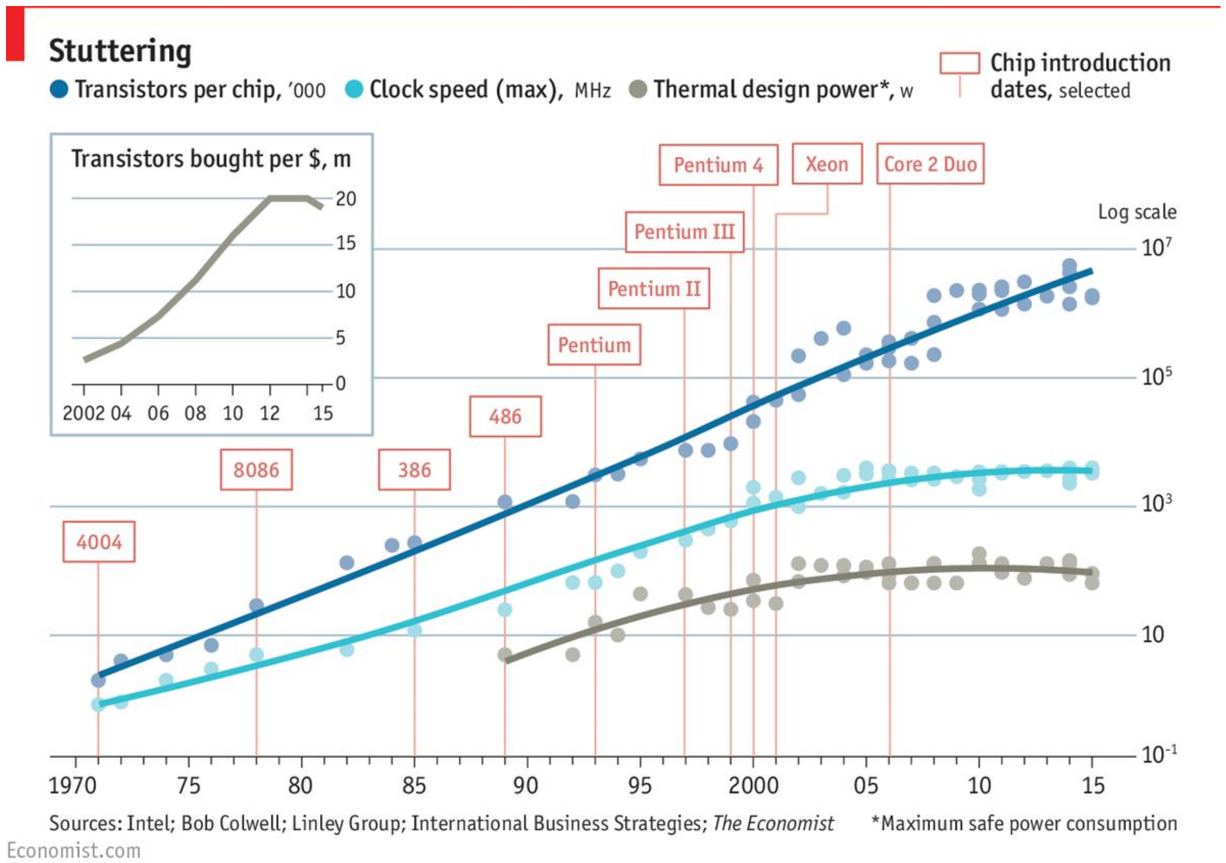
GPU Accelerated Data Analytics in Python

Mads R. B. Kristensen, NVIDIA


Stuttering
Transistors per chip, '000
Clock speed (max), MHz
Thermal design power*, w
Chip introduction dates, selected
Transistors bought per $, m
20
15
10
5
0
2002 04 06 08 10 12 15
4004
8086
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486
Pentium
Pentium II
Pentium III
Pentium 4
Xeon
Core 2 Duo
Log scale
10^7
10^5
10^3
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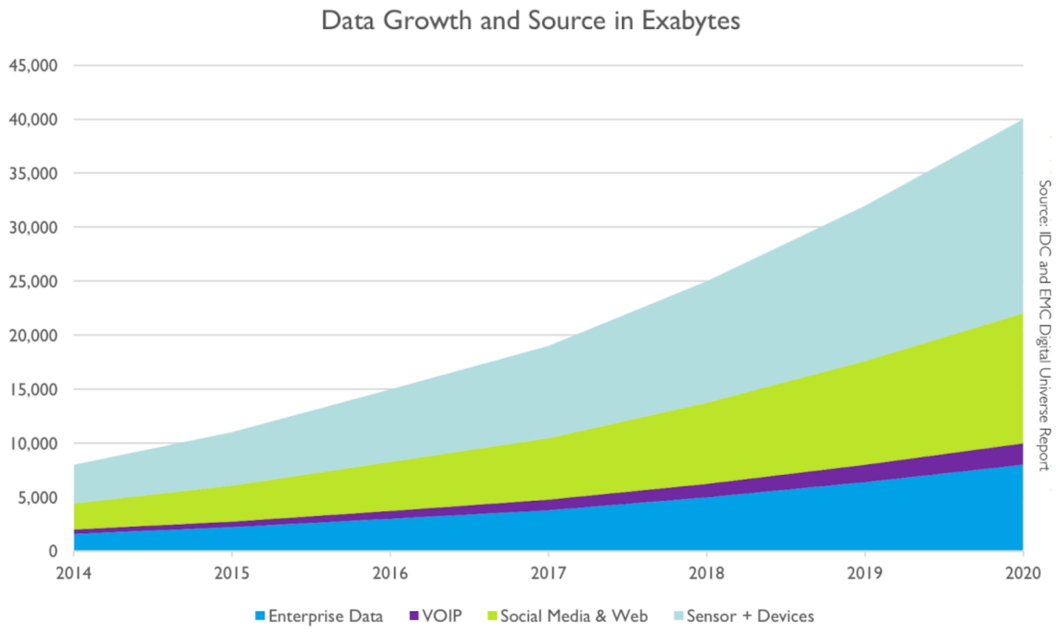
10^{-1}
1970 75 80 85 90 95 2000 05 10 15
Sources: Intel; Bob Colwell; Linley Group; International Business Strategies; *The Economist*
*Maximum safe power consumption
Economist.com


Data Growth and Source in Exabytes
45,000
40,000
35,000
30,000
25,000
20,000
15,000
10,000
5,000
0
2014 2015 2016 2017 2018 2019 2020
Enterprise Data
VOIP
Social Media & Web
Sensor + Devices
Source: IDC and EMC Digital Universe Report

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

Dask + RAPIDS

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

PyData

NumPy, Pandas, Scikit-Learn
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

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NumPy

scikit learn

pandas

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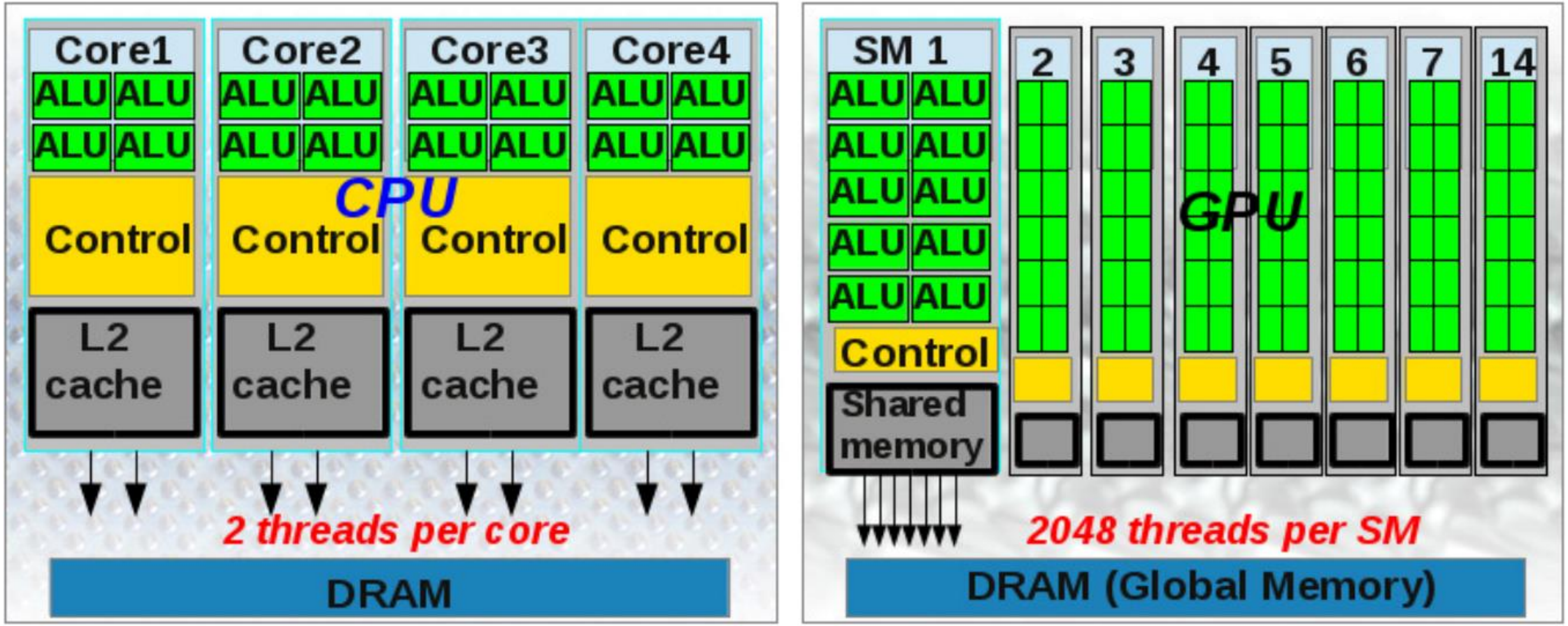
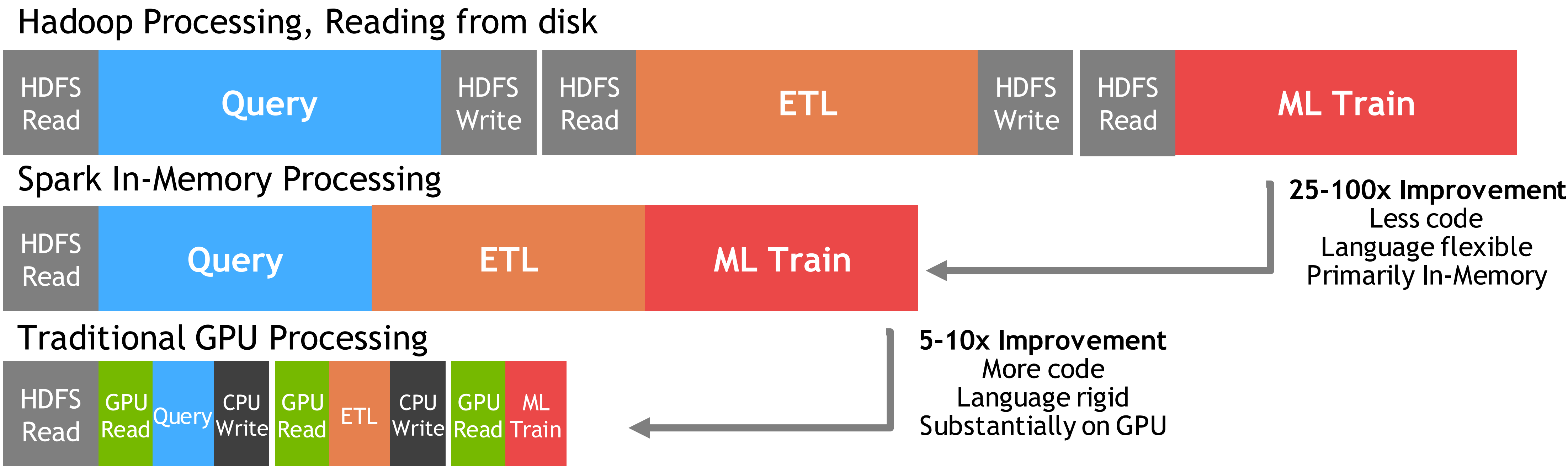
CPU vs GPU



DOI: 10.1016/j.cam.2013.12.032.

