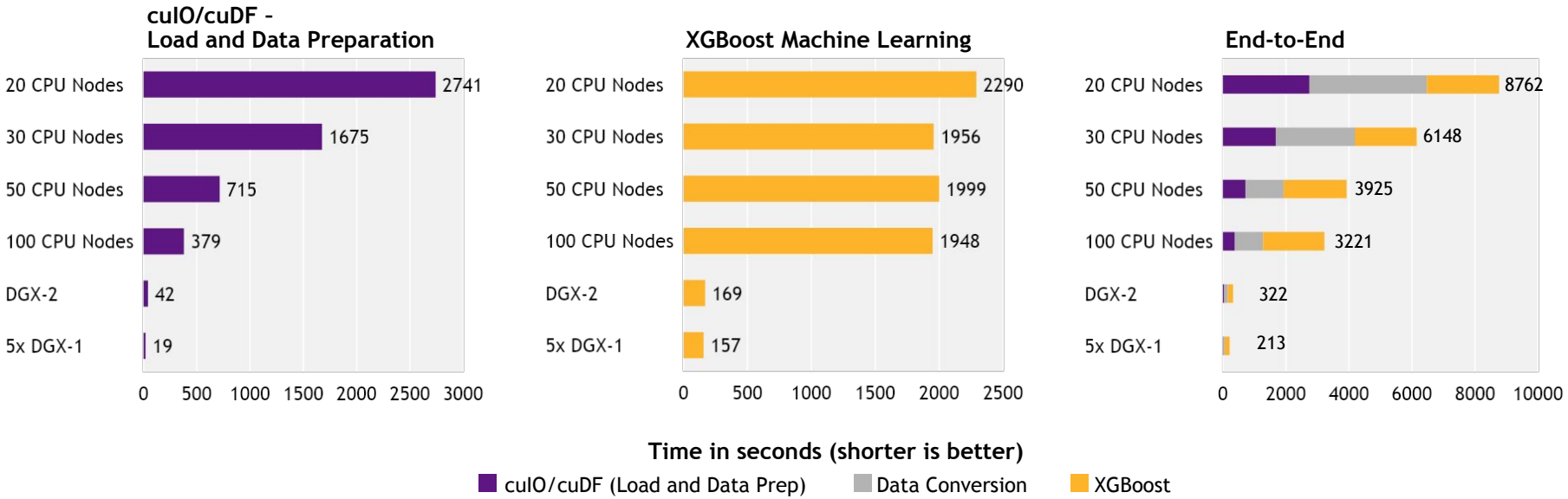
From Apache Arrow Home Page - https://arrow.apache.org/

Data Processing Evolution

Faster data access, less data movement



Faster Speeds, Real-World Benefits



Benchmark

200GB CSV dataset; Data prep includes joins, variable transformations

CPU Cluster Configuration

CPU nodes (61 GiB memory, 8 vCPUs, 64-bit platform), Apache Spark

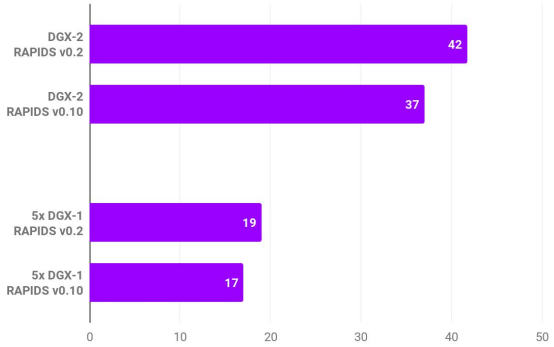
DGX Cluster Configuration

5x DGX-1 on InfiniBand network

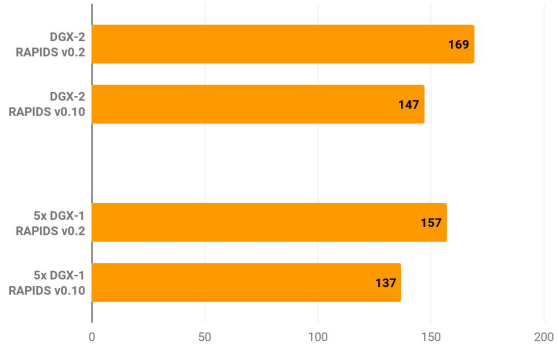
Faster Speeds, Real-World Benefits

Improving Over Time

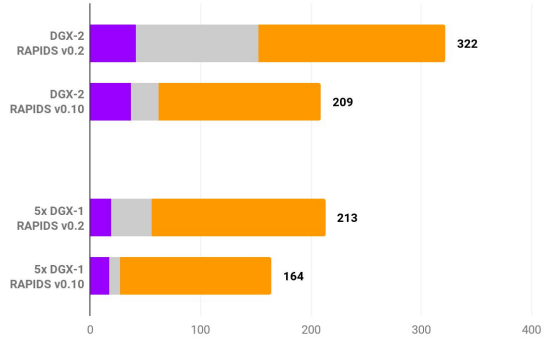
cuIO/cuDF – Load and Data Preparation



XGBoost Machine Learning



End-to-End



Time in seconds (shorter is better)

cuIO/cuDF (Load and Data Prep) | Data Conversion | XGBoost

Benchmark

200GB CSV dataset; Data prep includes joins, variable transformations

CPU Cluster Configuration

CPU nodes (61 GiB memory, 8 vCPUs, 64-bit platform), Apache Spark

DGX Cluster Configuration

5x DGX-1 on InfiniBand network

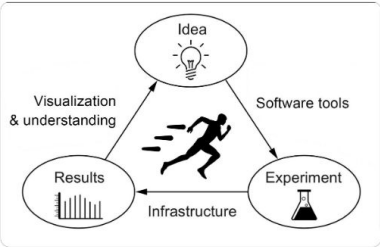
Speed, Ease of Use, and Iteration

The Way to Win at Data Science

François Chollet @fchollet — Following

Winners are those who went through *more iterations* of the "loop of progress" -- going from an idea, to its implementation, to actionable results. So the winning teams are simply those able to run through this loop *faster*.

And this is were Keras gives you an edge.



12:31 PM - 3 Apr 2019

50 Retweets 158 Likes

5 50 158

François Chollet @fchollet · Apr 3

We often talk about how following UX best practices for API design makes Keras more accessible and easier to use, and how this helps beginners.

But those who stand to benefit most from good UX *aren't* the beginners. It's actually the very best practitioners in the world.

1 7 50

François Chollet @fchollet · Apr 3

Because good UX reduces the overhead (development overhead & cognitive overhead) to setting up new experiments. It means you will be able to iterate faster. You will be able to try more ideas.

And ultimately, that's how you win competitions or get papers published.

2 11 78

François Chollet @fchollet · Apr 3

So I don't think it's mere personal preference if Kaggle champions are overwhelmingly using Keras.

Using Keras means you're more likely to win, and inversely, those who practice the sort of fast experimentation strategy that sets them up to win are more likely to prefer Keras.

8 8 74

Joshua Patterson @datametrician · Apr 3

Replying to @fchollet

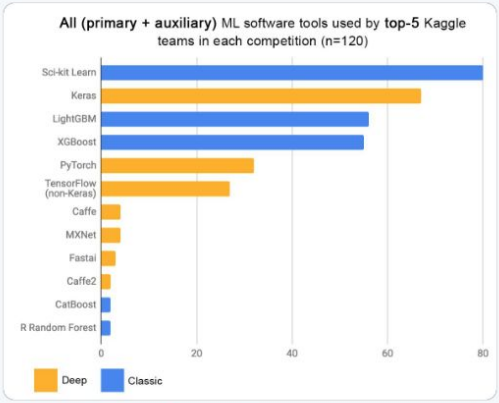
This is the fundamental believe that drives @RAPIDSai. @nvidia #GPU infrastructure is fast, people need to iterate quickly, people want a known #python interface. Combine them and you're off to the races!

2 11

François Chollet @fchollet · Apr 3

The second question asked about secondary frameworks -- usually teams win with an ensemble that involves many different ML frameworks. Here are *all* frameworks used.

Sklearn tops that ranking: everyone uses sklearn (although often as an auxiliary, for preprocessing or scoring).



