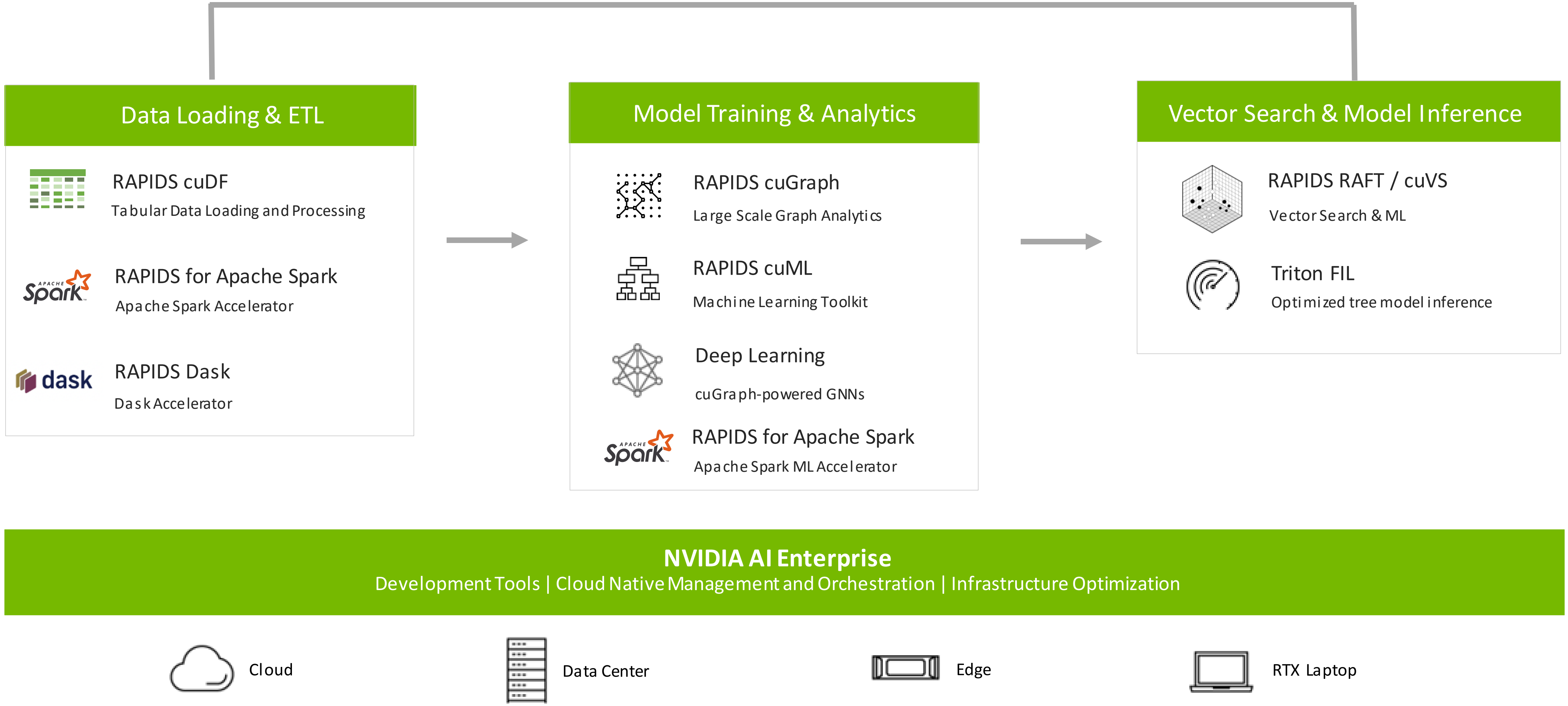
# RAPIDS: Accelerated Data Science and Data Processing