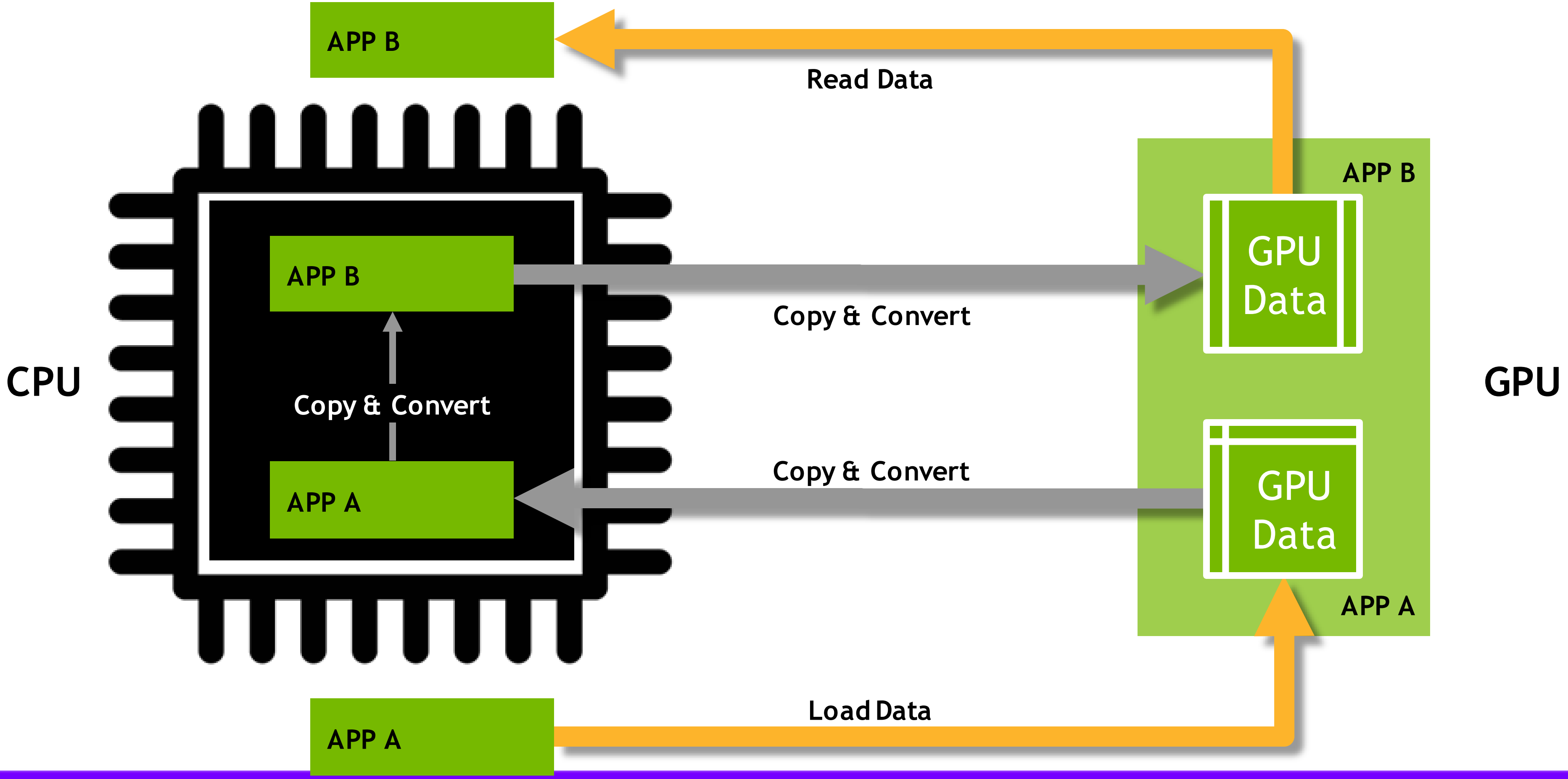
Data Processing Evolution

Faster data access, less data movement



Data Movement and Transformation

What if we could keep data on the GPU?



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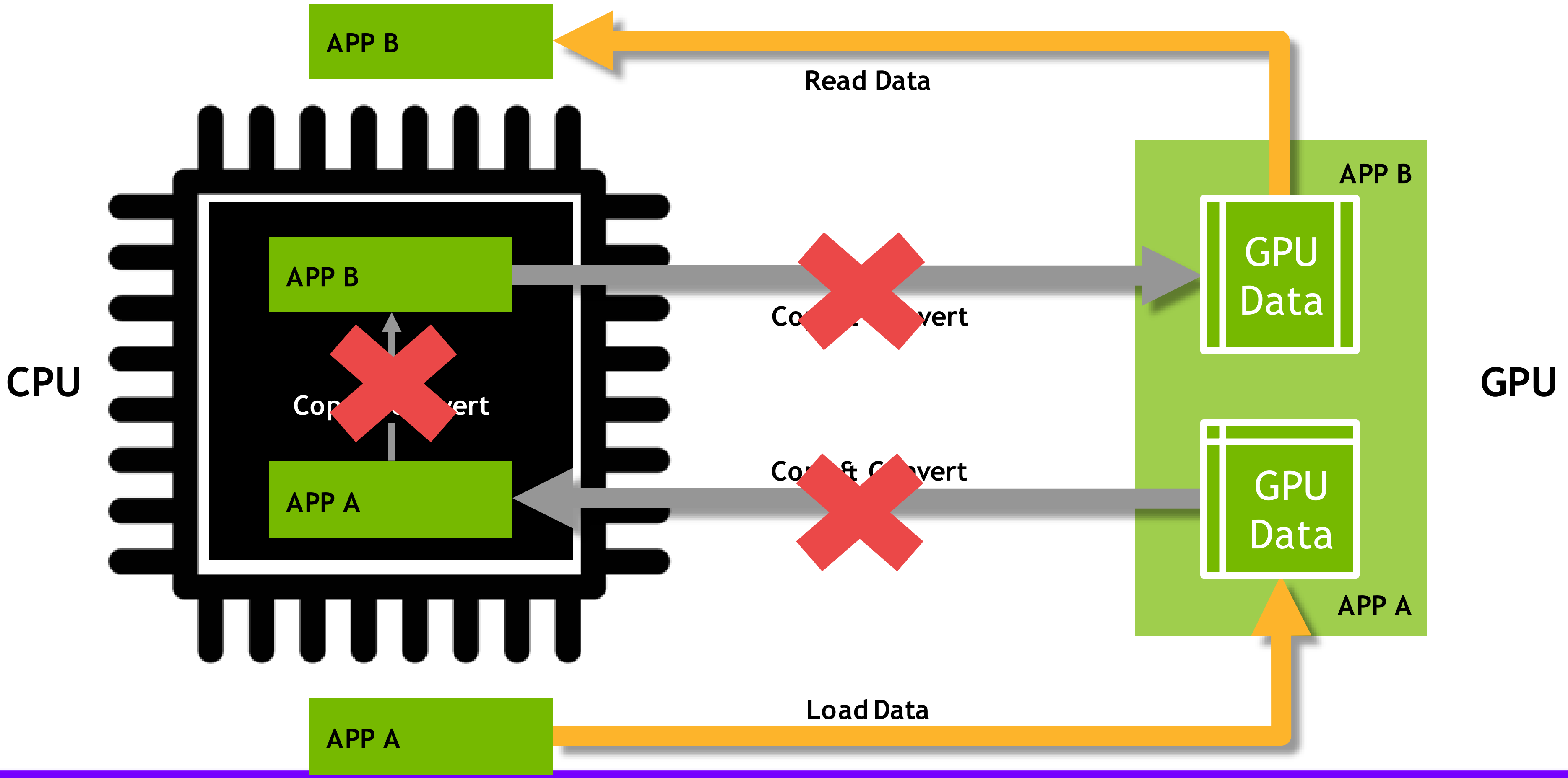