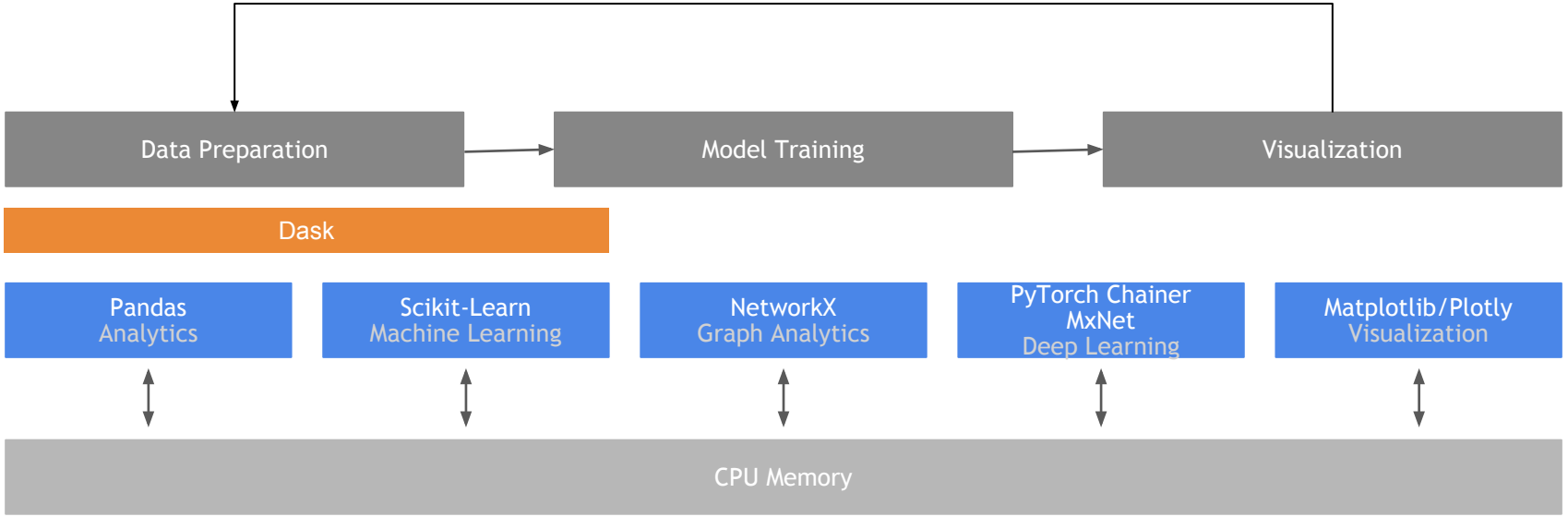
4 44 129

kaggle

RAPIDS Core

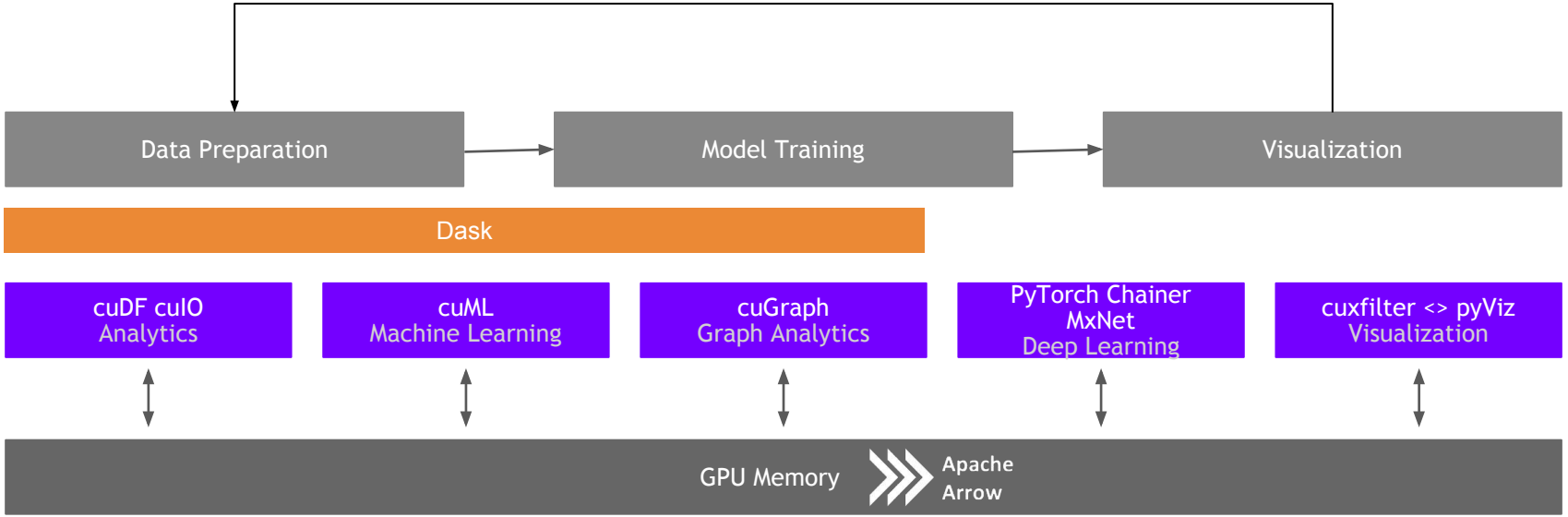
Open Source Data Science Ecosystem

Familiar Python APIs



RAPIDS

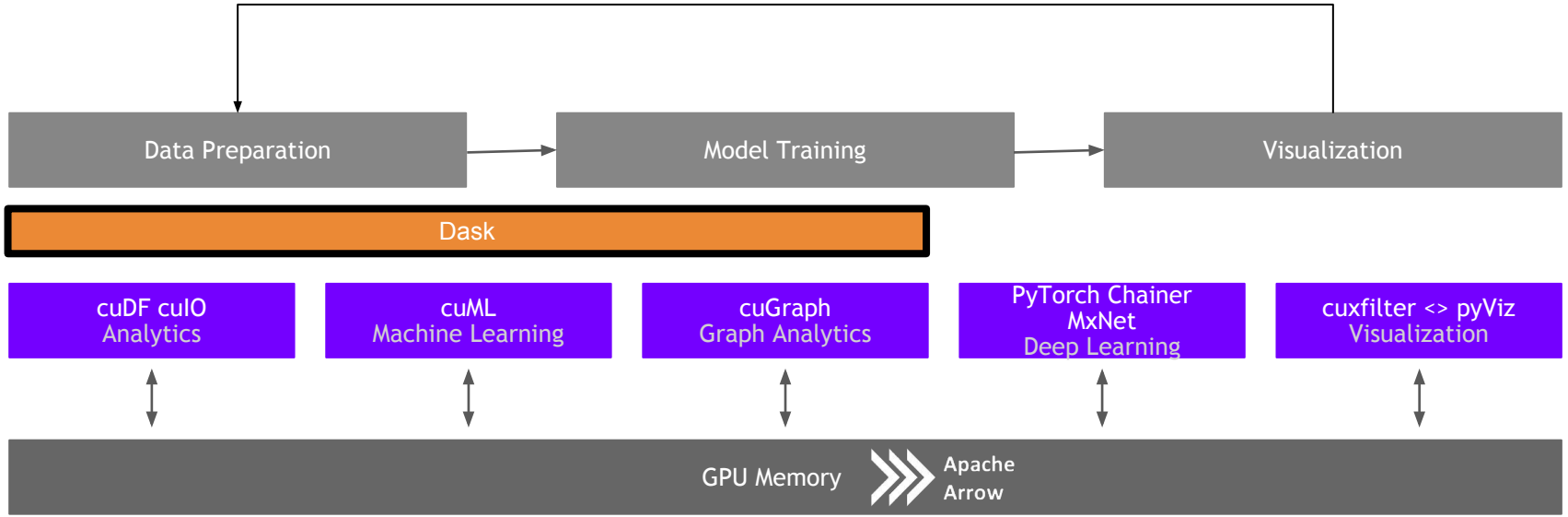
End-to-End Accelerated GPU Data Science



Dask

RAPIDS

Scaling RAPIDS with Dask



Why Dask?

PyData Native

- **Easy Migration:** Built on top of NumPy, Pandas Scikit-Learn, etc.
- **Easy Training:** With the same APIs
- **Trusted:** With the same developer community

Deployable

- **HPC:** SLURM, PBS, LSF, SGE
- **Cloud:** Kubernetes
- **Hadoop/Spark:** Yarn

Easy Scalability

- Easy to install and use on a laptop
- Scales out to thousand-node clusters

Popular

- Most common parallelism framework today in the PyData and SciPy community

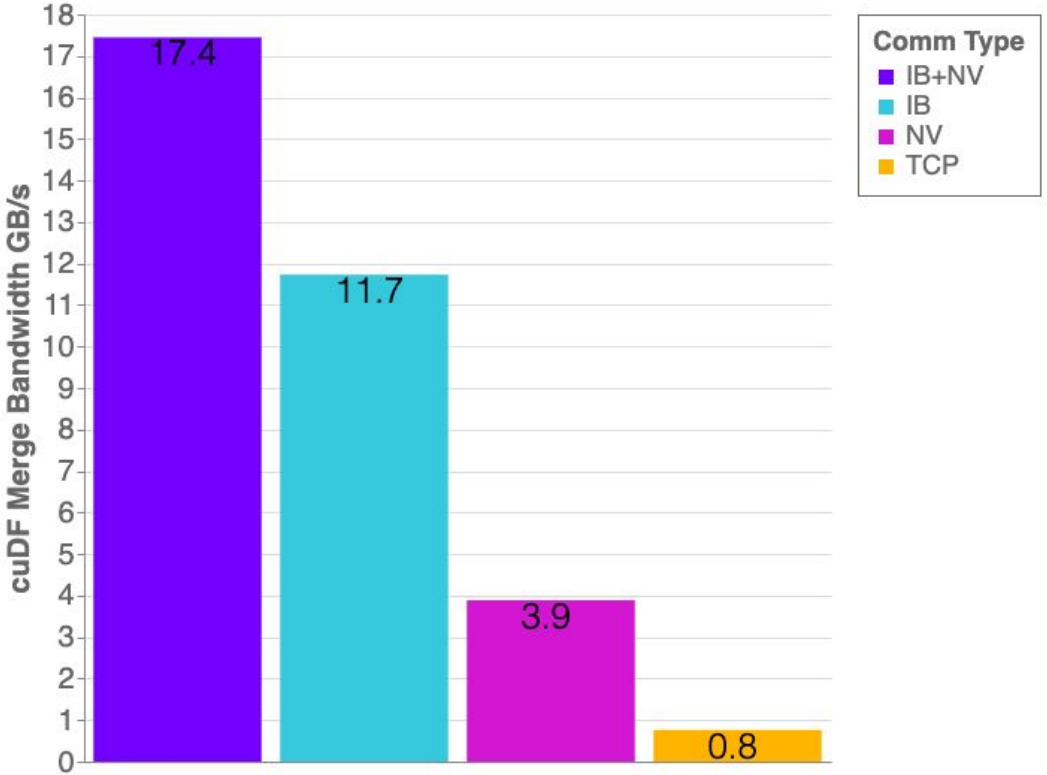
Why OpenUCX?

Bringing hardware accelerated communications to Dask

- TCP sockets are slow!
- UCX provides uniform access to transports (TCP, InfiniBand, shared memory, NVLink)
- Alpha Python bindings for UCX (ucx-py)
- Will provide best communication performance, to Dask based on available hardware on nodes/cluster

```
conda install -c conda-forge -c rapidsai \
  cudatoolkit=<CUDA version> ucx-proc=*=gpu ucx ucx-py
```

Benchmarks: Distributed cuDF Random Merge



cuDF v0.13, UCX-PY 0.13

Running on NVIDIA DGX-1 (8GPUs):

GPU: NVIDIA Tesla V100 32GB
CPU: Intel(R) Xeon(R) CPU 8168 @ 2.70GHz

Benchmark Setup:

DataFrames: Left/Right 1x int64 column key column, 1x int64 value columns

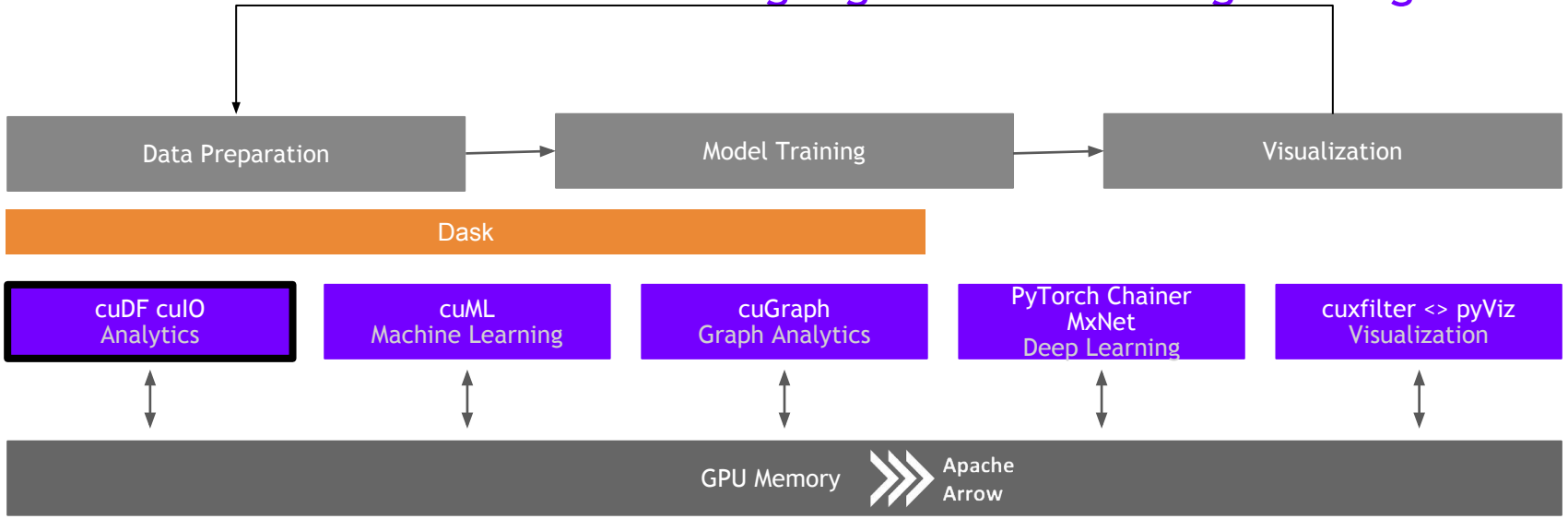
Merge: inner

30% of matching data balanced across each partition

cuDF

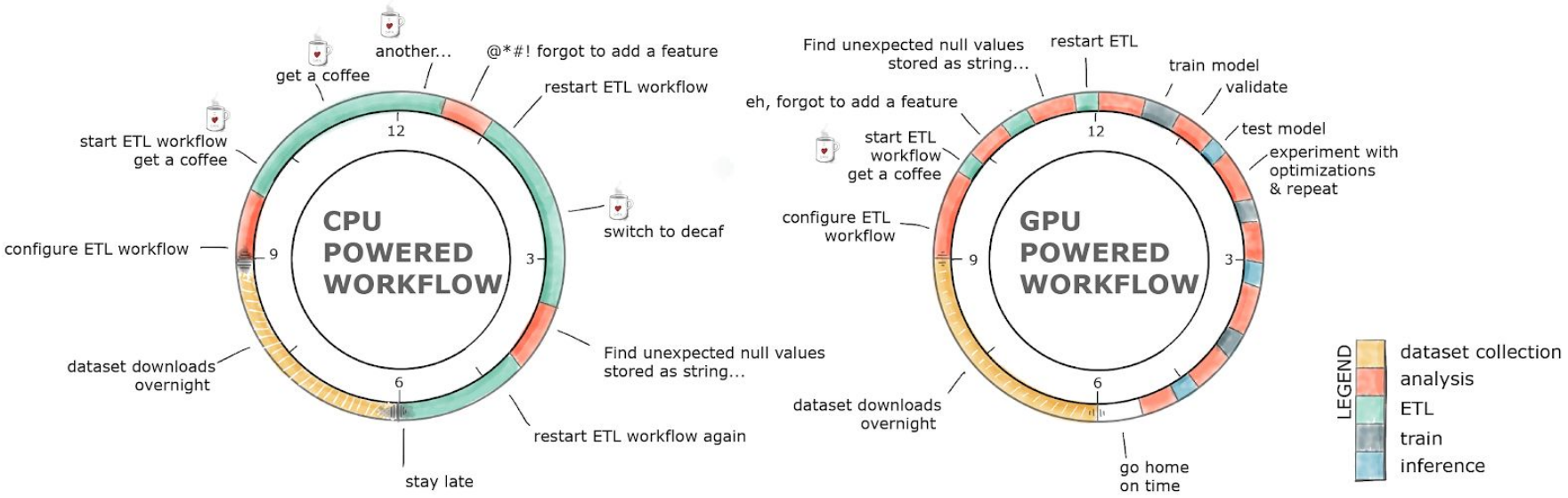
RAPIDS

GPU Accelerated data wrangling and feature engineering

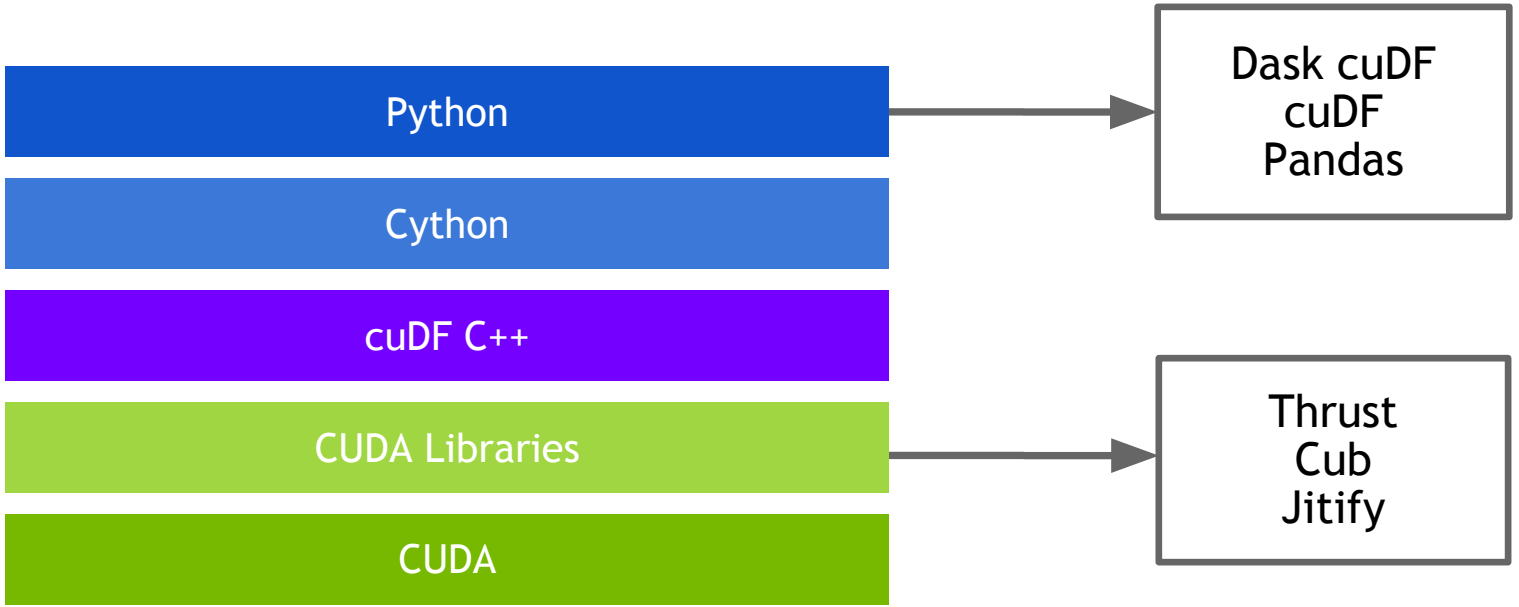


GPU-Accelerated ETL

The average data scientist spends 90+% of their time in ETL as opposed to training models



ETL Technology Stack



ETL: the Backbone of Data Science

libcuDF is…

CUDA C++ Library

- Table (dataframe) and column types and algorithms
- CUDA kernels for sorting, join, groupby, reductions, partitioning, elementwise operations, etc.
- Optimized GPU implementations for strings, timestamps, numeric types (more coming)
- Primitives for scalable distributed ETL

```
std::unique_ptr<table>
gather(table_view const& input,
       column_view const& gather_map, …)
{
     // return a new table containing
    // rows from input indexed by
    // gather_map
}
```

ETL: the Backbone of Data Science

cuDF is…

```
In [2]: #Read in the data. Notice how it decompresses as it reads the data into memory.
        gdf = cudf.read_csv('/rapids/Data/black-friday.zip')

In [3]: #Taking a look at the data. We use "to_pandas()" to get the pretty printing.
        gdf.head().to_pandas()
```

Out[3]:

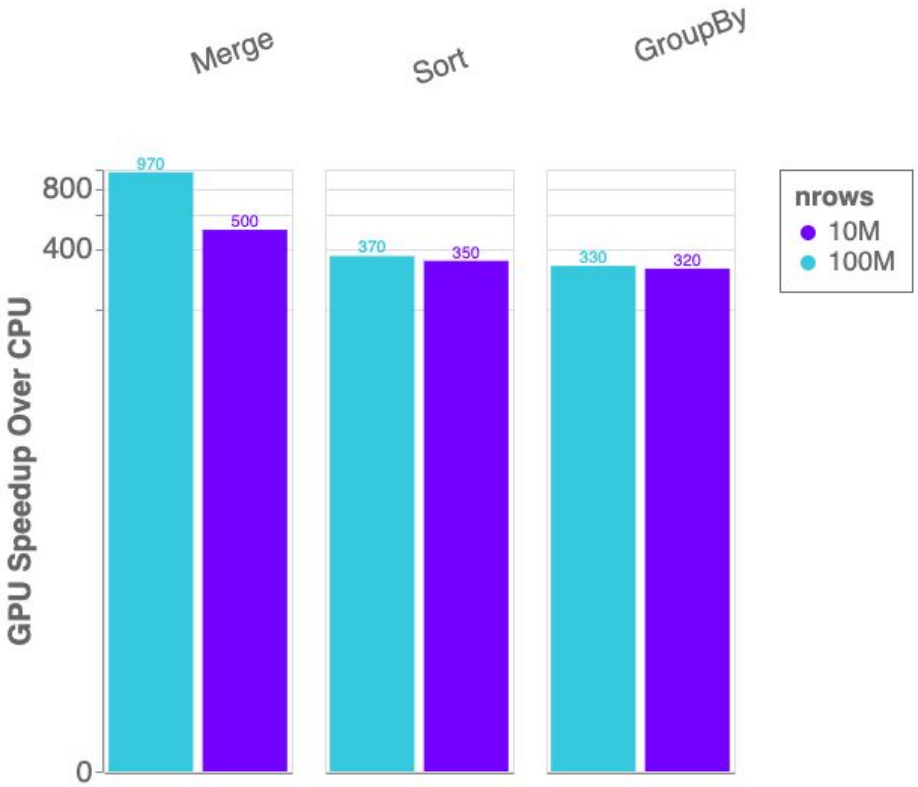
	User_ID	Product_ID	Gender	Age	Occupation	City_Category	Stay_In_Current_City_Years	Marital_Status	Product_Cat
0	1000001	P00069042	F	0-17	10	A	2	0	3
1	1000001	P00248942	F	0-17	10	A	2	0	1
2	1000001	P00087842	F	0-17	10	A	2	0	12
3	1000001	P00085442	F	0-17	10	A	2	0	12
4	1000002	P00285442	M	55+	16	C	4+	0	8

```
In [6]: #grabbing the first character of the years in city string to get rid of plus sign, and converting
         to int
        gdf['city_years'] = gdf.Stay_In_Current_City_Years.str.get(0).stoi()

In [7]: #Here we can see how we can control what the value of our dummies with the replace method and turn
        strings to ints
        gdf['City_Category'] = gdf.City_Category.str.replace('A', '1')
        gdf['City_Category'] = gdf.City_Category.str.replace('B', '2')
        gdf['City_Category'] = gdf.City_Category.str.replace('C', '3')
        gdf['City_Category'] = gdf['City_Category'].str.stoi()
```

Python Library

- A Python library for manipulating GPU DataFrames following the Pandas API
- Python interface to CUDA C++ library with additional functionality
- Creating GPU DataFrames from Numpy arrays, Pandas DataFrames, and PyArrow Tables
- JIT compilation of User-Defined Functions (UDFs) using Numba

Benchmarks: single-GPU Speedup vs. Pandas



cuDF v0.13, Pandas 0.25.3

Running on NVIDIA DGX-1:

GPU: NVIDIA Tesla V100 32GB
CPU: Intel(R) Xeon(R) CPU E5-2698 v4 @ 2.20GHz

Benchmark Setup:

RMM Pool Allocator Enabled

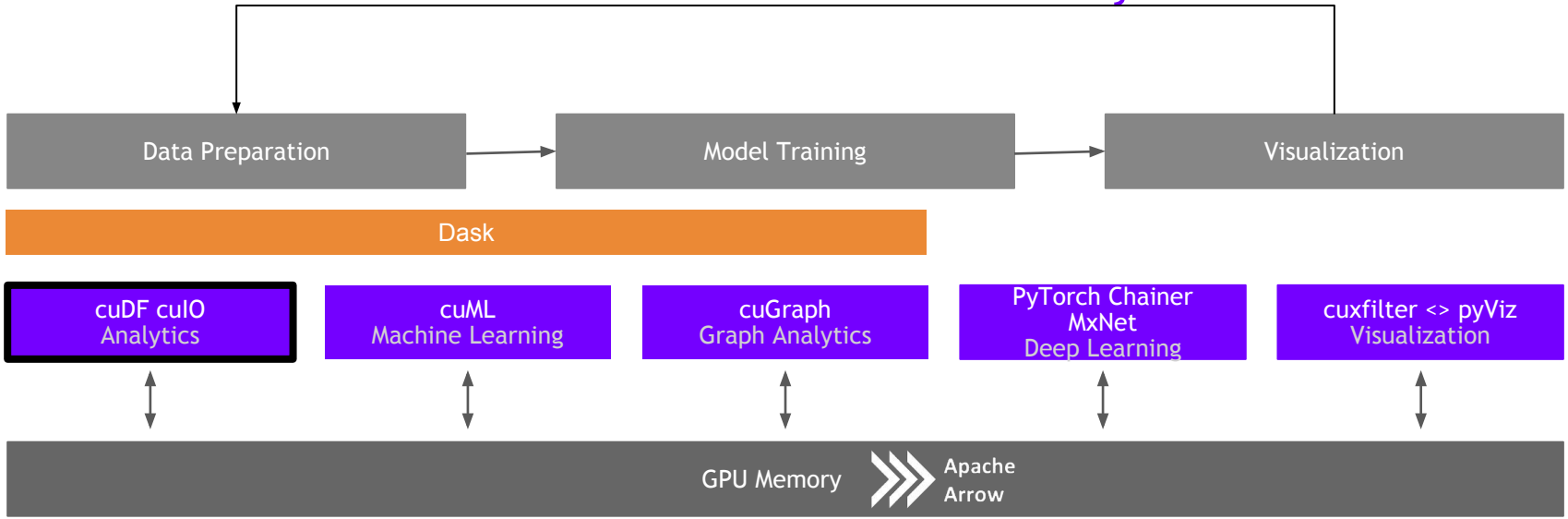
DataFrames: 2x int32 columns key columns, 3x int32 value columns

Merge: inner

GroupBy: count, sum, min, max calculated for each value column

ETL: the Backbone of Data Science

cuDF is not the end of the story



ETL: the Backbone of Data Science

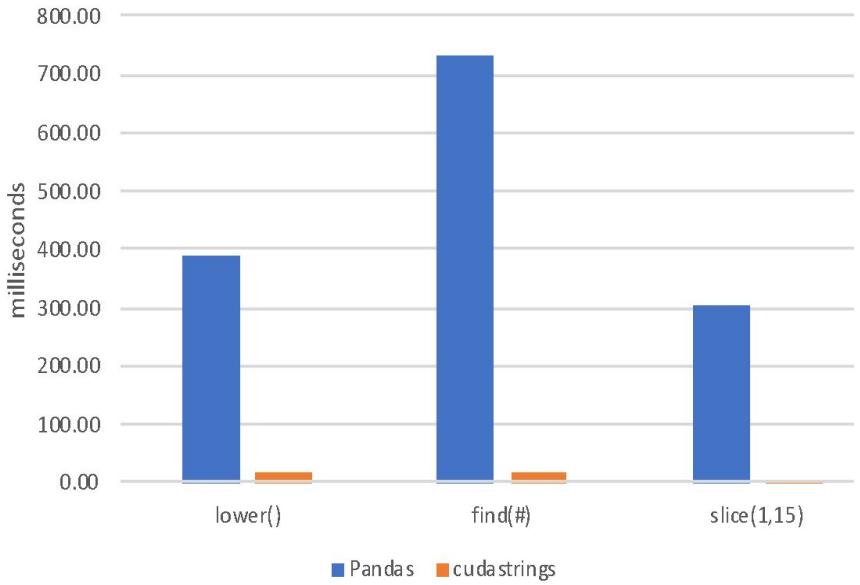
String Support

Current v0.13 String Support

- Regular Expressions
- Element-wise operations
  - Split, Find, Extract, Cat, Typecasting, etc…
- String GroupBys, Joins, Sorting, etc.
- Categorical columns fully on GPU
- Native String type in libcudf C++

Future v0.14+ String Support

- Further performance optimization
- JIT-compiled String UDFs



Extraction is the Cornerstone

cuDF I/O for Faster Data Loading

- Follow Pandas APIs and provide >10x speedup

- CSV Reader - v0.2, CSV Writer v0.8
- Parquet Reader – v0.7, Parquet Writer v0.12
- ORC Reader – v0.7, ORC Writer v0.10
- JSON Reader - v0.8
- Avro Reader - v0.9

- GPU Direct Storage integration in progress for bypassing PCIe bottlenecks!

- Key is GPU-accelerating both parsing and decompression wherever possible

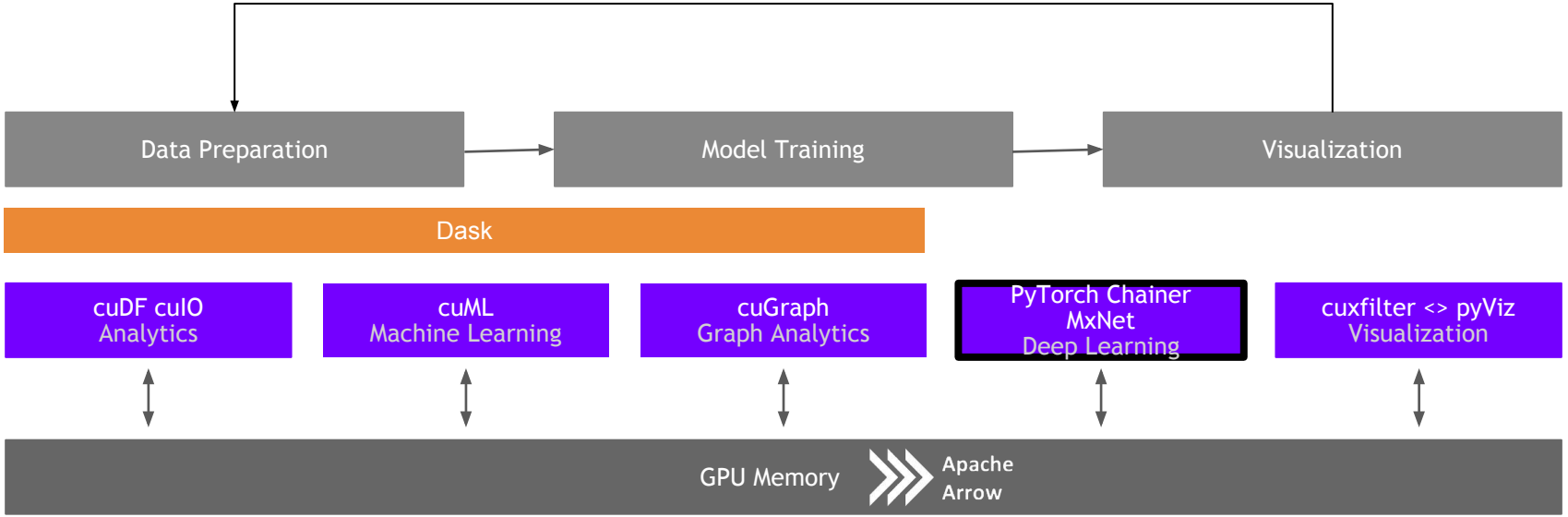
```
1]: import pandas, cudf

2]: %time len(pandas.read_csv('data/nyc/yellow_tripdata_2015-01.csv'))
CPU times: user 25.9 s, sys: 3.26 s, total: 29.2 s
Wall time: 29.2 s
2]: 12748986

3]: %time len(cudf.read_csv('data/nyc/yellow_tripdata_2015-01.csv'))
CPU times: user 1.59 s, sys: 372 ms, total: 1.96 s
Wall time: 2.12 s
3]: 12748986

4]: !du -hs data/nyc/yellow_tripdata_2015-01.csv
1.9G    data/nyc/yellow_tripdata_2015-01.csv
```

Source: Apache Crail blog: SQL Performance: Part 1 - Input File Formats

ETL is not just DataFrames!