Mads R. B. Kristensen, NVIDIA

# RAPIDS Accelerates Data Science End-to-End



## Data Loading & ETL

RAPIDS cuDF
Tabular Data Loading and Processing

RAPIDS for Apache Spark
Apache Spark Accelerator

RAPIDS Dask
Dask Accelerator

## Model Training & Analytics

RAPIDS cuGraph
Large Scale Graph Analytics

RAPIDS cuML
Machine Learning Toolkit

Deep Learning
cuGraph-powered GNNs

RAPIDS for Apache Spark
Apache Spark ML Accelerator

## Vector Search & Model Inference

RAPIDS RAFT / cuVS
Vector Search & ML

Triton FIL
Optimized tree model inference

**NVIDIA AI Enterprise**
Development Tools | Cloud Native Management and Orchestration | Infrastructure Optimization

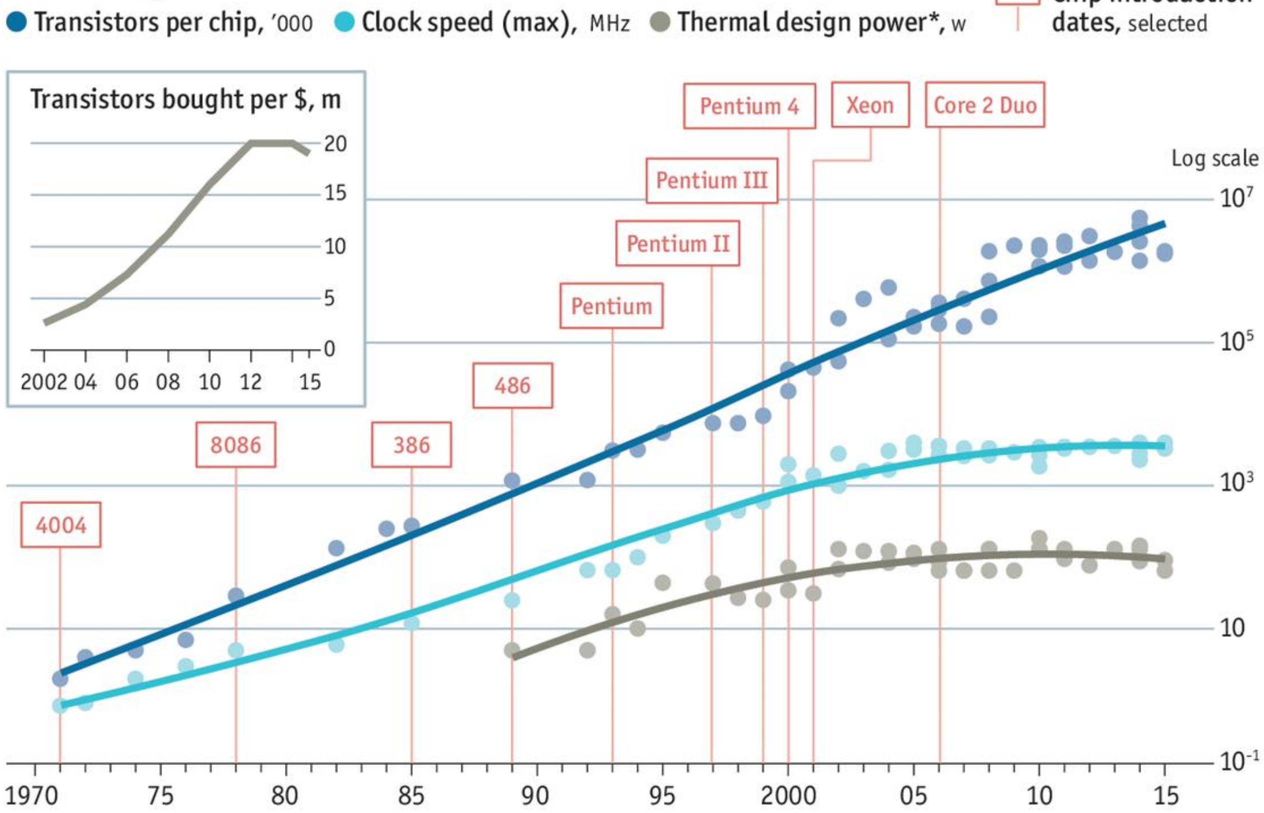
Cloud

Data Center

Edge

RTX Laptop

## Stuttering

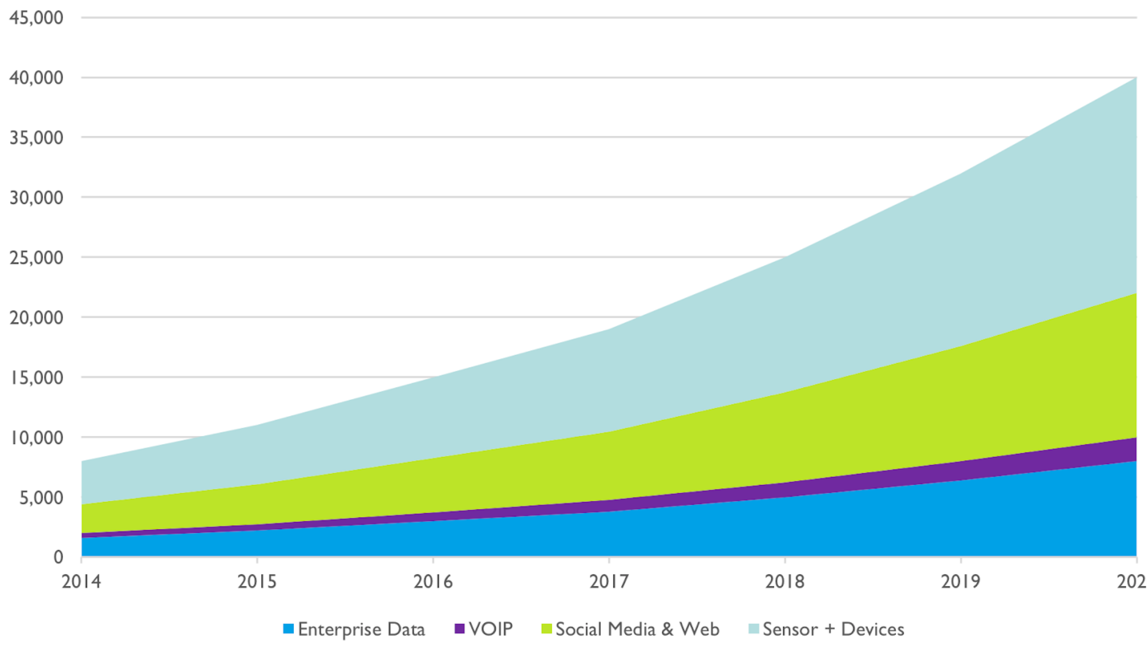


Sources: Intel; Bob Colwell; Linley Group; International Business Strategies; *The Economist*