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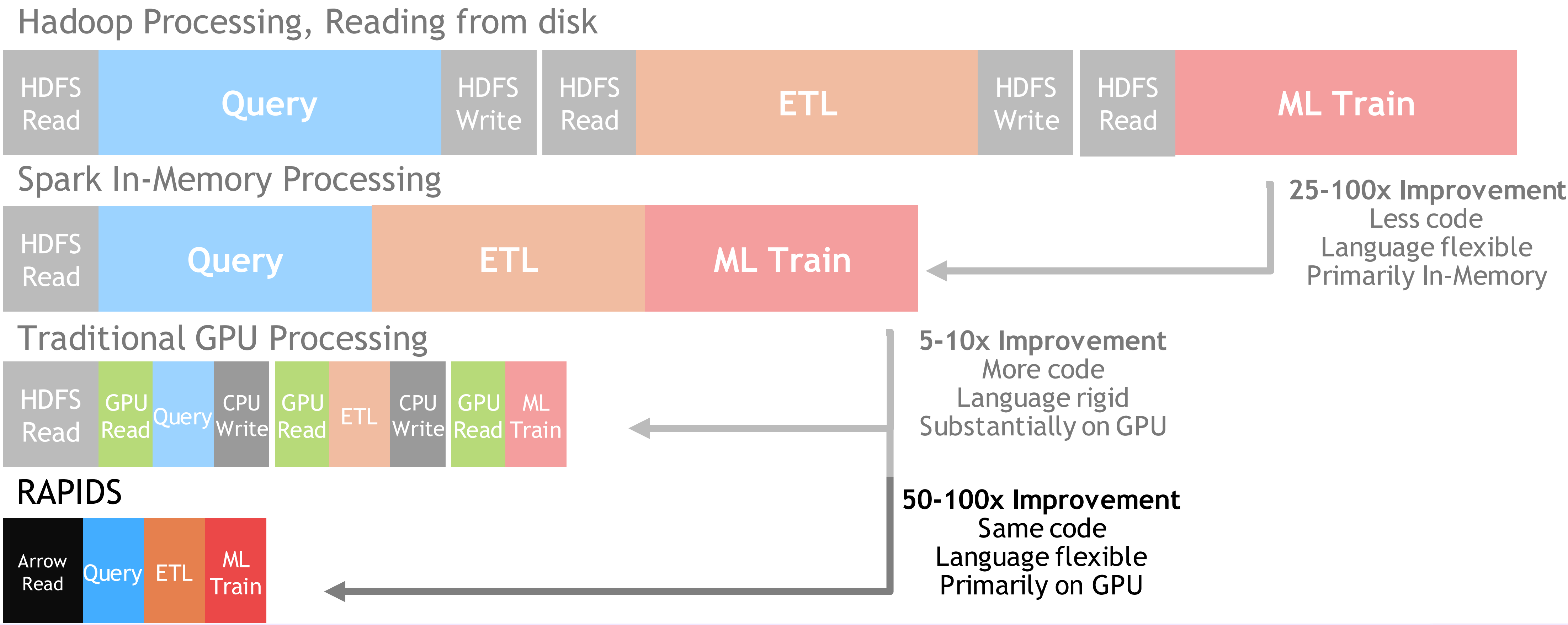
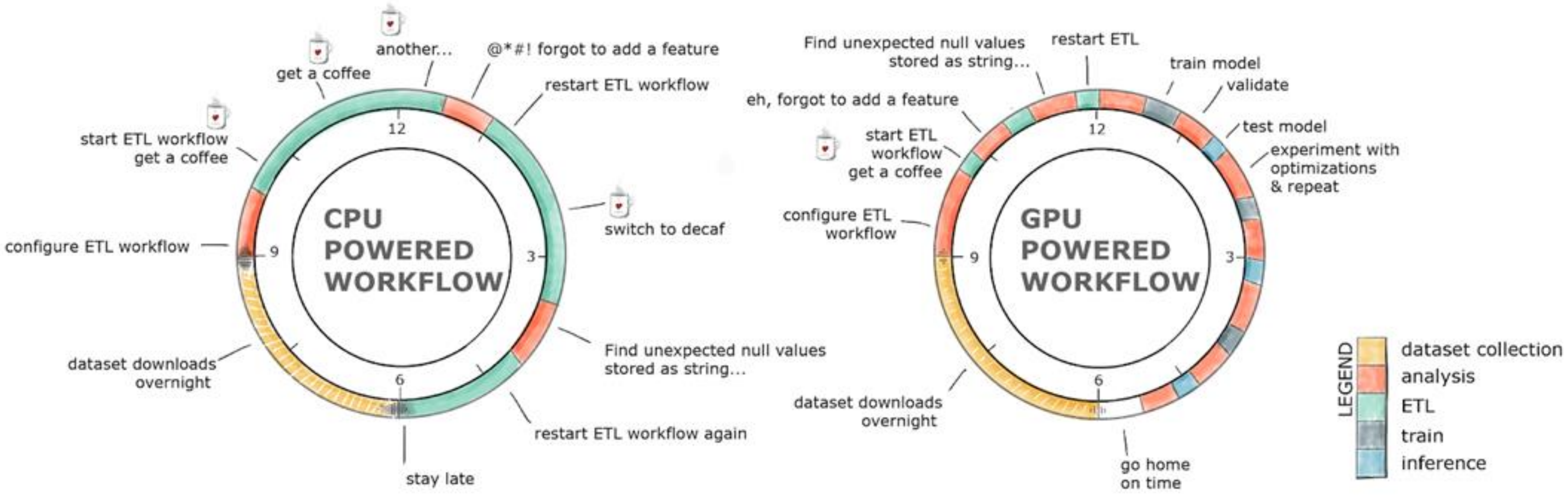


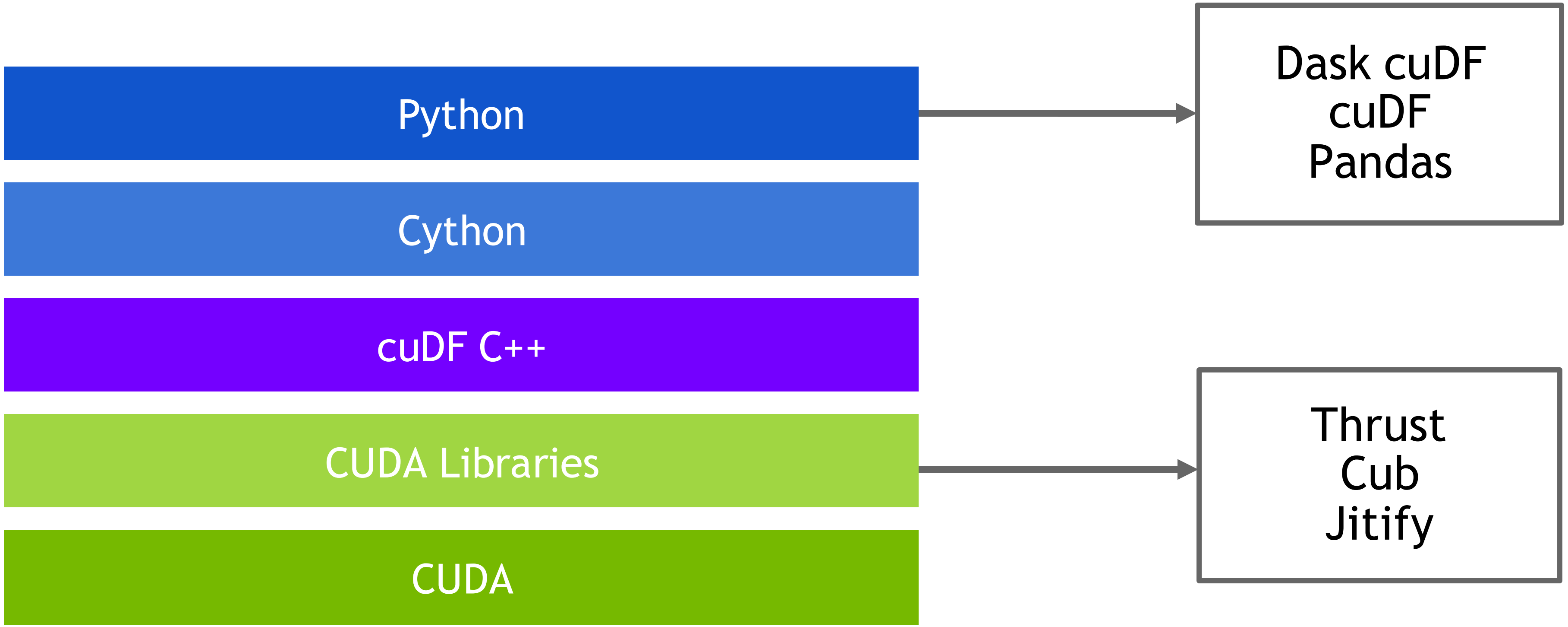
CuDF – Pandas on GPU

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

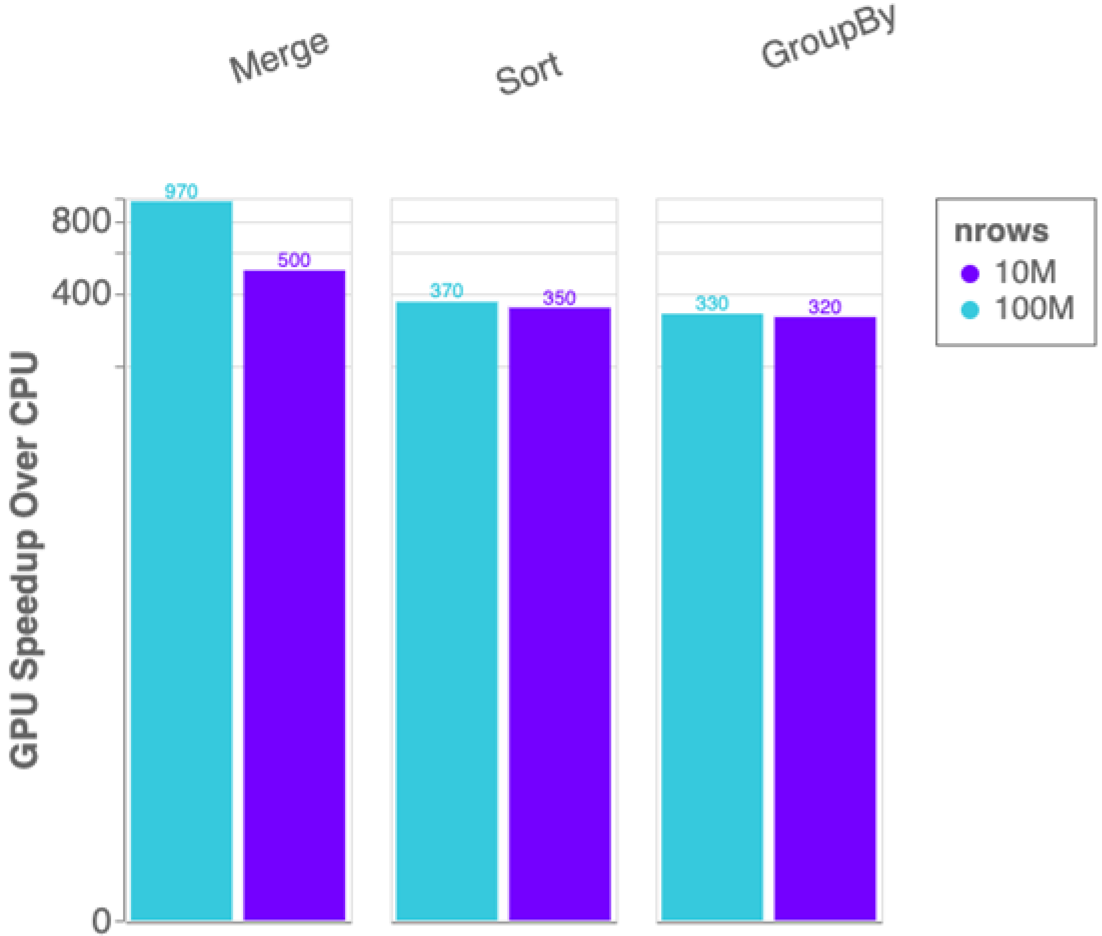
```
In [6]: #grabbing the first character of the years in city string to get rid of plus sign, and converting
  to int
gdf['city_years'] = gdf.Stay_In_Current_City_Years.str.get(0).stoi()
```

```
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

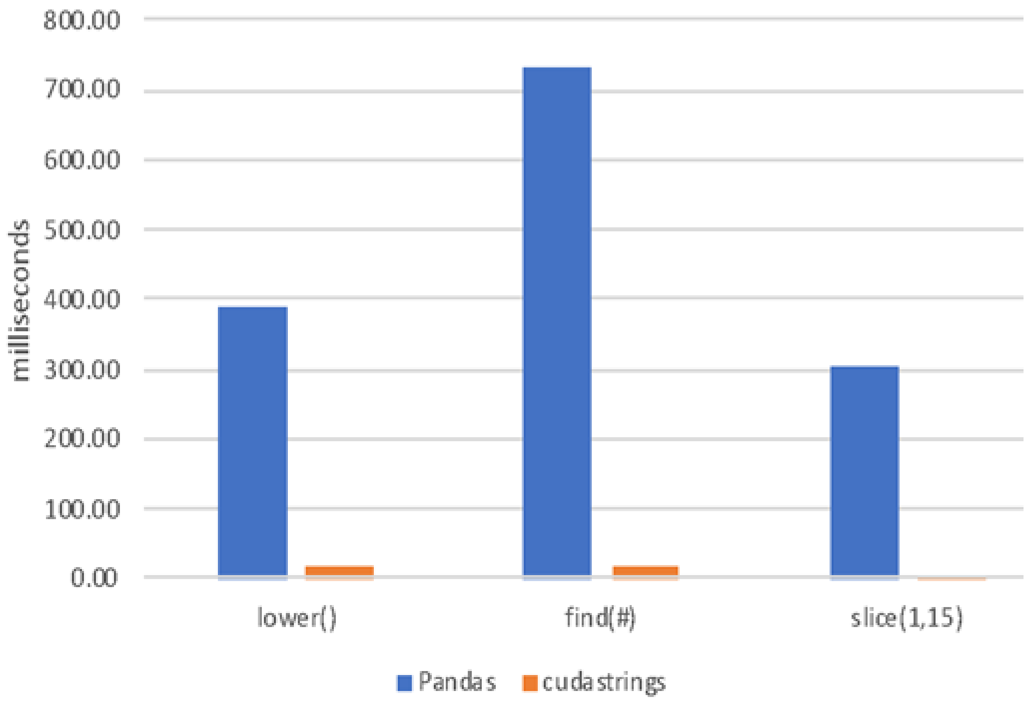
String Support

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

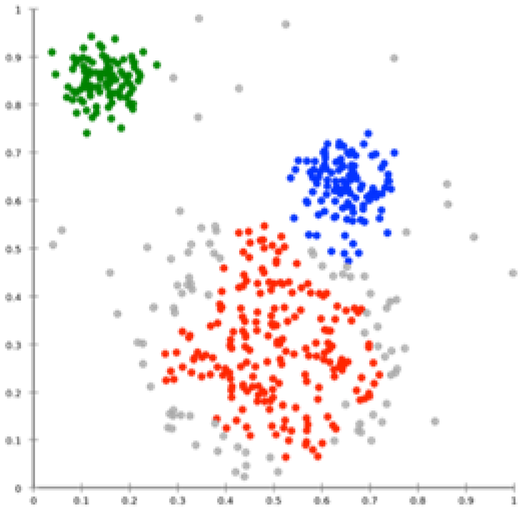
- Further performance optimization
- JIT-compiled String UDFs



CuML – Scikit-Learn on GPU

Algorithms

GPU-accelerated Scikit-Learn



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

Cross Validation

Hyper-parameter Tuning

More to come!

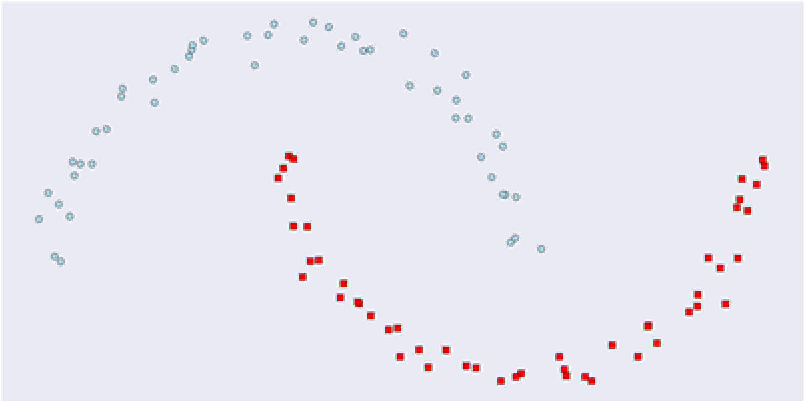
Key:
- Preexisting
- **NEW or enhanced for 0.13**

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)
```