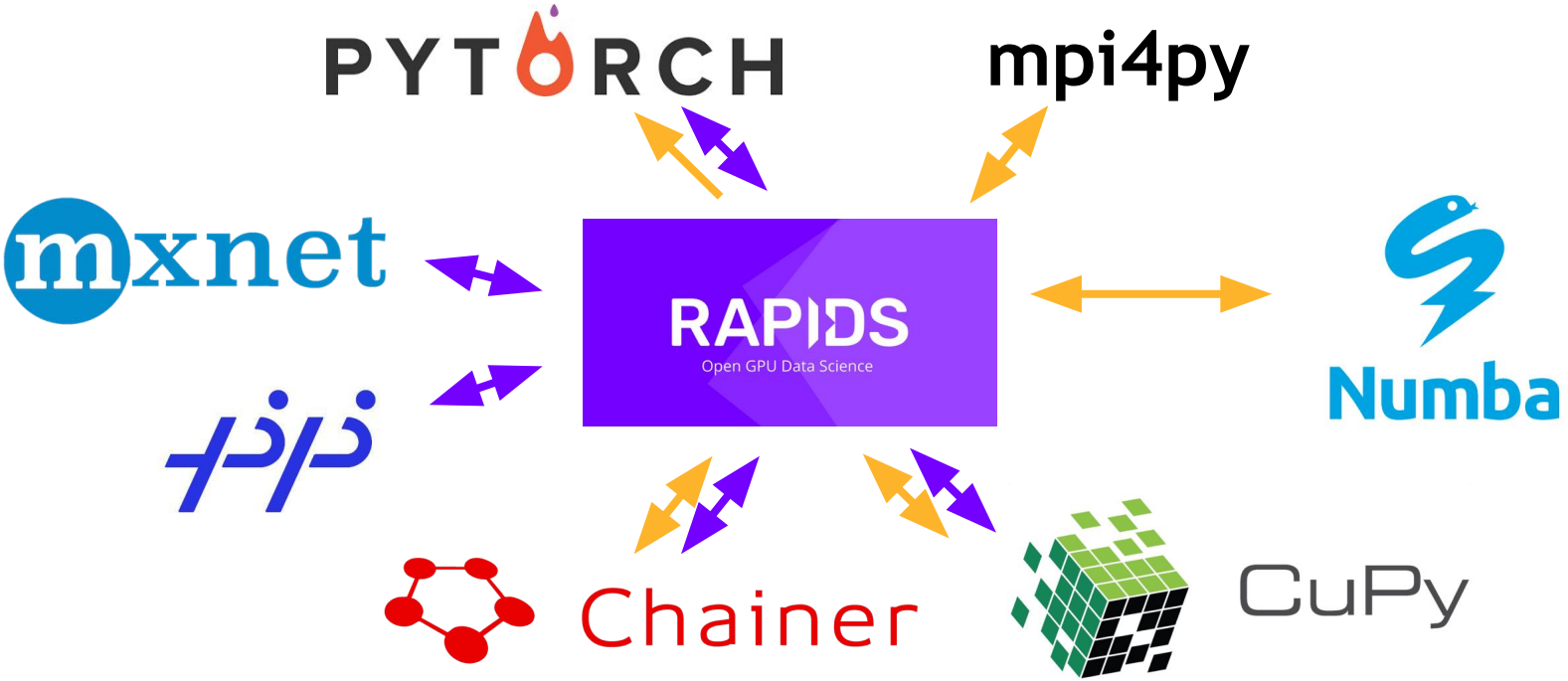
RAPIDS

Building bridges into the array ecosystem



Interoperability for the Win

DLPack and __cuda_array_interface__



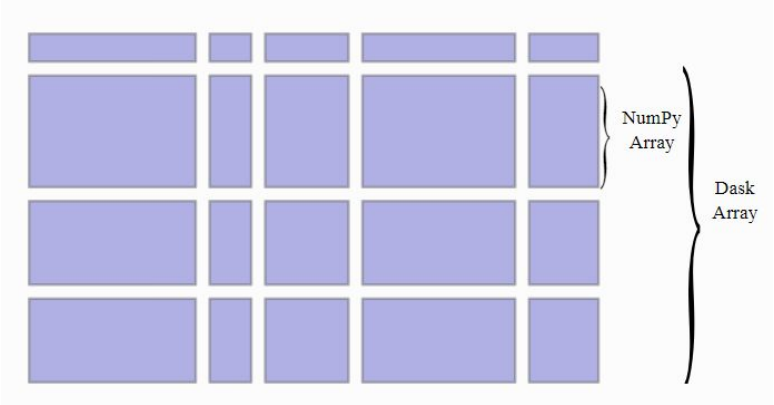
ETL: Arrays and DataFrames

Dask and CUDA Python arrays

Chainer

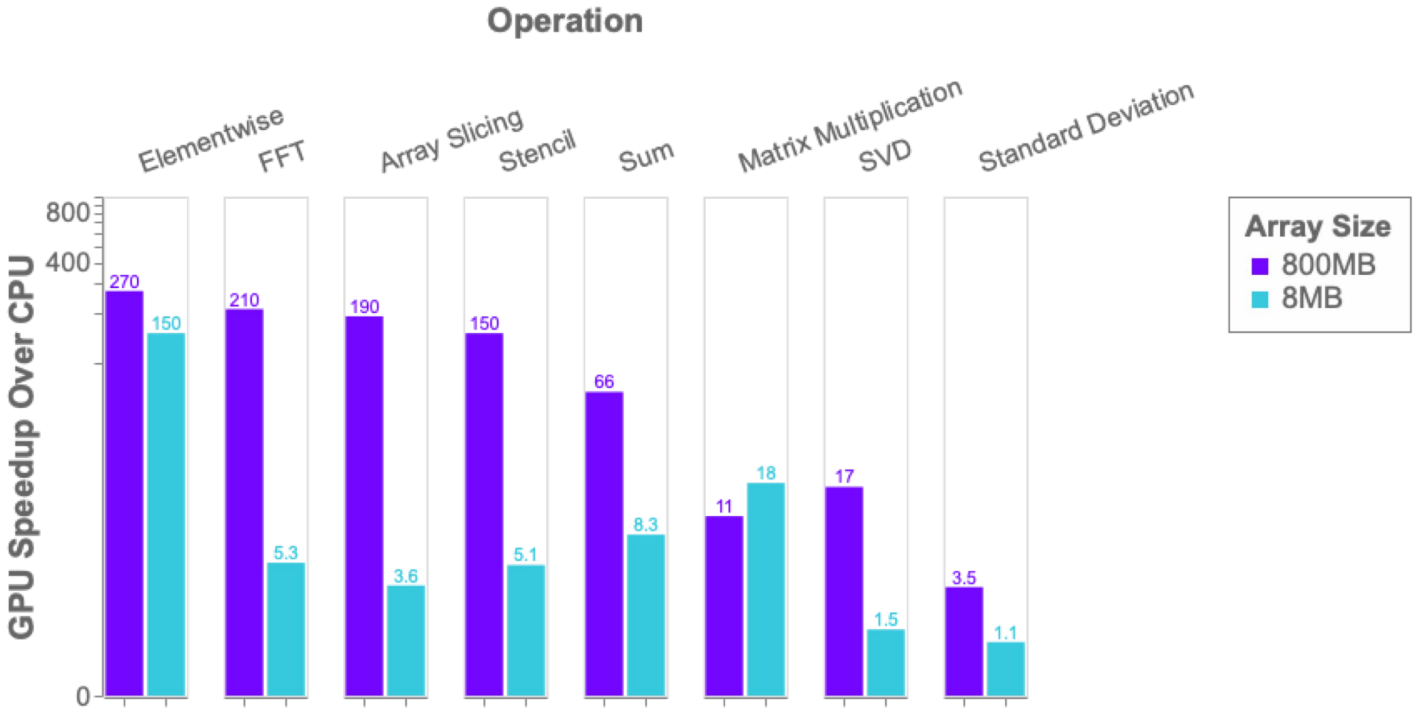
CuPy

Numba



- Scales NumPy to distributed clusters
- Used in climate science, imaging, HPC analysis up to 100TB size
- Now seamlessly accelerated with GPUs

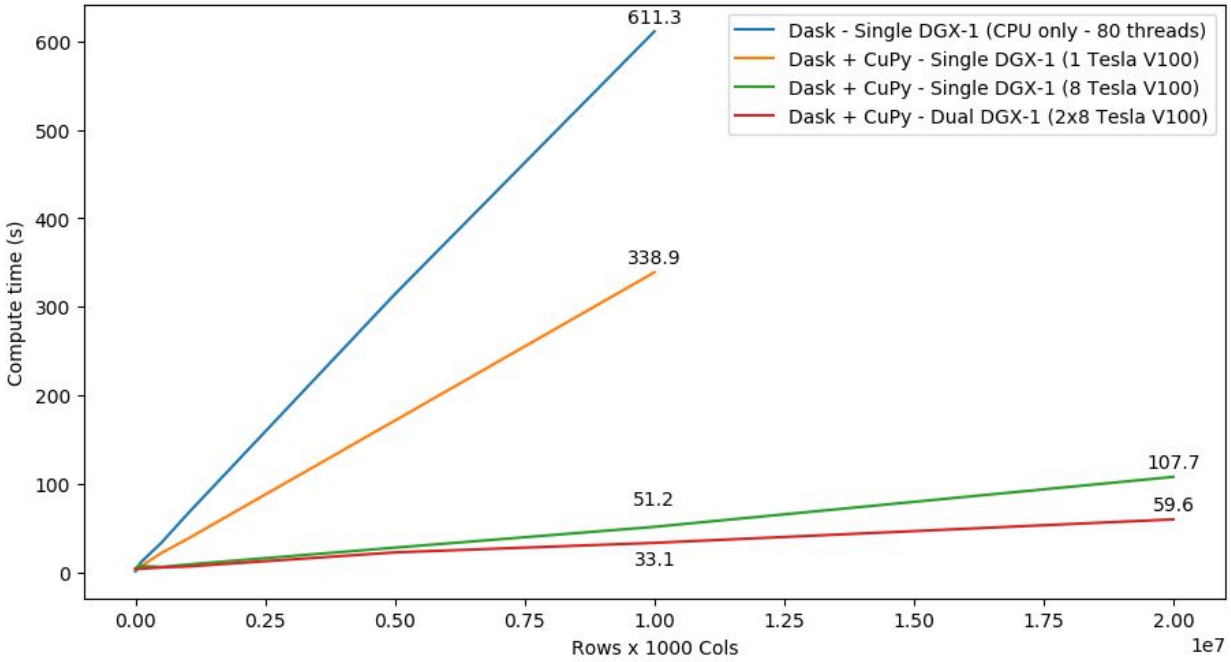
Benchmark: single-GPU CuPy vs NumPy



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

SVD Benchmark

Dask and CuPy Doing Complex Workflows



Petabyte Scale Analytics with Dask and CuPy

Architecture	Time
Single CPU Core	2hr 39min
Forty CPU Cores	11min 30s
One GPU	1min 37s
Eight GPUs	19s

https://blog.dask.org/2019/01/03/dask-array-gpus-first-steps

3.2 PETABYTES IN LESS THAN 1 HOUR

Distributed GPU array | parallel reduction | using 76x GPUs

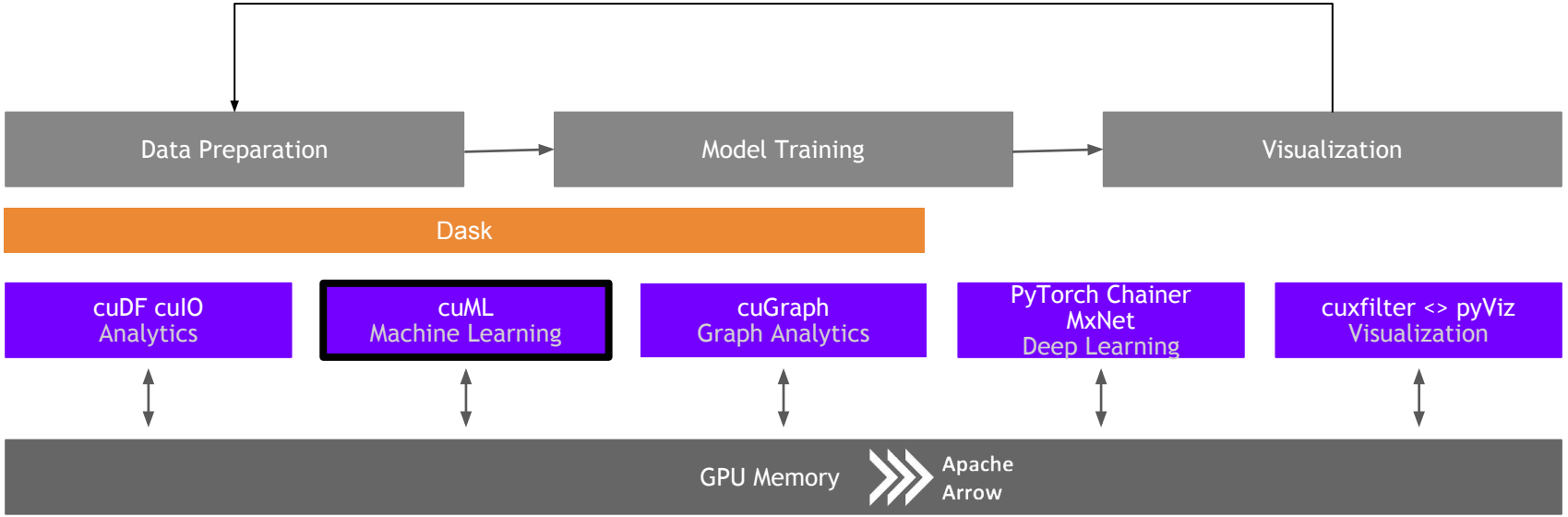
Array size	Wall Time (data creation + compute)
3.2 PB (20M x 20M doubles)	54 min 51 s