*Maximum safe power consumption

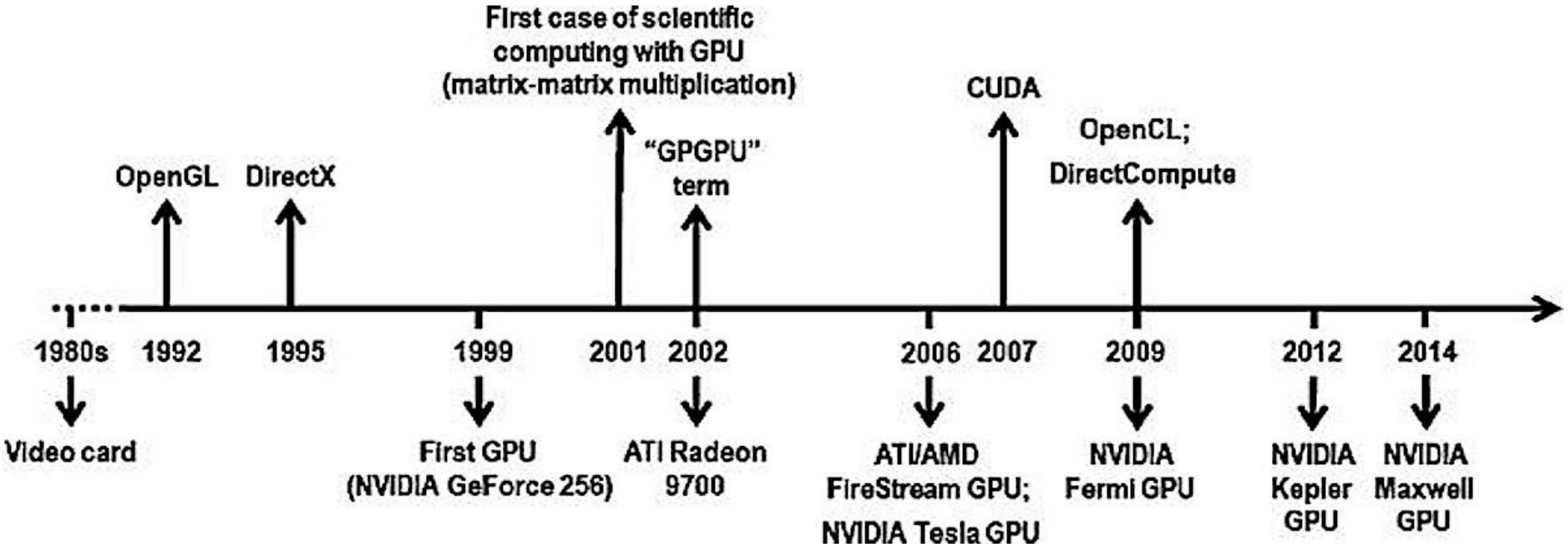
Economist.com

### Data Growth and Source in Exabytes



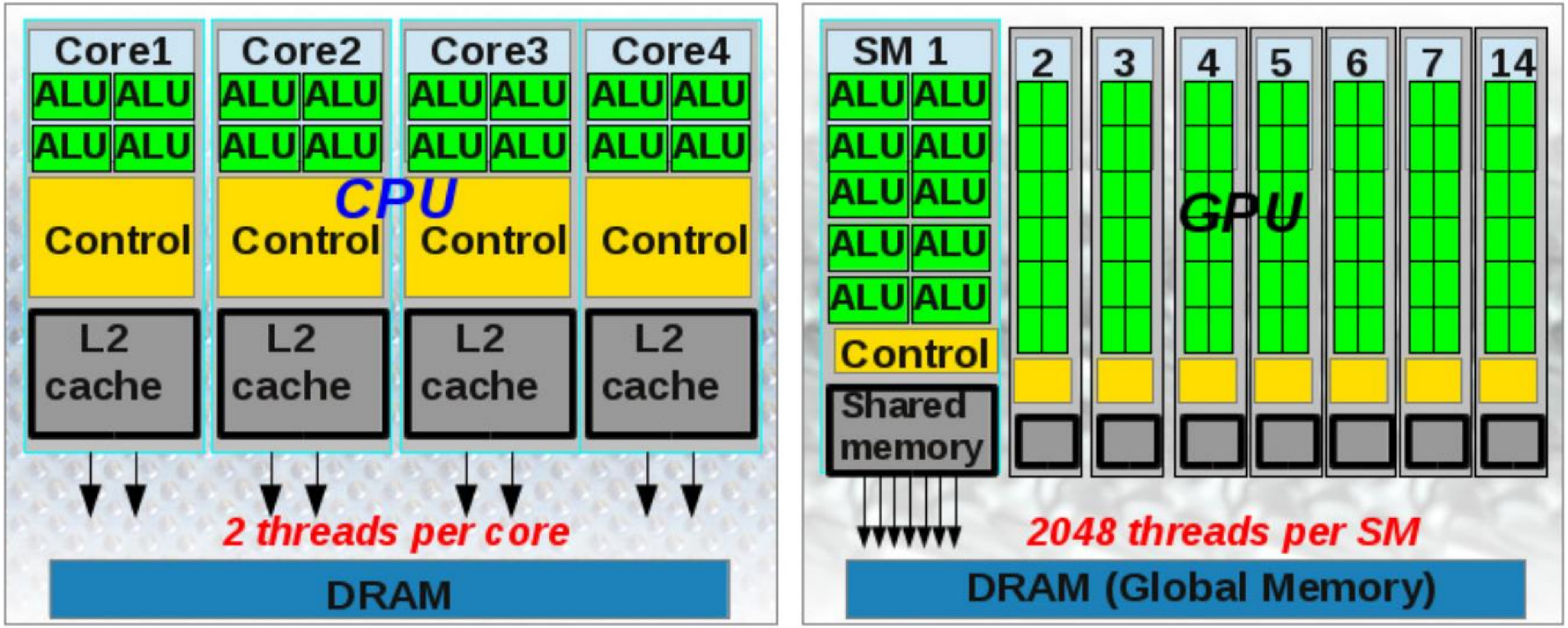
Source: IDC and EMC Digital Universe Report

# History of the GPU



**DOI:** https://doi.org/10.1007/978-3-319-17885-1_1606

# CPU vs GPU

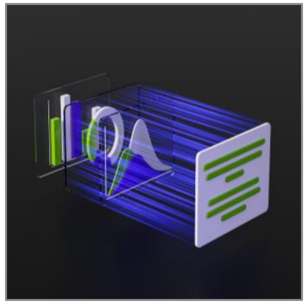


DOI:
10.1016/j.cam.2013.12.032.