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GPU-Accelerated Clustering

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import cudf

X, y = make_moons(n_samples=int(1e2),
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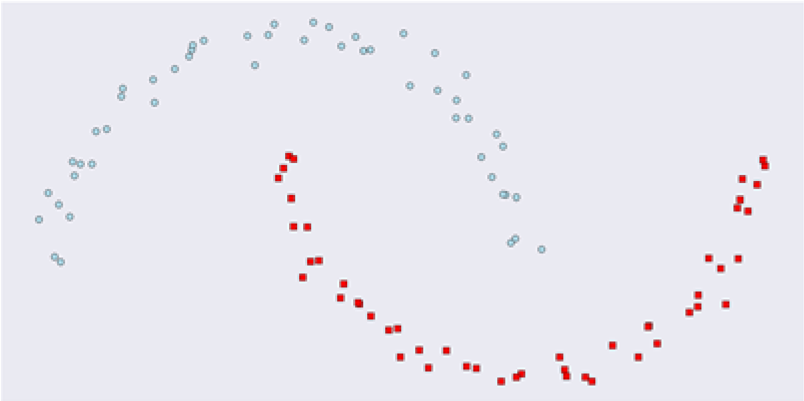
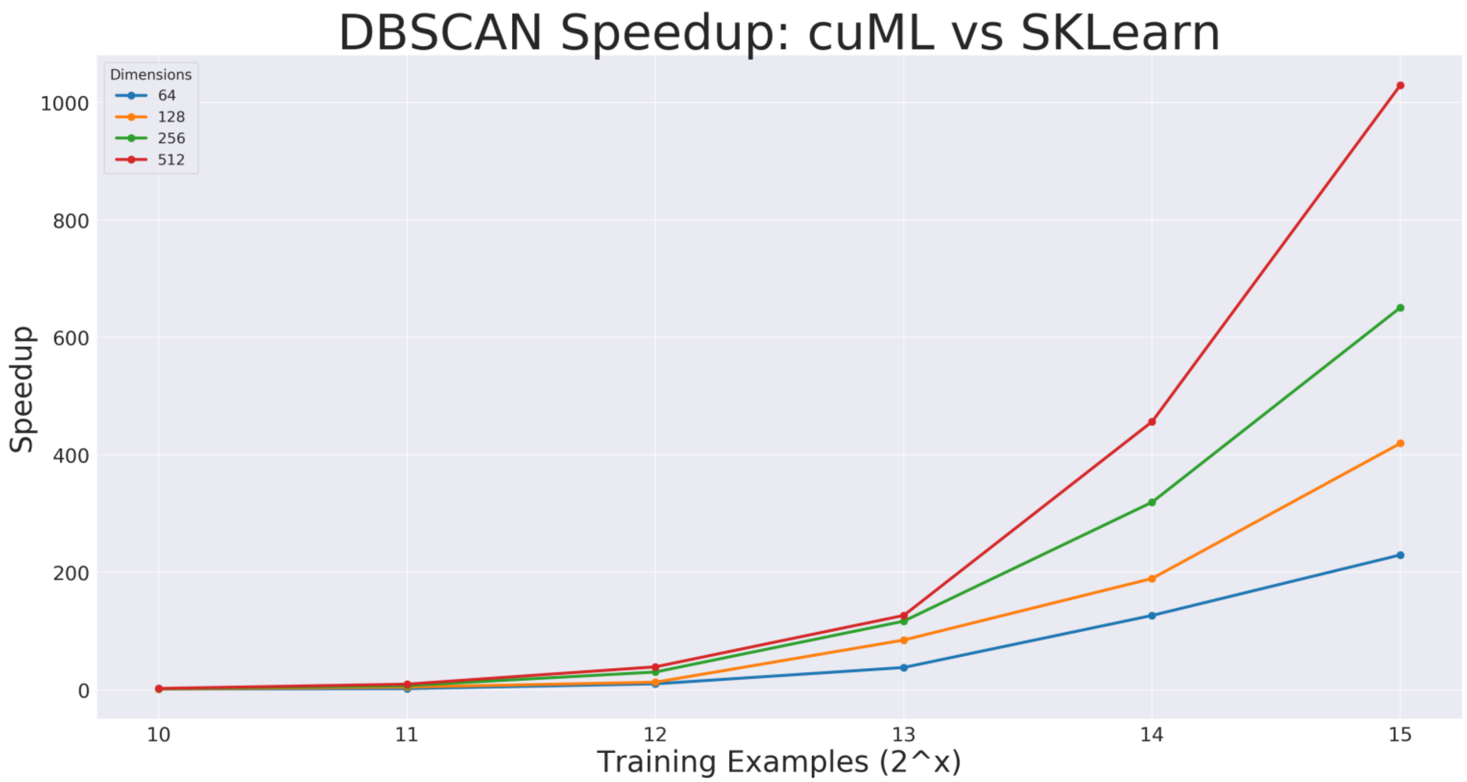
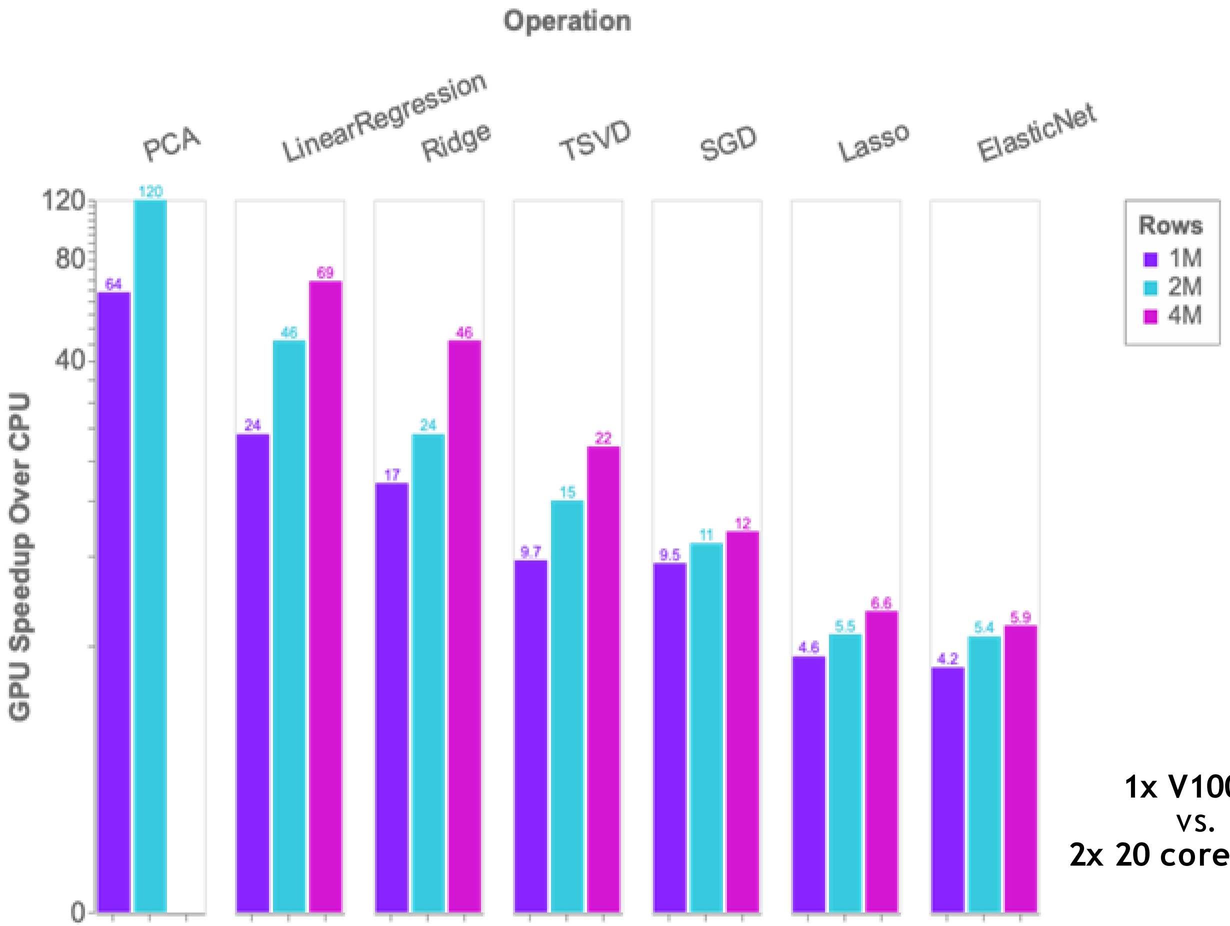