Cluster configuration: 20x GCP instances, each instance has:
CPU: 1 VM socket (Intel Xeon CPU @ 2.30GHz), 2-core, 2 threads/core, 132GB mem, GbE ethernet, 950 GB disk
GPU: 4x NVIDIA Tesla P100-16GB-PCIe (total GPU DRAM across nodes 1.22 TB)
Software: Ubuntu 18.04, RAPIDS 0.5.1, Dask=1.1.1, Dask-Distributed=1.1.1, CuPY=5.2.0, CUDA 10.0.130

cuML

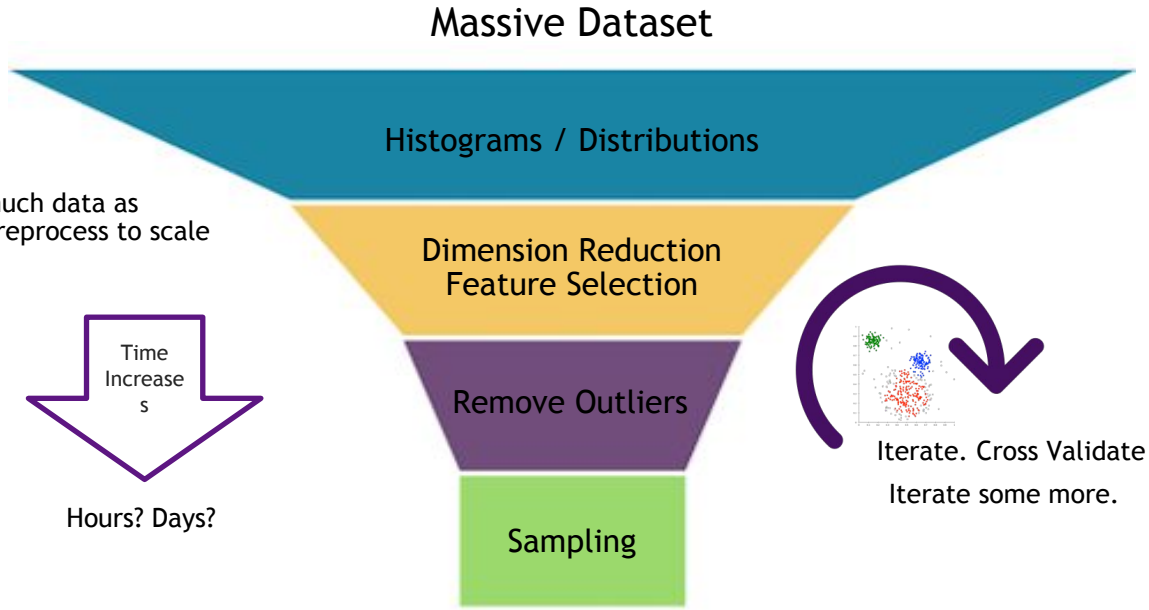
Machine Learning

More models more problems



Problem

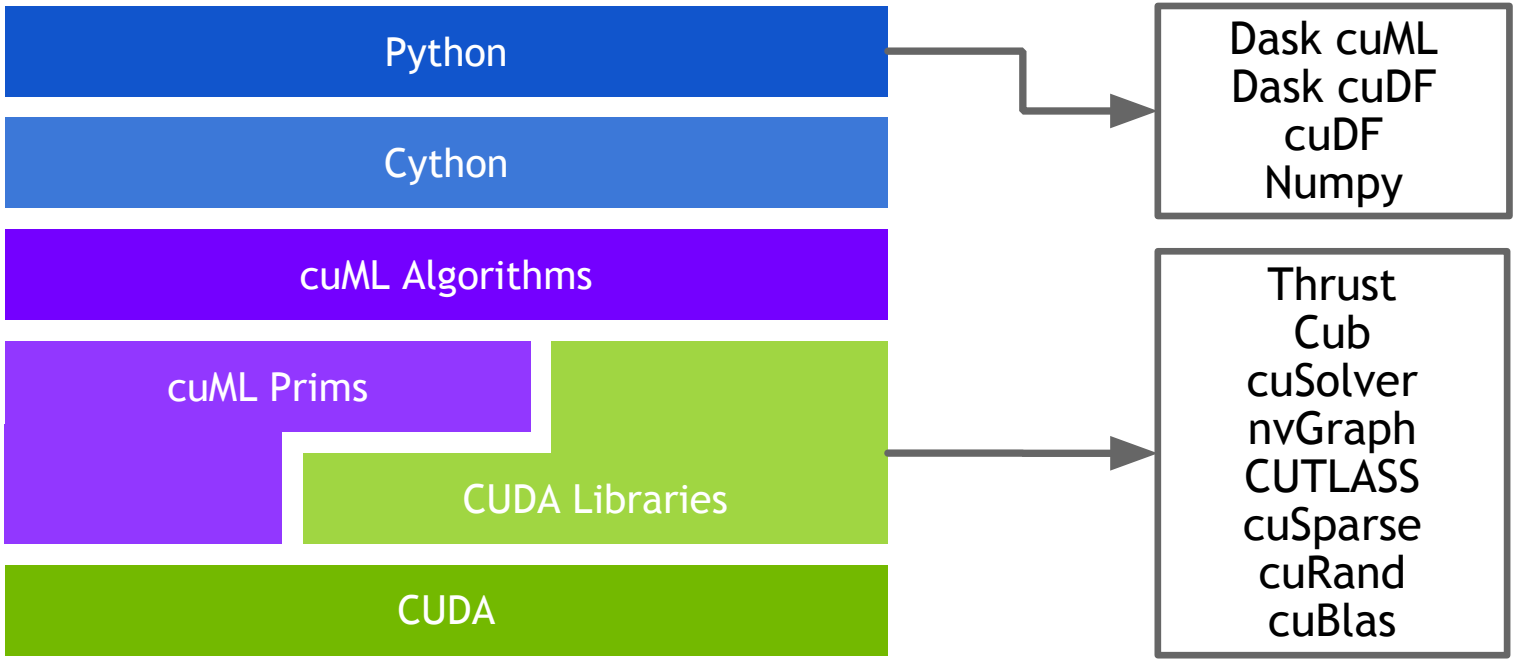
Data sizes continue to grow



Better to start with as much data as possible and explore / preprocess to scale to performance needs.

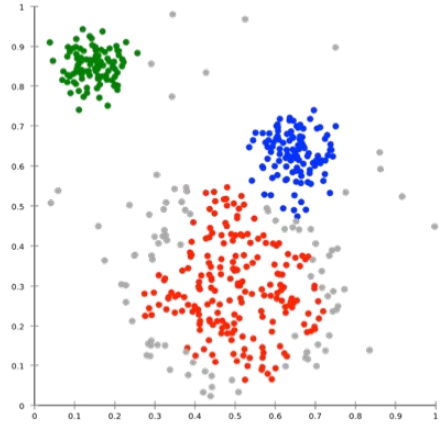
Meet reasonable speed vs accuracy tradeoff

ML Technology Stack



Algorithms

GPU-accelerated Scikit-Learn



Cross Validation

Hyper-parameter Tuning

More to come!

Classification / Regression

Decision Trees / **Random Forests**
Linear Regression
Logistic Regression
K-Nearest Neighbors
Support Vector Machines

Inference

Random forest / GBDT inference

Clustering

K-Means
DBSCAN
Spectral Clustering

Decomposition & Dimensionality Reduction

Principal Components
Singular Value Decomposition
UMAP
Spectral Embedding
T-SNE

Time Series

Holt-Winters
Seasonal ARIMA

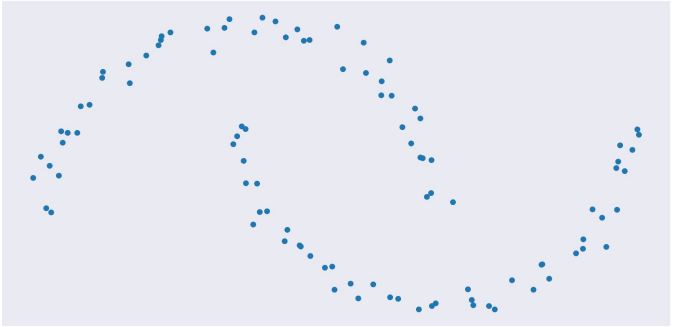
Key:

- Preexisting
- **NEW or enhanced for 0.13**

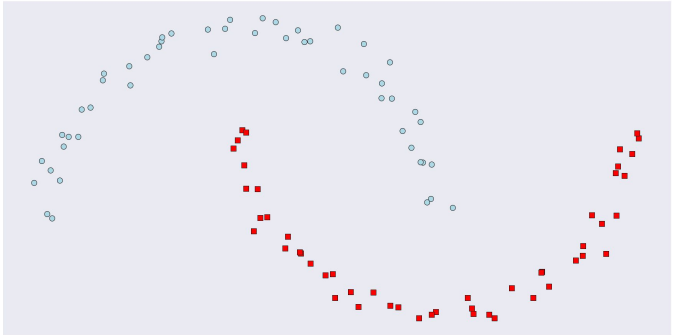
RAPIDS matches common Python APIs

CPU-Based Clustering

```
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)
```

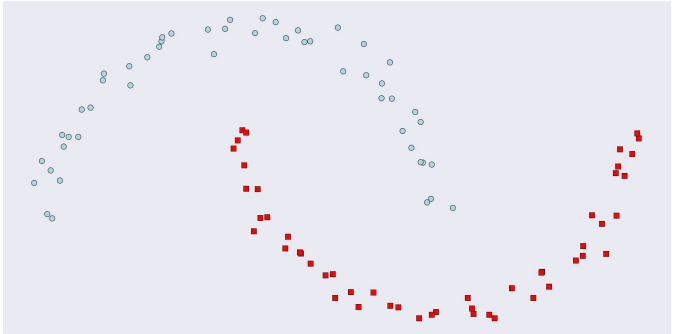


RAPIDS matches common Python APIs

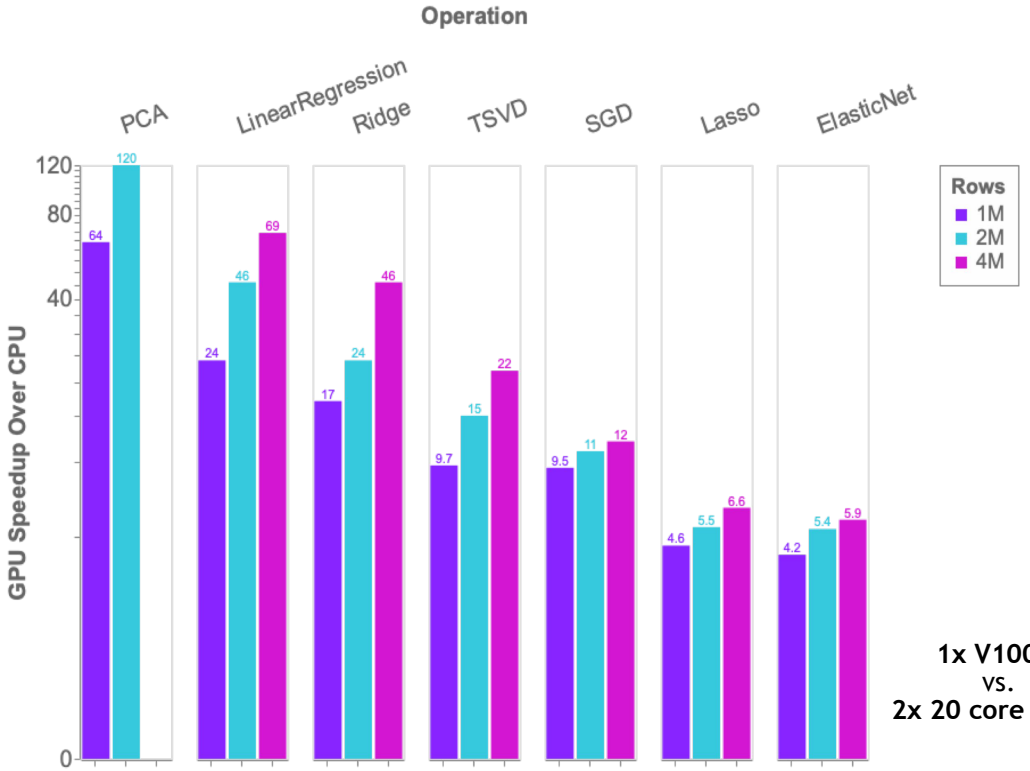
GPU-Accelerated Clustering

```
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])})
```