# Modern Enterprise Applications Need Accelerated Computing

Internet scale data | Massive models | Real-time performance

Recommenders



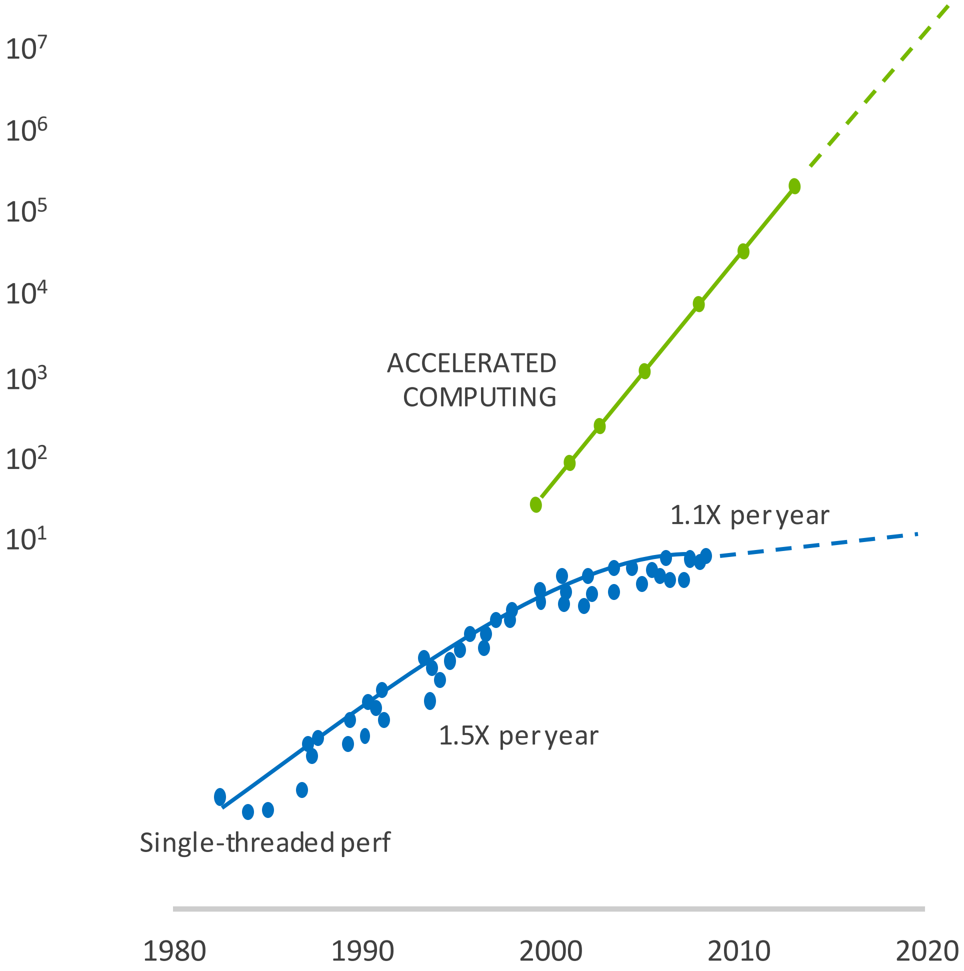
LLMs

Forecasting

Fraud Detection

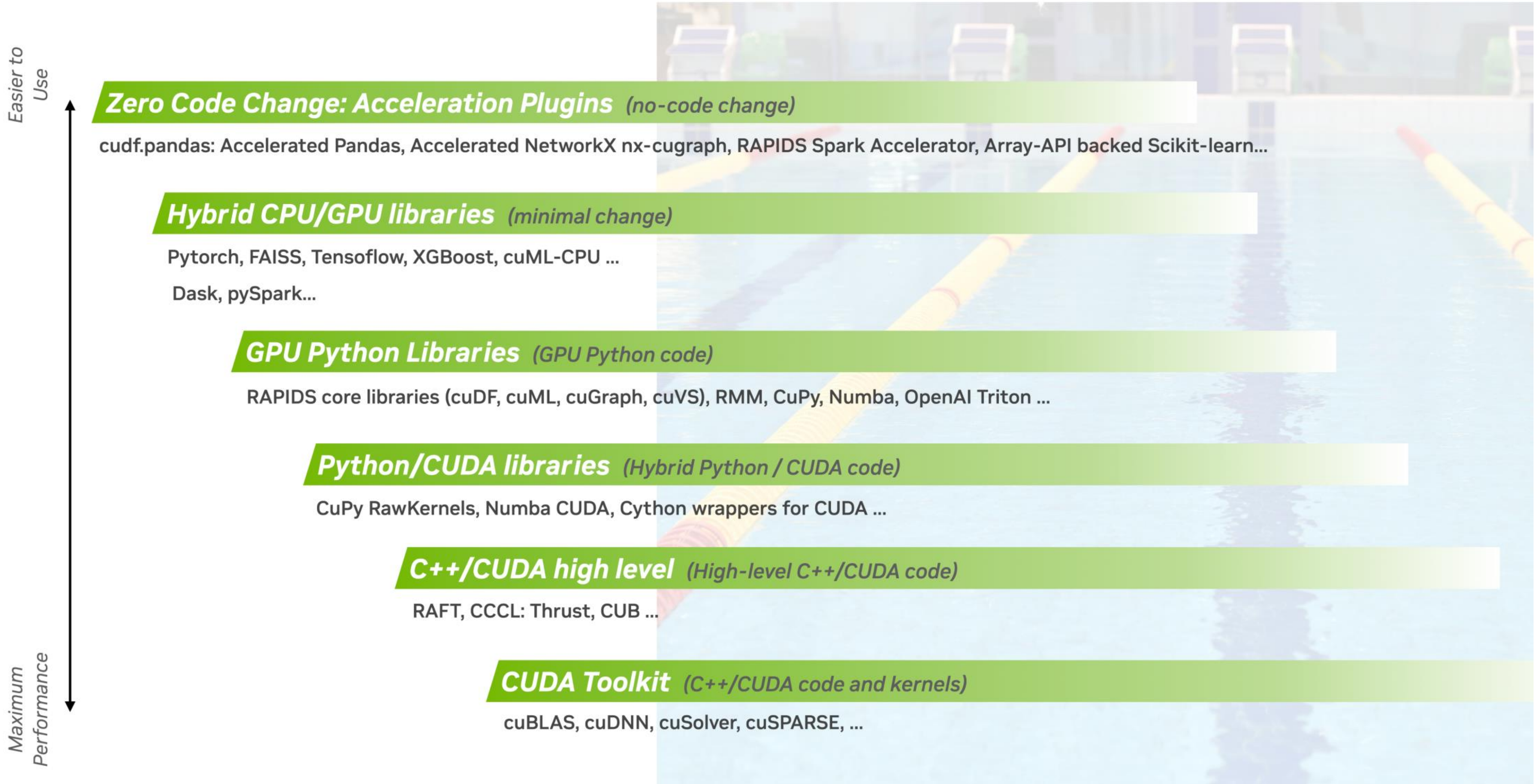
Genomic Analysis

Cybersecurity



# Accelerated Computing Swim Lanes

RAPIDS makes accelerated computing more seamless while enabling specialization for maximum performance



Easier to Use

**Zero Code Change: Acceleration Plugins** *(no-code change)*

cudf.pandas: Accelerated Pandas, Accelerated NetworkX nx-cugraph, RAPIDS Spark Accelerator, Array-API backed Scikit-learn…

**Hybrid CPU/GPU libraries** *(minimal change)*

Pytorch, FAISS, Tensoflow, XGBoost, cuML-CPU …