CLUSTERING

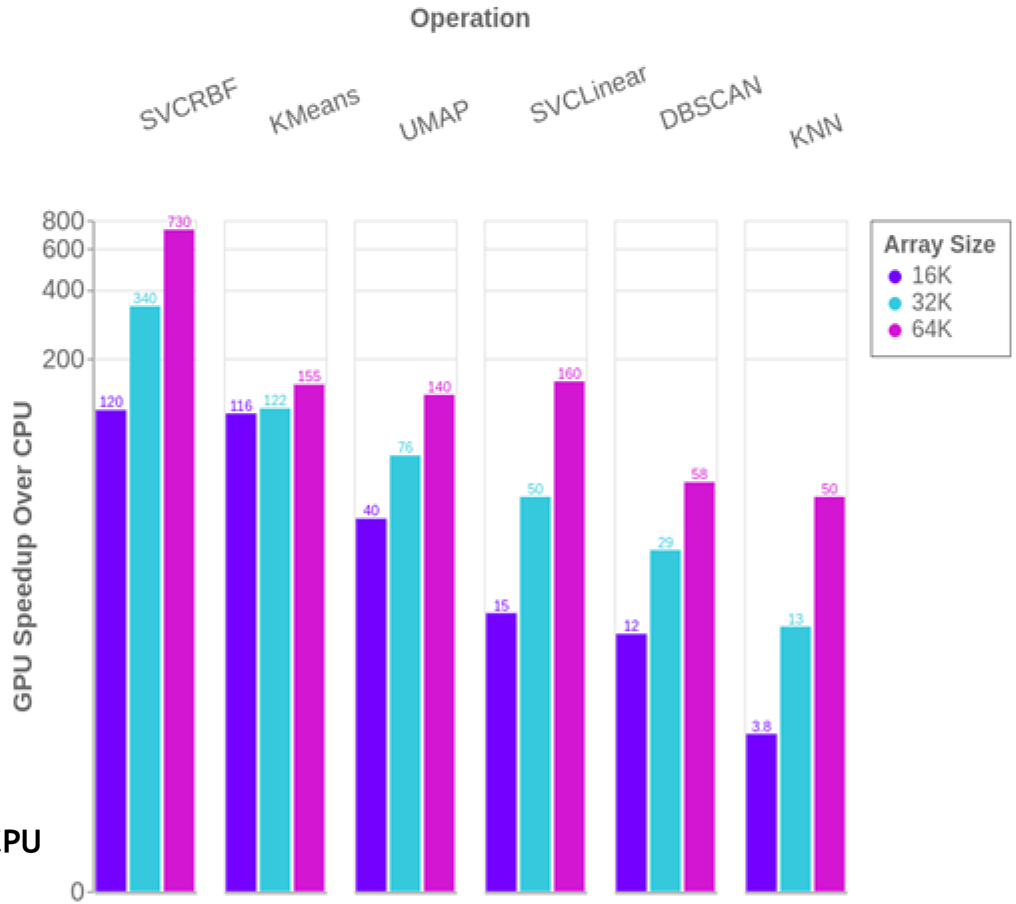
Benchmark



Benchmarks: single-GPU cuML vs scikit-learn



1x V100
vs.
2x 20 core CPU



Scale up and out with RAPIDS and Dask

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Scale out / Parallelize

Dask
Distributing Python Libraries

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Scale out / Parallelize

Dask Parallelizes

Natively

- **Support existing data science libraries**
  - Built on top of NumPy, Pandas, Scikit-Learn, … (easy to migrate)
  - With the same APIs (easy to train)
- **Scales**
  - Scales out to thousand-node clusters
  - Easy to install and use on a laptop
- **Popular**
  - Most common parallelism framework today at PyData and SciPy conferences
- **Deployable**
  - HPC: SLURM, PBS, LSF, SGE
  - Cloud: Kubernetes
  - Hadoop/Spark: Yarn

Parallel NumPy

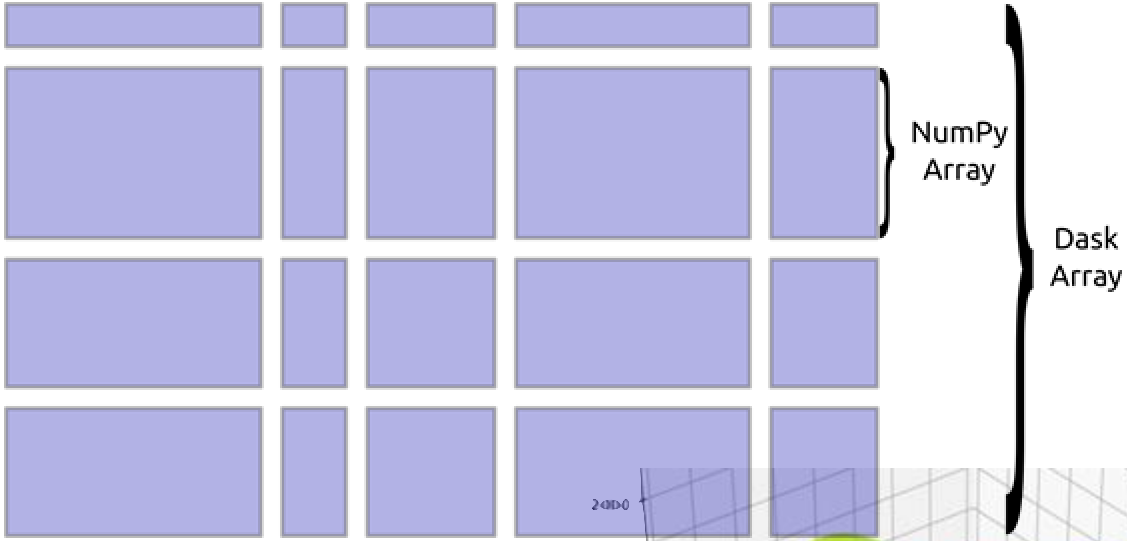
For imaging, simulation analysis, machine learning

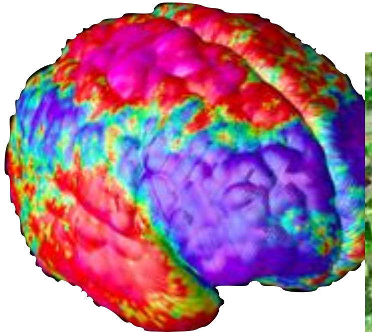
- Same API as NumPy

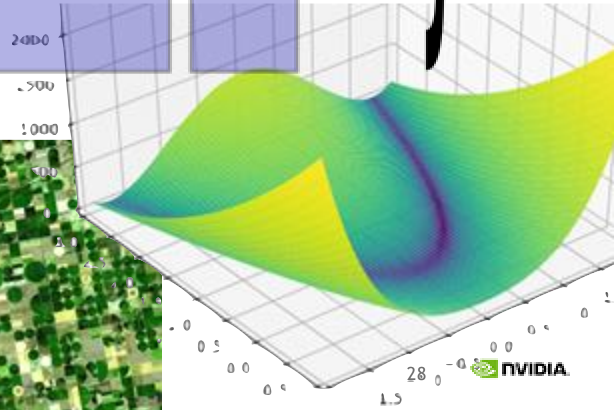
```
import dask.array as da
x = da.from_hdf5(...)
x + x.T - x.mean(axis=0)
```

- One Dask Array is built from many NumPy arrays

  Either lazily fetched from disk
  Or distributed throughout a cluster







Parallel Pandas

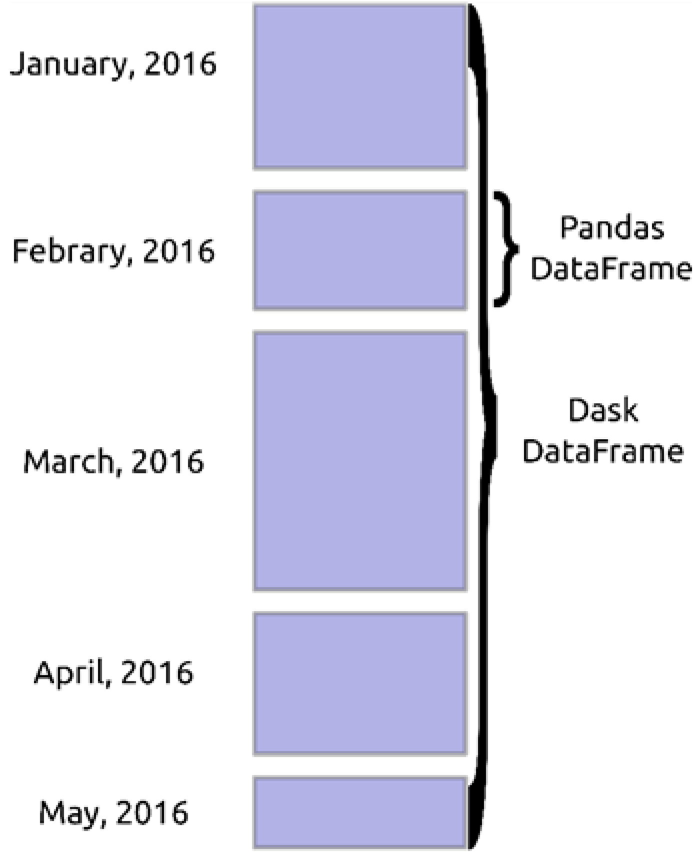
For ETL, time series, data munging

- Same API as Pandas

```
import dask.dataframe as dd
df = dd.read_csv(...)
df.groupby('name').balance.max()
```

- One Dask DataFrame is built from many Pandas DataFrames

  Either lazily fetched from disk
  Or distributed throughout a cluster

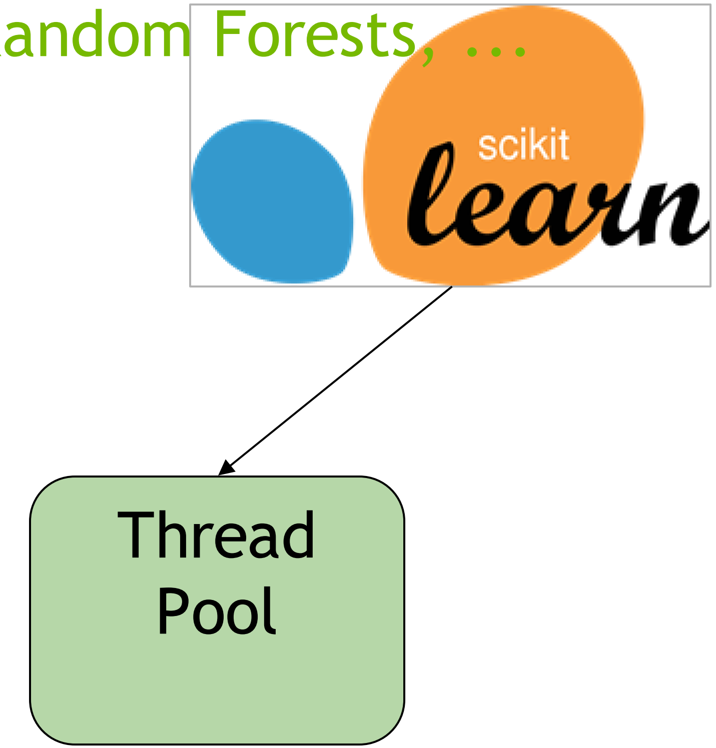


Parallel Scikit-Learn

For Hyper-Parameter Optimization, Random Forests, ...