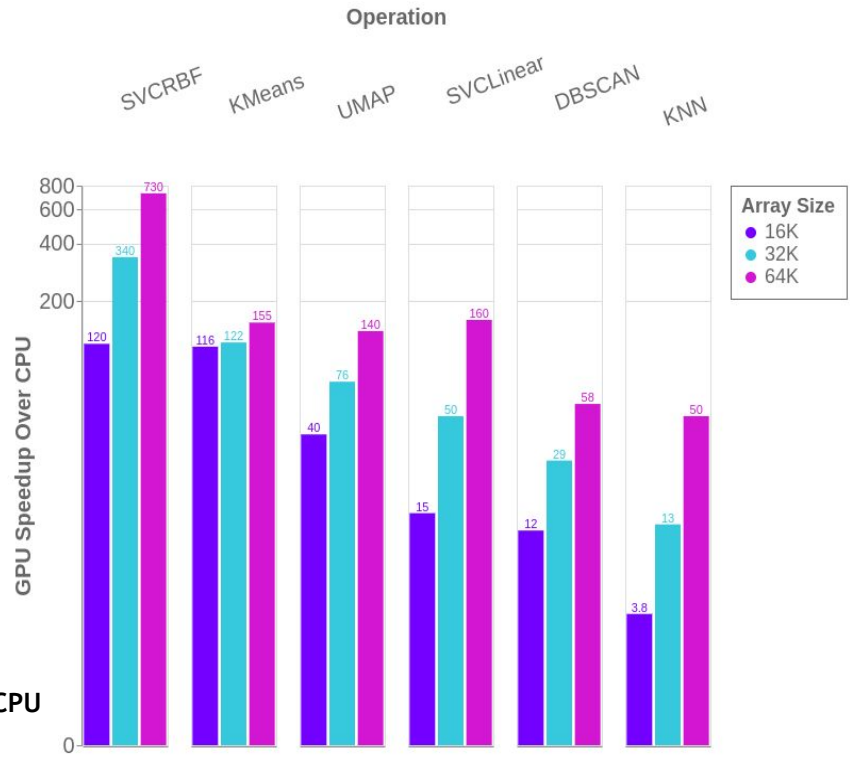
```
from cuml           import DBSCAN
dbscan = DBSCAN(eps = 0.3, min_samples = 5)

dbscan.fit(X)

y_hat = dbscan.predict(X)
```



Benchmarks: single-GPU cuML vs scikit-learn



1x V100
vs.
2x 20 core CPU

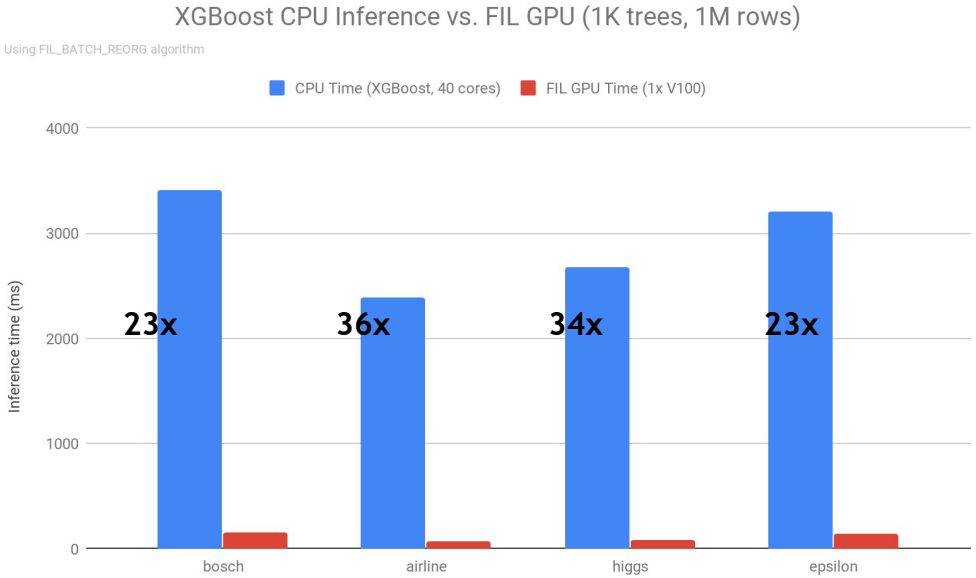


Forest Inference

Taking models from training to production

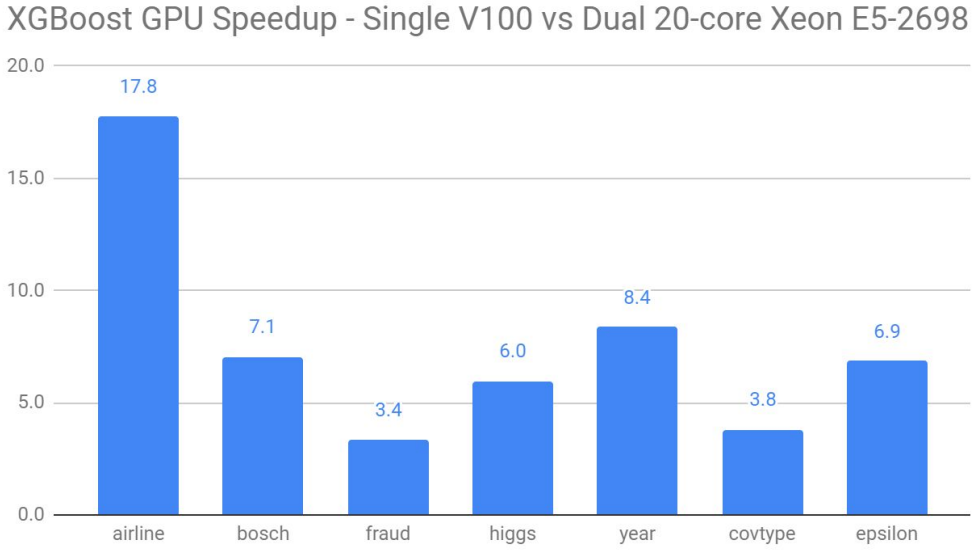
cuML's **Forest Inference Library** accelerates prediction (inference) for random forests and boosted decision trees:

- Works with existing saved models (XGBoost, LightGBM, scikit-learn RF cuML RF soon)
- Lightweight Python API
- Single V100 GPU can infer up to 34x faster than XGBoost dual-CPU node
- Over 100 million forest inferences per sec (with 1000 trees) on a DGX-1 for large (sparse) or dense models



RAPIDS + dmlc XGBoost

- RAPIDS works closely with the XGBoost community to accelerate GBDTs on GPU
- The default rapids conda metapackage includes XGBoost
- XGBoost can seamlessly load data from cuDF dataframes and cuPy arrays
- Dask allows XGBoost to scale to arbitrary numbers of GPUs
- With the *gpu_hist* tree method, a single GPU can outpace 10s to 100s of CPUs
- Version 1.0 of XGBoost launched with the RAPIDS 0.13 stack.



Road to 1.0

March 2020 - RAPIDS 0.13

cuML	Single-GPU	Multi-GPU	Multi-Node-Multi-GPU
Gradient Boosted Decision Trees (GBDT)			
Linear Regression			
Logistic Regression			
Random Forest			
K-Means			
K-NN			
DBSCAN			
UMAP			
Holt-Winters			
ARIMA			
t-SNE			
Principal Components			
Singular Value Decomposition			
SVM			

Road to 1.0

2020 - RAPIDS 1.0

cuML	Single-GPU	Multi-Node-Multi-GPU
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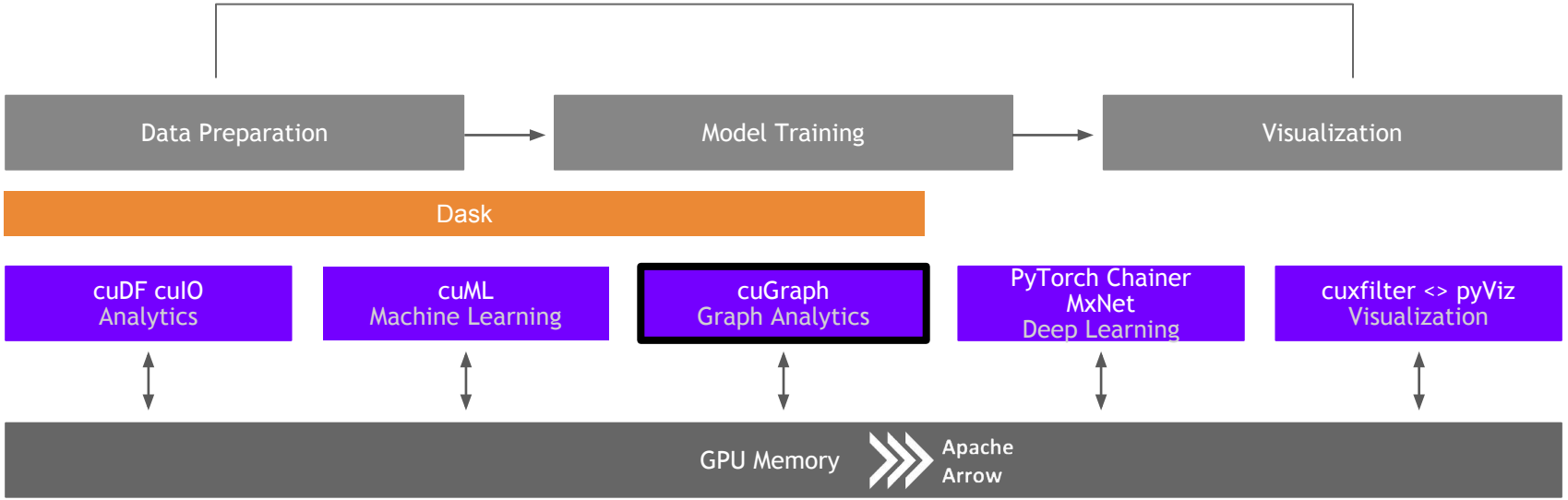
SVM		

cuGraph

Graph Analytics

More connections more insights



Goals and Benefits of cuGraph

Focus on Features and User Experience

Breakthrough Performance

- Up to 500 million edges on a single 32GB GPU
- Multi-GPU support for scaling into the billions of edges