Dask, pySpark…

**GPU Python Libraries** *(GPU Python code)*

RAPIDS core libraries (cuDF, cuML, cuGraph, cuVS), RMM, CuPy, Numba, OpenAI Triton …

**Python/CUDA libraries** *(Hybrid Python / CUDA code)*

CuPy RawKernels, Numba CUDA, Cython wrappers for CUDA …

**C++/CUDA high level** *(High-level C++/CUDA code)*

RAFT, CCCL: Thrust, CUB …

**CUDA Toolkit** *(C++/CUDA code and kernels)*

cuBLAS, cuDNN, cuSolver, cuSPARSE, …

Maximum Performance

# RAPIDS ETL

Extract, transform, and load

# Pandas

## Python’s Preeminent DataFrame Library

**9.5M**

Pandas users

**65%**

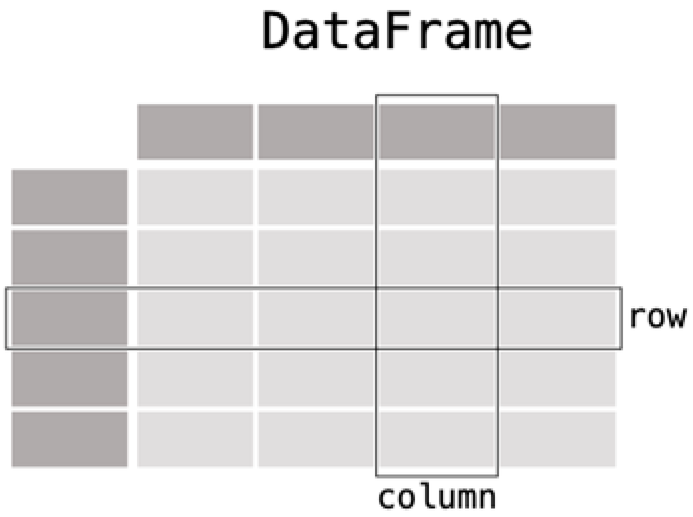
Users love using pandas (HuggingFace most loved at 72%)