- Same API

```
estimator = RandomForest()
estimator.fit(data, labels)
```



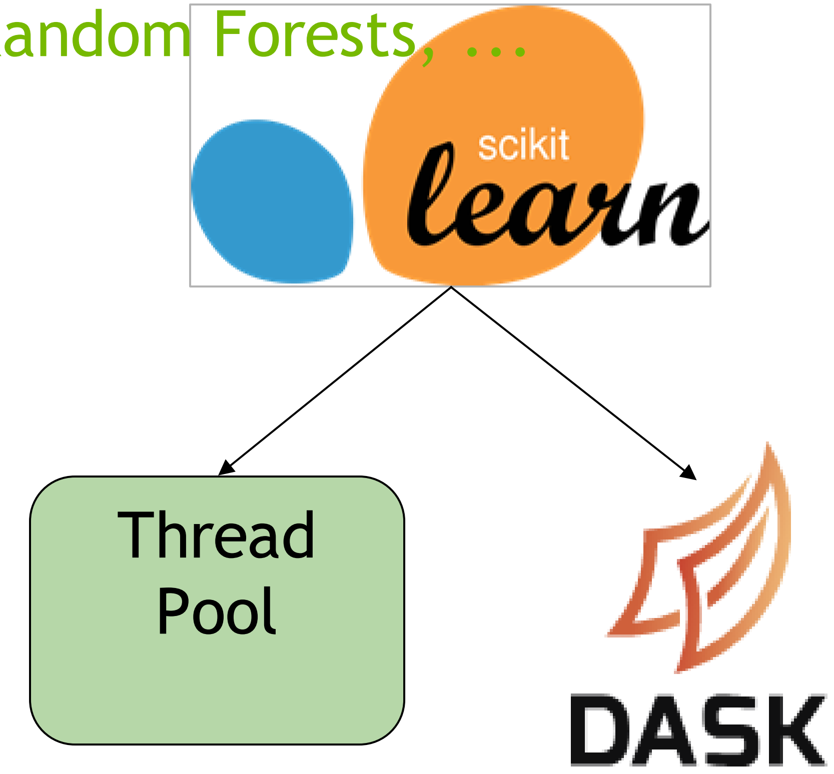
Parallel Scikit-Learn

For Hyper-Parameter Optimization, Random Forests, ...

- Same API

```
from scikit_learn.externals import joblib
with joblib.parallel_backend('dask'):
    estimator = RandomForest()
    estimator.fit(data, labels)
```

- Same exact code, just wrap in a "with" block
- Replaces default threaded execution with Dask
  Allowing scaling onto clusters
- Available in most Scikit-Learn algorithms where joblib is used



Parallel Python

For custom systems, ML algorithms, workflow engines

- Parallelize existing codebases

```
results = {}

for x in X:
  for y in Y:
    if x < y:
      result = f(x, y)
    else:
      result = g(x, y)
    results.append(result)
```

Parallel Python

For custom systems, ML algorithms, workflow engines

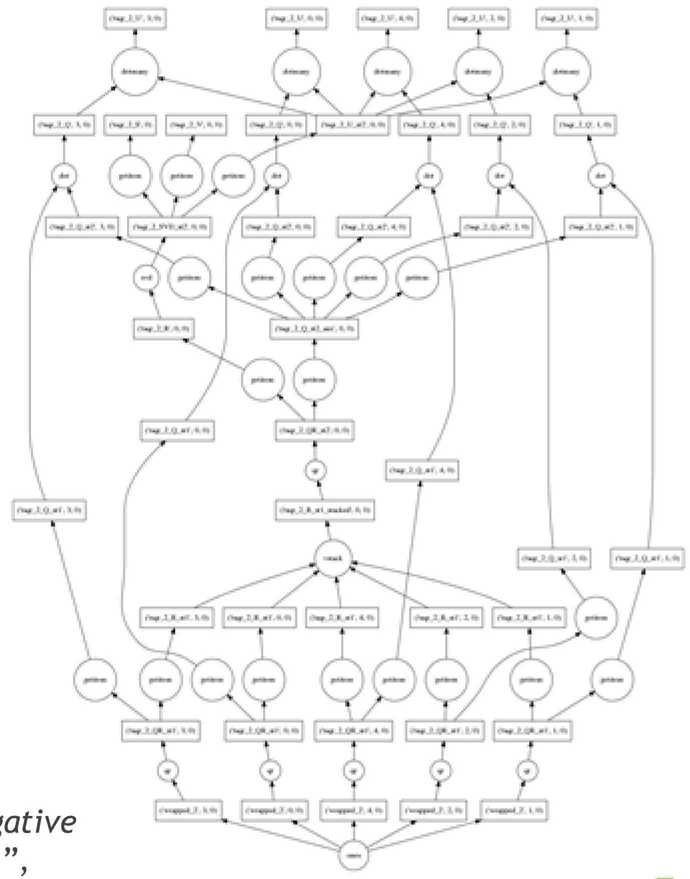
- Parallelize existing codebases

```
f = dask.delayed(f)
g = dask.delayed(g)

results = {}

for x in X:
  for y in Y:
    if x < y:
      result = f(x, y)
    else:
      result = g(x, y)
    results.append(result)

result = dask.compute(results)
```



M Tepper, G Sapiro "*Compressed nonnegative matrix factorization is fast and accurate*", IEEE Transactions on Signal Processing, 2016

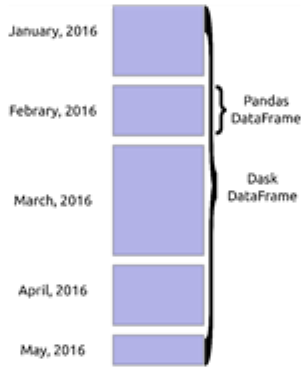
Dask Connects Python users to Hardware

User

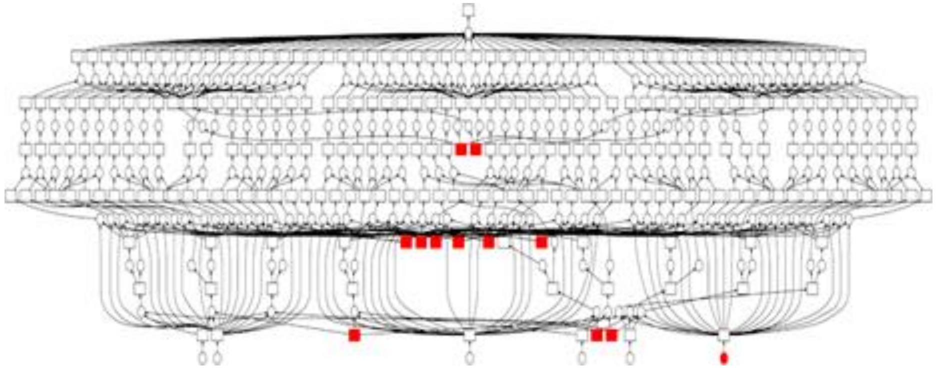
Execute on distributed hardware

Dask Connects Python users to Hardware

User



Writes high level code (NumPy/Pandas/Scikit-Learn)



Turns into a task graph

Execute on distributed hardware

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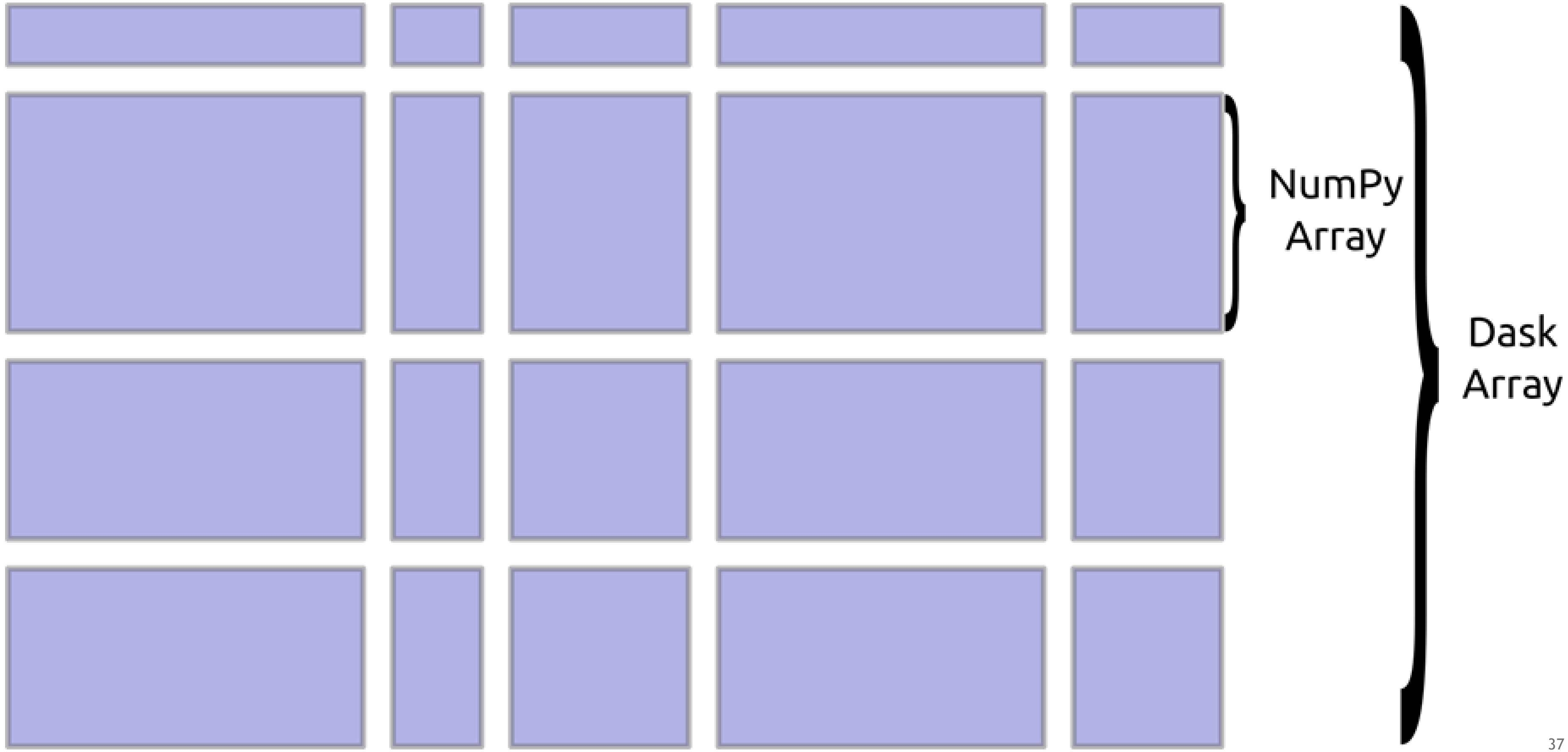
Combine Dask with CuPy