Multiple APIs

- **Python**: Familiar NetworkX-like API
- **C/C++:** lower-level granular control for application developers

Seamless Integration with cuDF and cuML

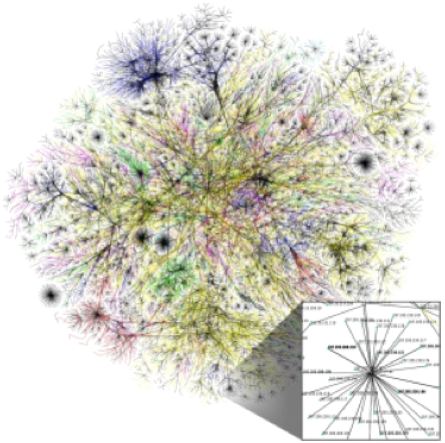
- Property Graph support via DataFrames

Growing Functionality

- Extensive collection of algorithm, primitive, and utility functions

Algorithms

GPU-accelerated NetworkX



Graph Classes

Renumbering
Auto-renumbering

Structure	Community	Spectral Clustering Balanced-Cut Modularity Maximization Louvain Ensemble Clustering for Graphs Subgraph Extraction KCore and KCore Number Triangle Counting ***K-Truss***
Multi-GPU	Components	Weakly Connected Components Strongly Connected Components
Utilities	Link Analysis	Page Rank (Multi-GPU) Personal Page Rank
More to come!	Link Prediction	Jaccard Weighted Jaccard Overlap Coefficient
	Traversal	Single Source Shortest Path (SSSP) Breadth First Search (BFS)
	Centrality	Katz ***Betweenness Centrality***

Multi-GPU PageRank Performance

PageRank portion of the HiBench benchmark suite

HiBench Scale	Vertices	Edges	CSV File (GB)	# of V100 GPUs	# of CPU Threads	PageRank for 3 Iterations (secs)
Huge	5,000,000	198,000,000	3	1		1.1
BigData	50,000,000	1,980,000,000	34	3		5.1
BigData x2	100,000,000	4,000,000,000	69	6		9.0
BigData x4	200,000,000	8,000,000,000	146	12		18.2
BigData x8	400,000,000	16,000,000,000	300	16		31.8
BigData x8	400,000,000	16,000,000,000	300		800*	5760*

*BigData x8, 100x 8-vCPU nodes, Apache Spark GraphX ⇒ 96 mins!

Community

Ecosystem Partners

CONTRIBUTORS

ADOPTERS

OPEN SOURCE

Building on top of RAPIDS

A bigger, better, stronger ecosystem for all

Streamz

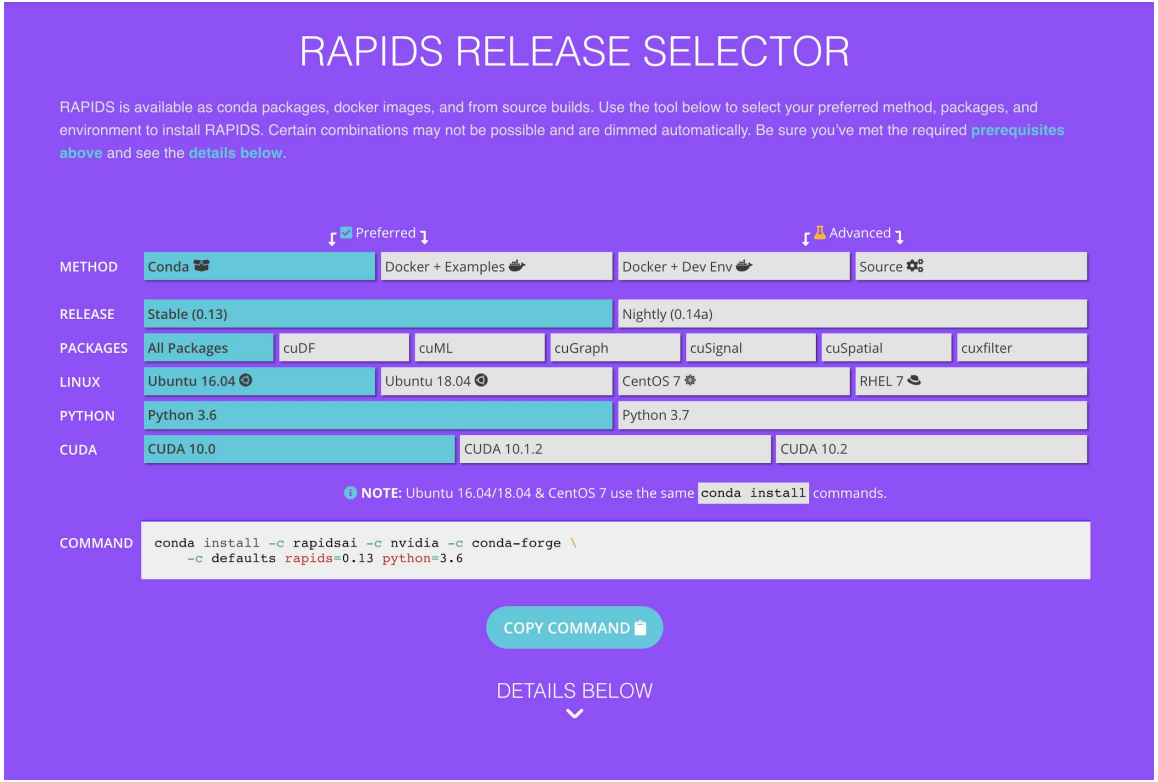
High-Performance Serverless event and data processing that utilizes RAPIDS for GPU Acceleration

GPU accelerated SQL engine built on top of RAPIDS

Distributed stream processing using RAPIDS and Dask

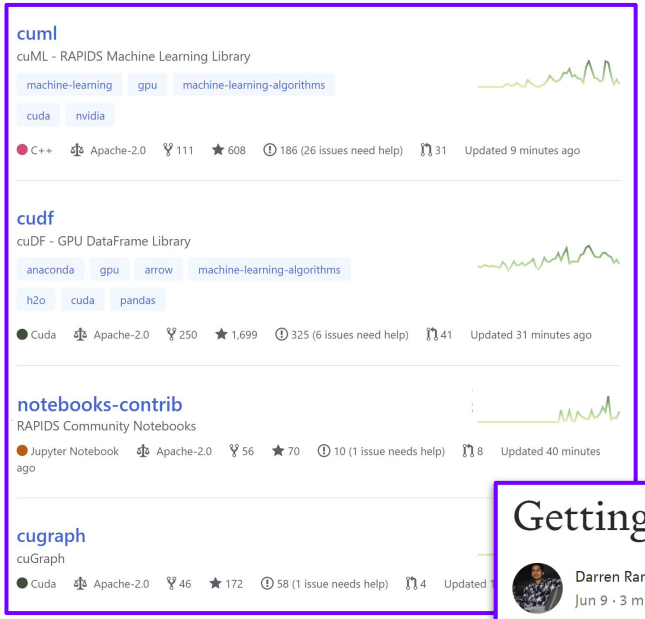
Easy Installation

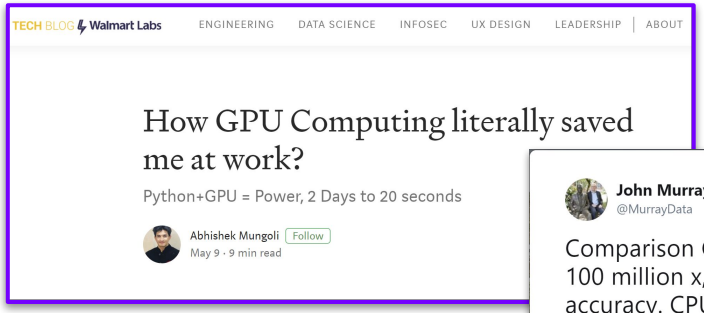
Interactive Installation Guide

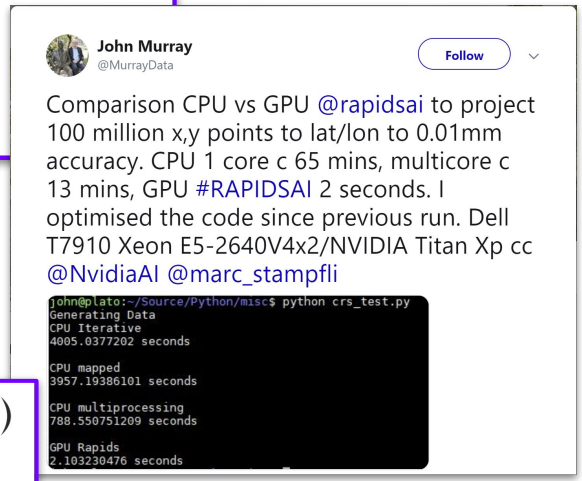


Contribute Back

Issues, feature requests, PRs, Blogs, Tutorials, Videos, QA...bring your best!



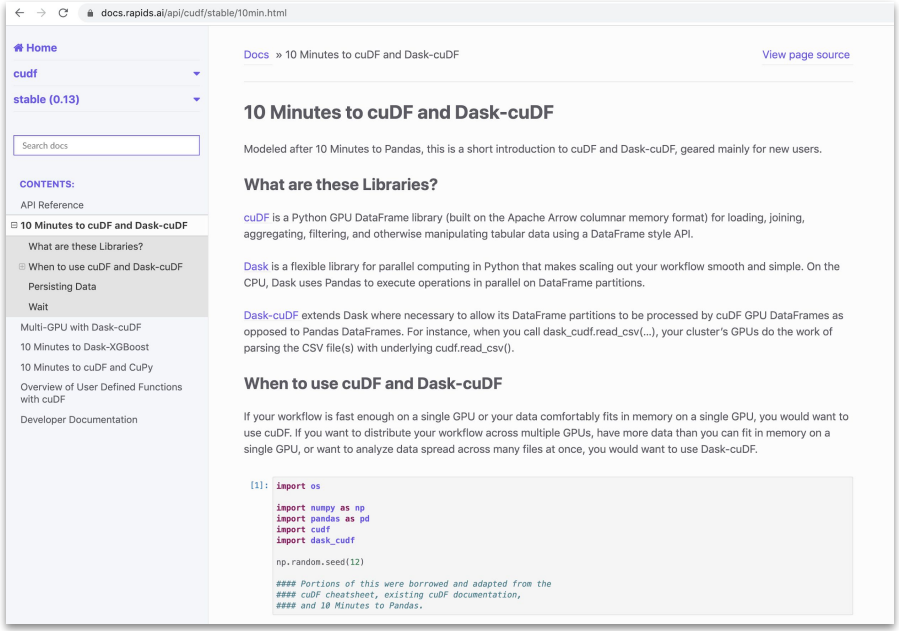




Getting Started

RAPIDS Docs

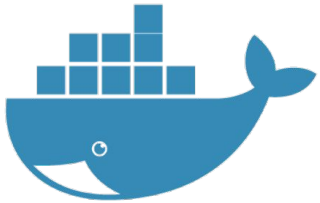
Improved and easier to use!



https://docs.rapids.ai

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/

THANK YOU

Nick Becker

nicholas@nvidia.com

RAPIDS