**135M+**

Monthly downloads

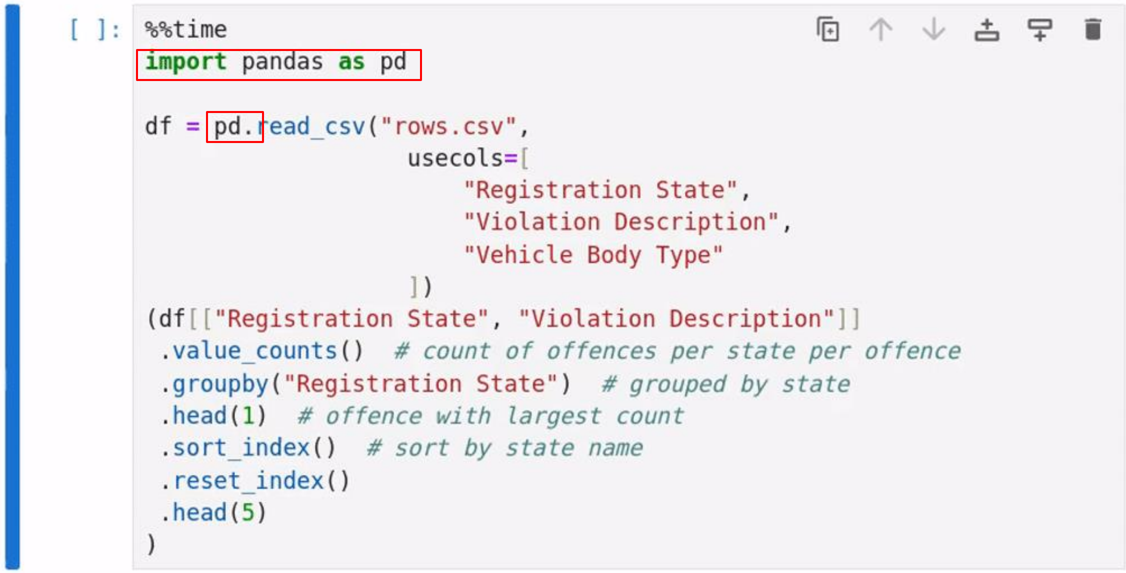
**25%**

Y/Y downloads growth

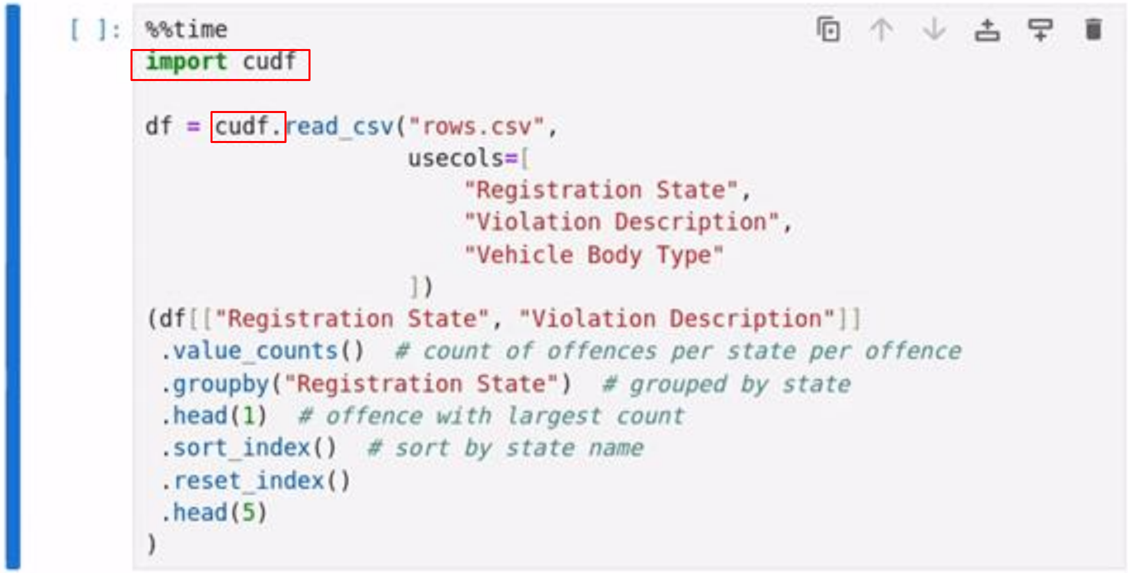


```
import pandas as pd

df = (
    pd.read_csv('data.csv')
    .melt(id_vars=['id', 'name'])
    .rename(columns={
        'variable':'var',
        'value':'val'})
    .query('val >= 200')
    .sort_values('val', ascending=False)
)
```