Many GPU arrays form a Distributed GPU array



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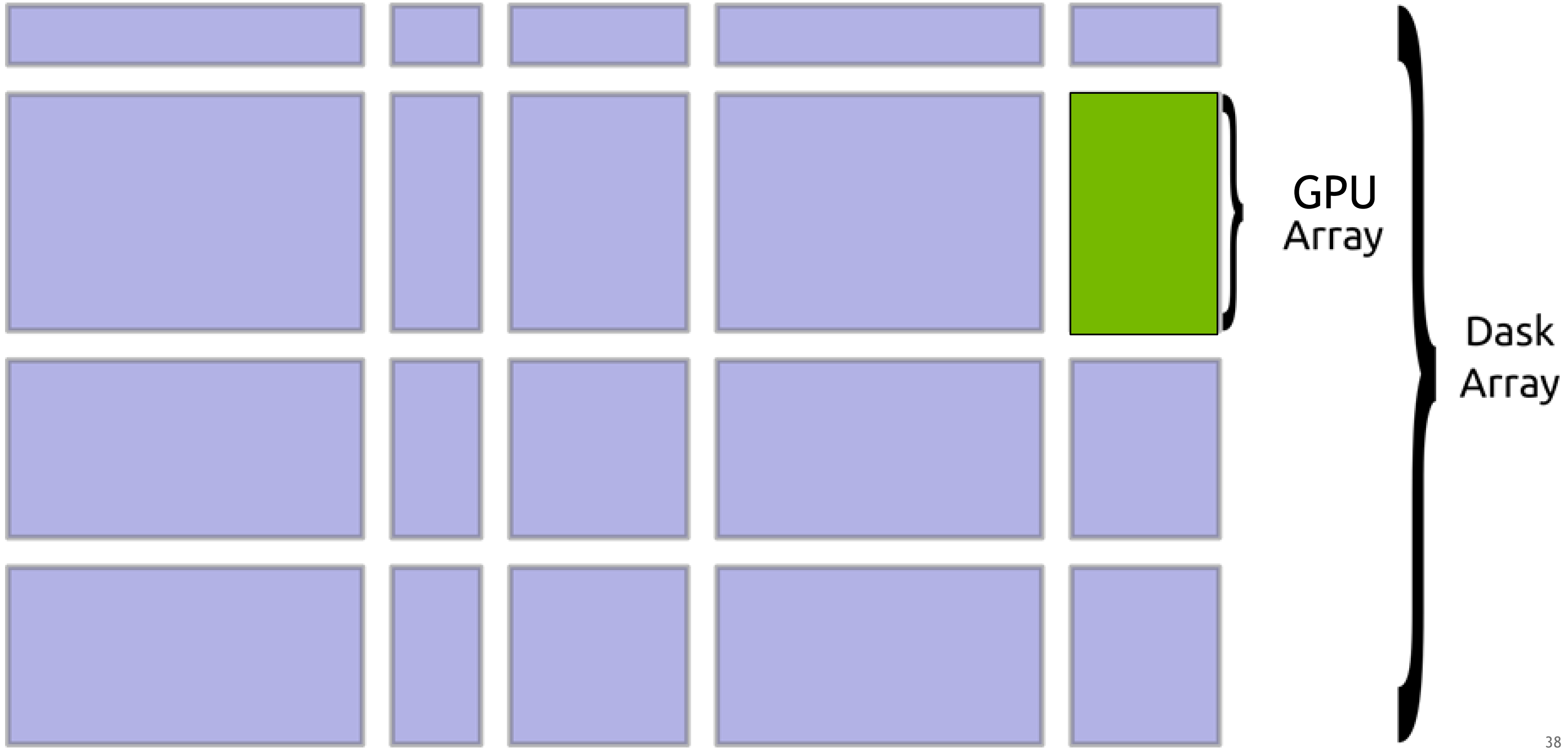
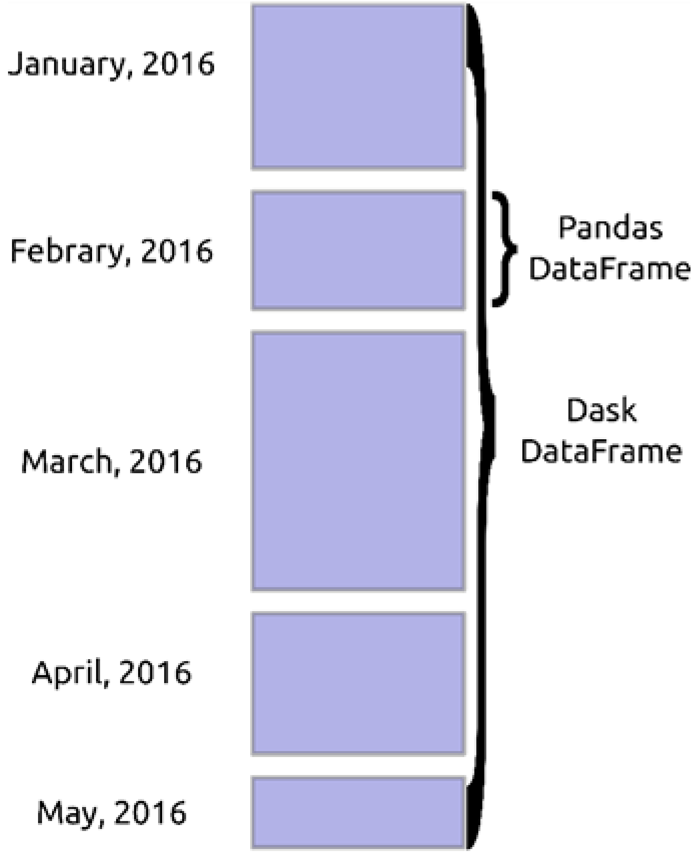


Combine Dask with cuDF

Many GPU DataFrames form a distributed DataFrame



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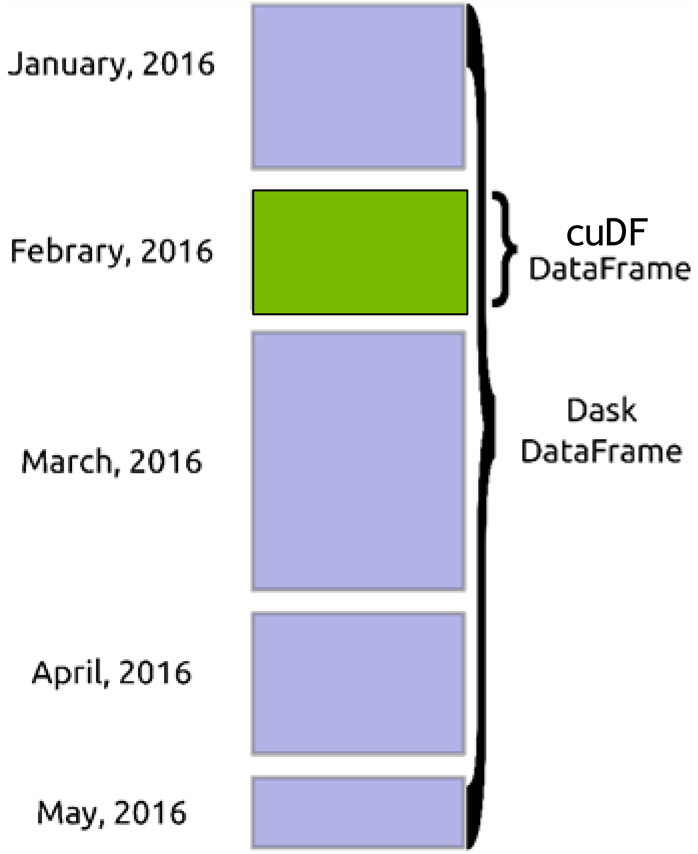
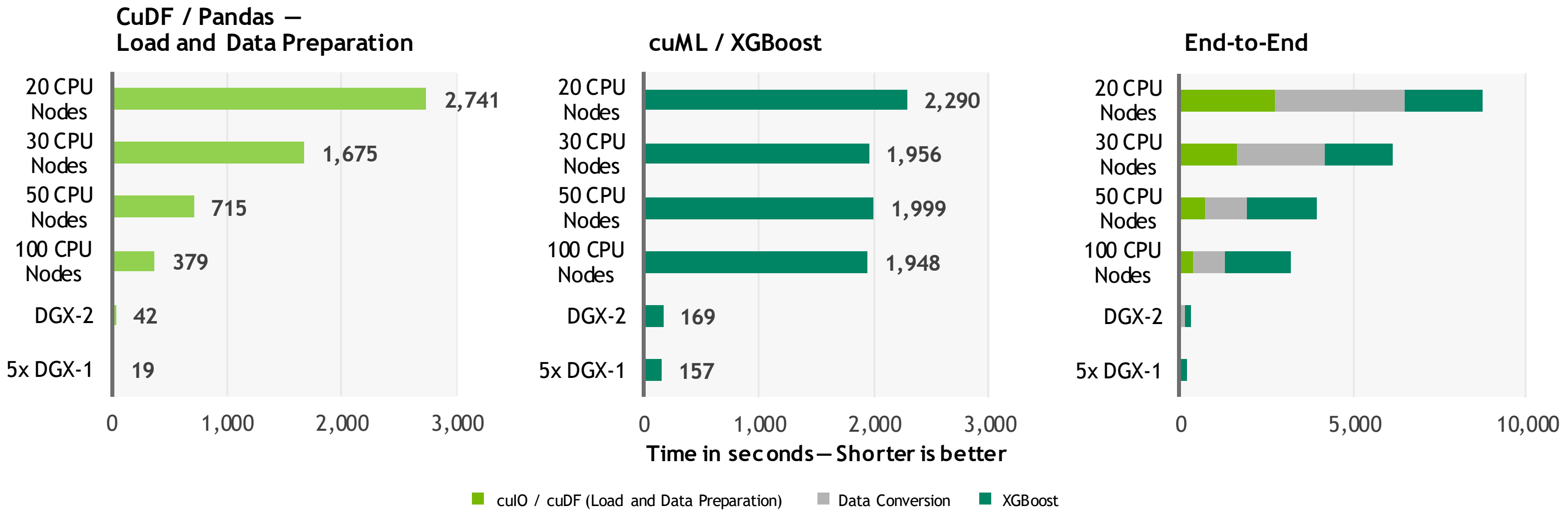


END-TO-END BENCHMARKS



Benchmark

200GB CSV dataset; Data preparation includes joins, variable transformations.