# cuDF - GPU DataFrames

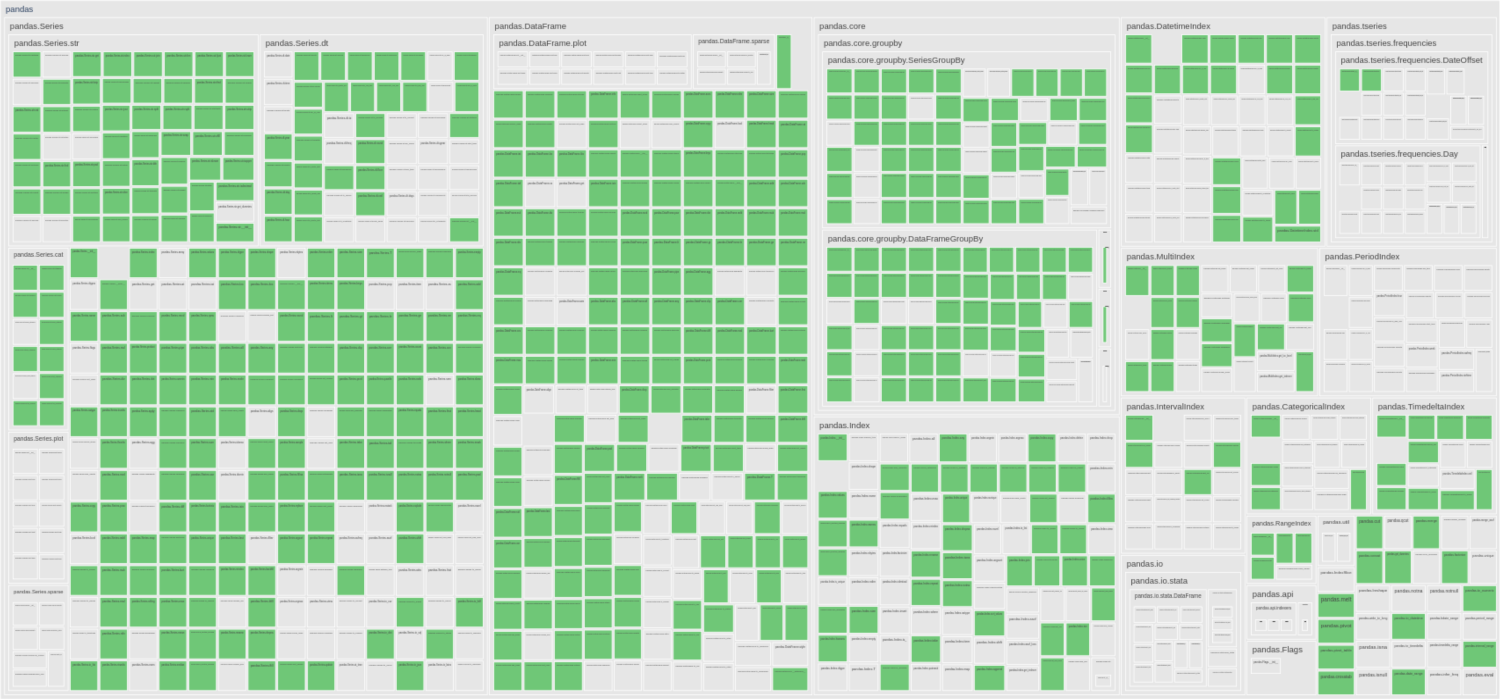


```
%%time
import pandas as pd

df = pd.read_csv("rows.csv",
                   usecols=[
                       "Registration State",
                       "Violation Description",
                       "Vehicle Body Type"
                   ])
(df[["Registration State", "Violation Description"]]
 .value_counts()  # count of offences per state per offence
 .groupby("Registration State")  # grouped by state
 .head(1)  # offence with largest count
 .sort_index()  # sort by state name
 .reset_index()
 .head(5)
)
```



```
%%time
import cudf

df = cudf.read_csv("rows.csv",
                   usecols=[
                       "Registration State",
                       "Violation Description",
                       "Vehicle Body Type"
                   ])
(df[["Registration State", "Violation Description"]]
 .value_counts()  # count of offences per state per offence
 .groupby("Registration State")  # grouped by state
 .head(1)  # offence with largest count
 .sort_index()  # sort by state name
 .reset_index()
 .head(5)
)
```

# cuDF Problems



*cuDF coverage of the Pandas API (green=implemented, gray=not implemented)*

***"We just don't have time to rewrite our code in a new paradigm."***

# cuDF

A GPU DataFrame library in Python with a pandas-like API built into the PyData ecosystem

## Pandas-like API on the GPU

CPU

pandas

```
>>> import pandas as pd
>>> df = pd.read_csv("filepath")
>>> df.groupby(“col”).mean()
>>> df.rolling(window=3).sum()
```

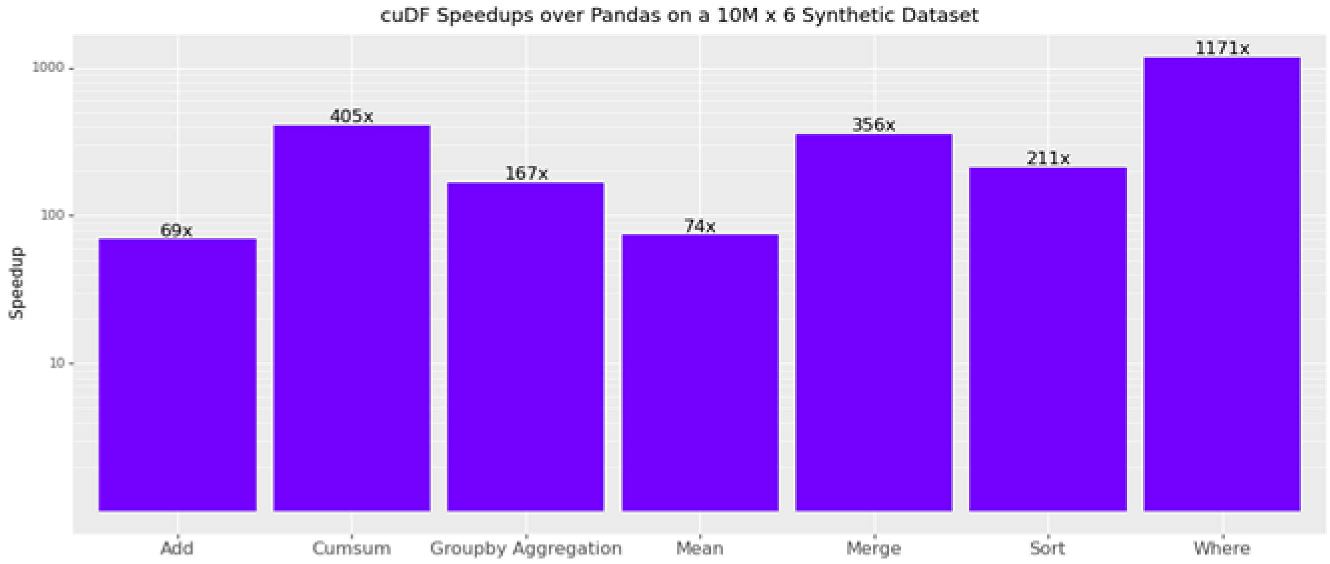
GPU

cuDF

```
>>> import cudf
>>> df = cudf.read_csv("filepath")
>>> df.groupby(“col”).mean()
>>> df.rolling(window=3).sum()
```