CPU Cluster Configuration

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

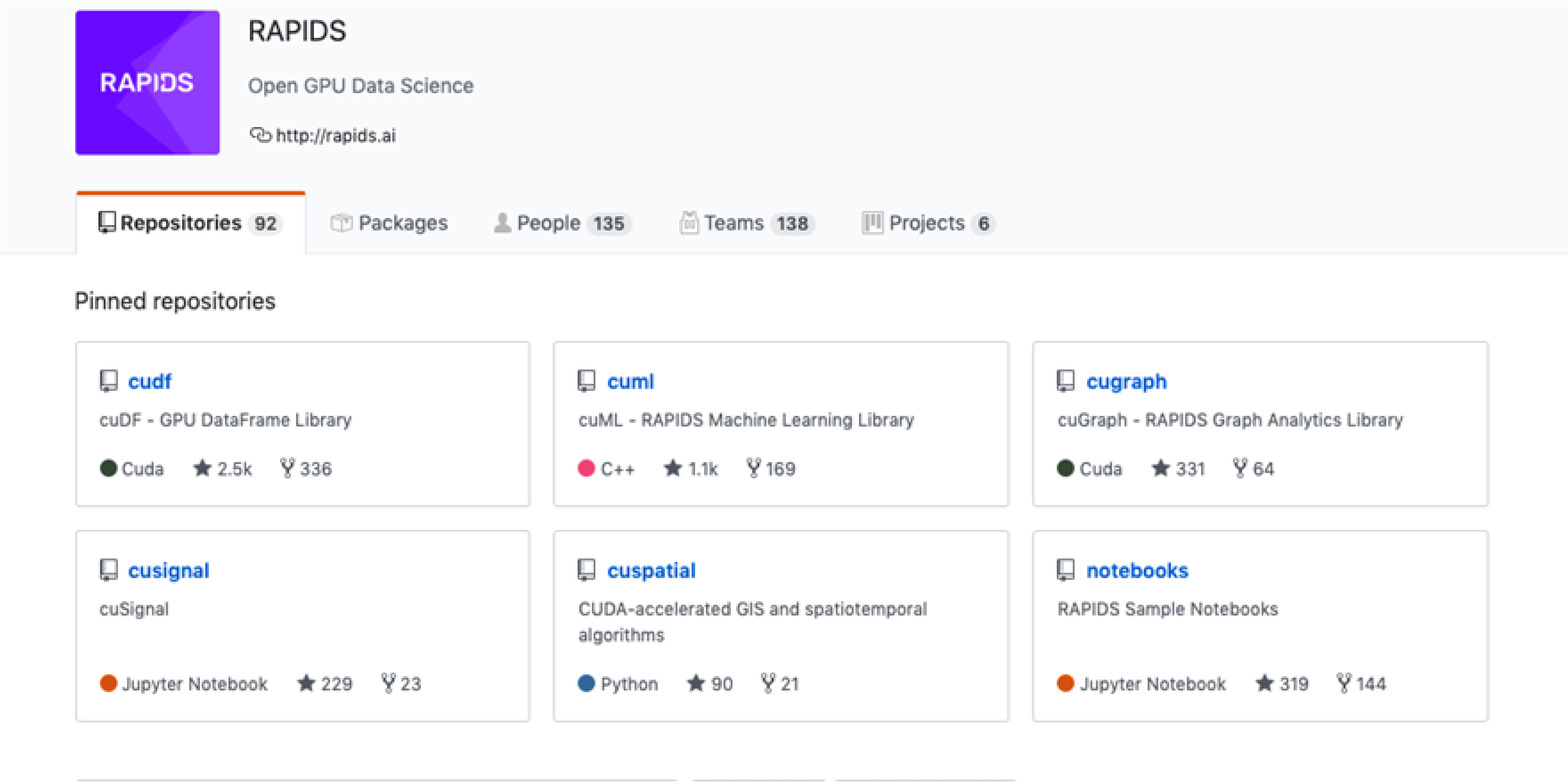
DGX Cluster Configuration

5x DGX-1 on InfiniBand network

Getting Started

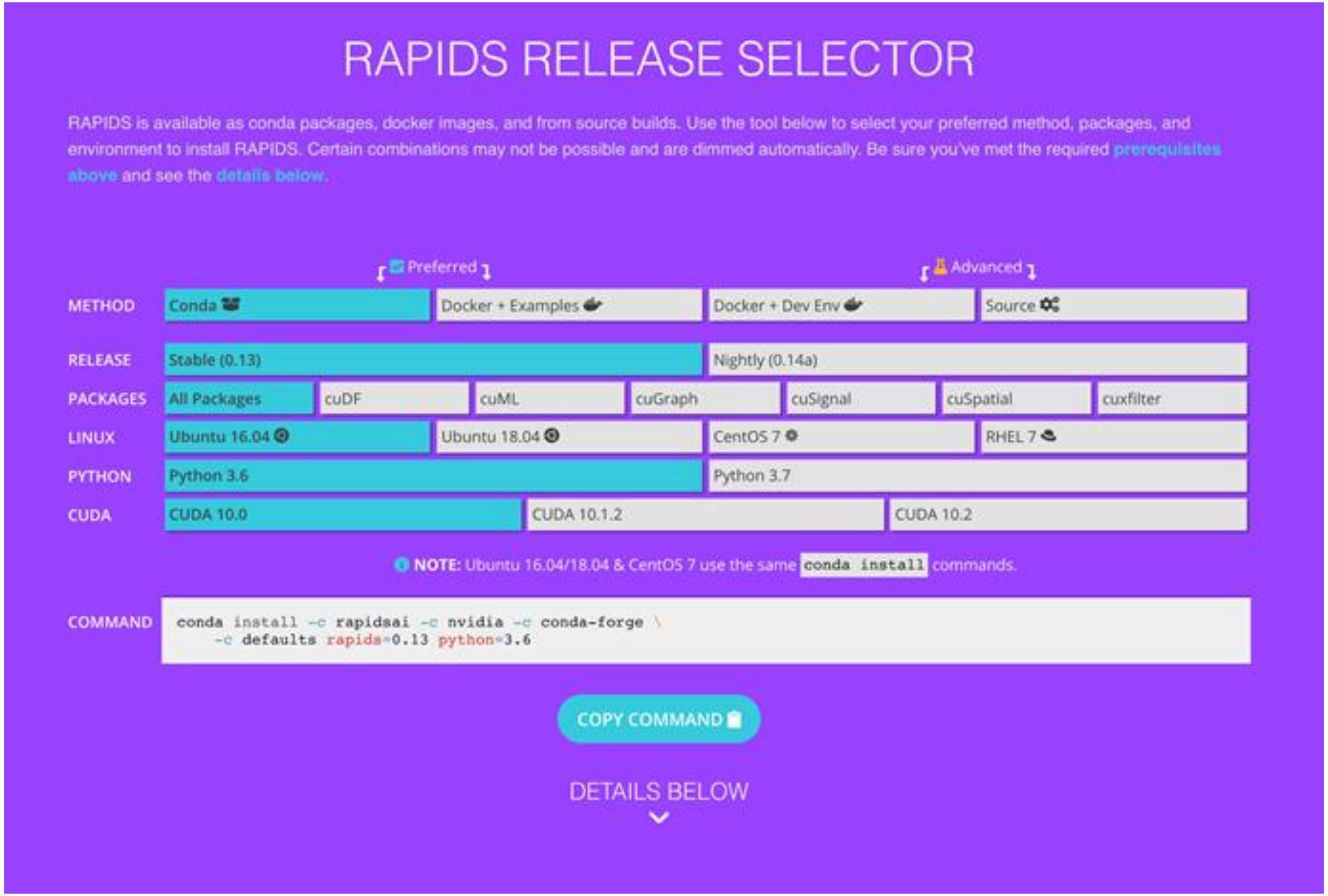
Explore: RAPIDS Github

https://github.com/rapidsai



Easy Installation

Interactive Installation Guide



Explore: RAPIDS Code and Blogs

Check out our code and how we use it


README.md

RAPIDS cuDF - GPU DataFrames

build running

NOTE: For the latest stable README.md ensure you are on the `master` branch.

Built based on the Apache Arrow columnar memory format, cuDF is a GPU DataFrame library for loading, joining, aggregating, filtering, and otherwise manipulating data.

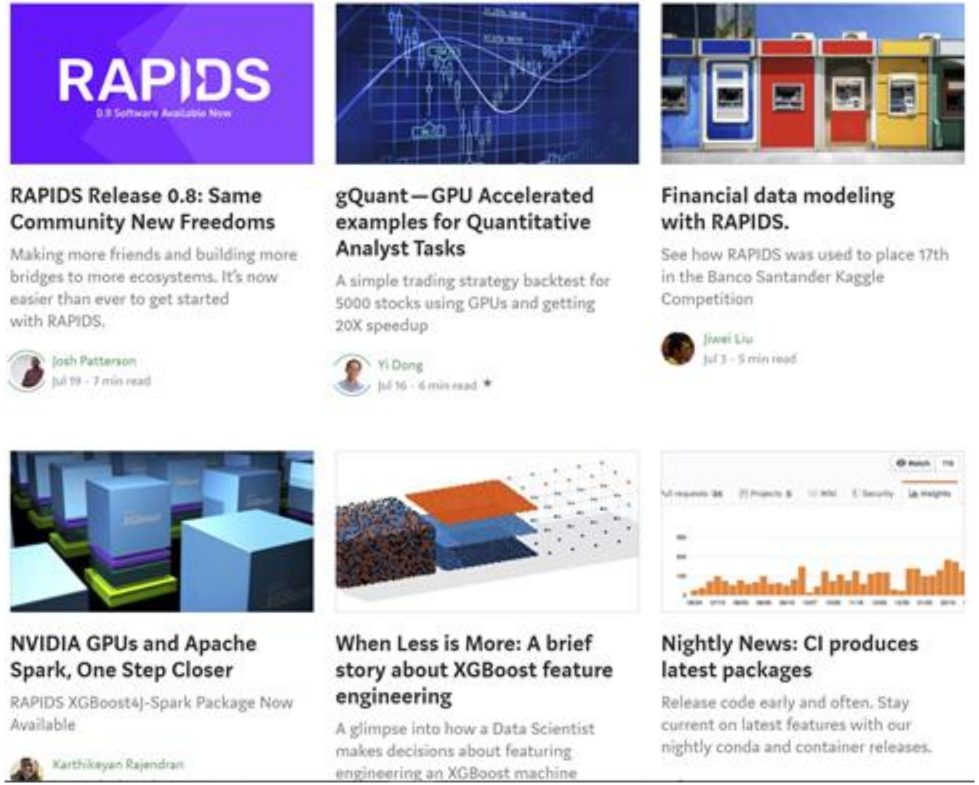
cuDF provides a pandas-like API that will be familiar to data engineers & data scientists, so they can use it to easily accelerate their workflows without going into the details of CUDA programming.

For example, the following snippet downloads a CSV, then uses the GPU to parse it into rows and columns and run calculations:

```
import cudf, io, requests
from io import StringIO

url="https://github.com/plotly/datasets/raw/master/tips.csv"
content = requests.get(url).content.decode('utf-8')

tips_df = cudf.read_csv(StringIO(content))
tips_df['tip_percentage'] = tips_df['tip']/tips_df['total_bill']*100

# display average tip by dining party size
print(tips_df.groupby('size').tip_percentage.mean())
```

Output:

```
size
```



https://github.com/rapidsai

https://medium.com/rapids-ai