Average Speed-Ups: *10-100x*

## Best-in-Class Performance (Benchmark)



Groupby | Strings and Regex | UDFs | Nested Types | Time Series

Indexing | Missing Data | CuPy Interoperability | Rolling Windows

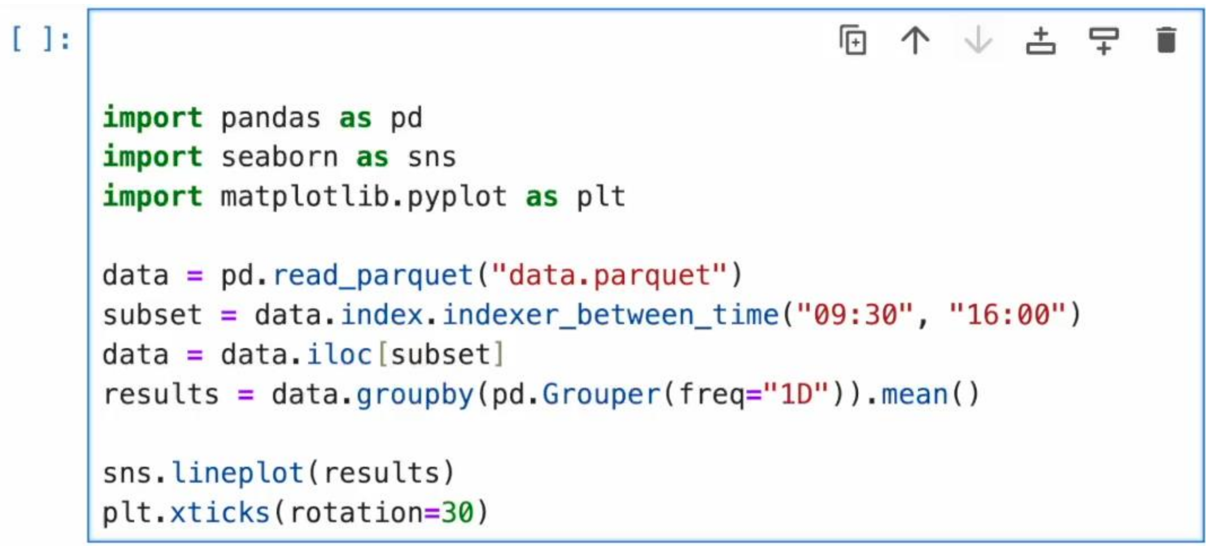
10 Minutes to cuDF

NVIDIA A100 vs. AMD EPYC 7642 48-Core Processor
cuDF Python vs. Pandas

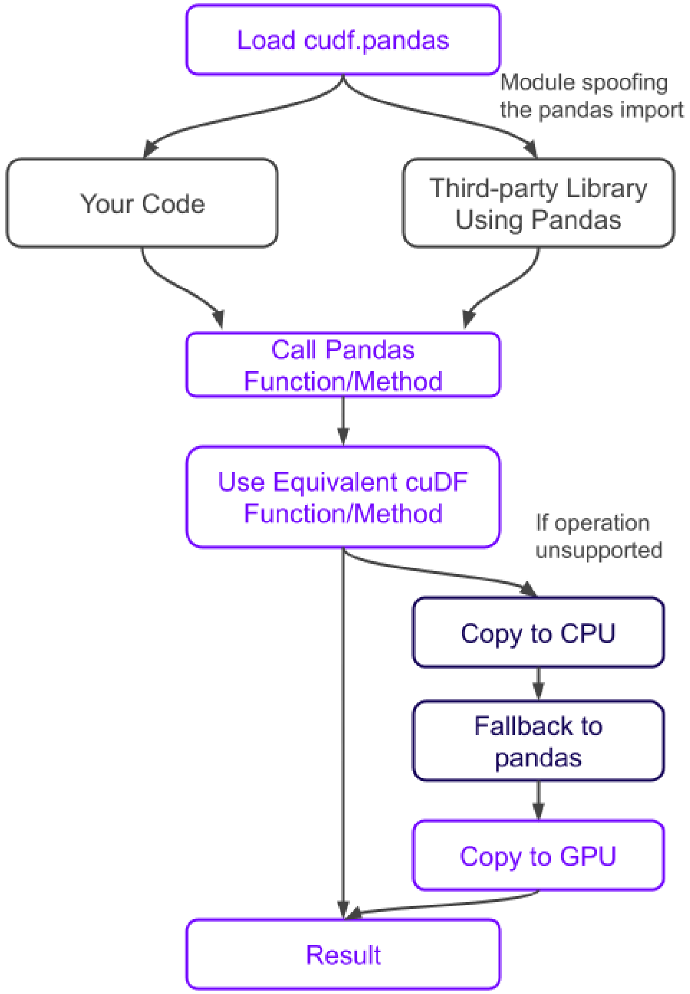
# Accelerated pandas

## cudf.pandas: the zero code change GPU accelerator for pandas built on cuDF

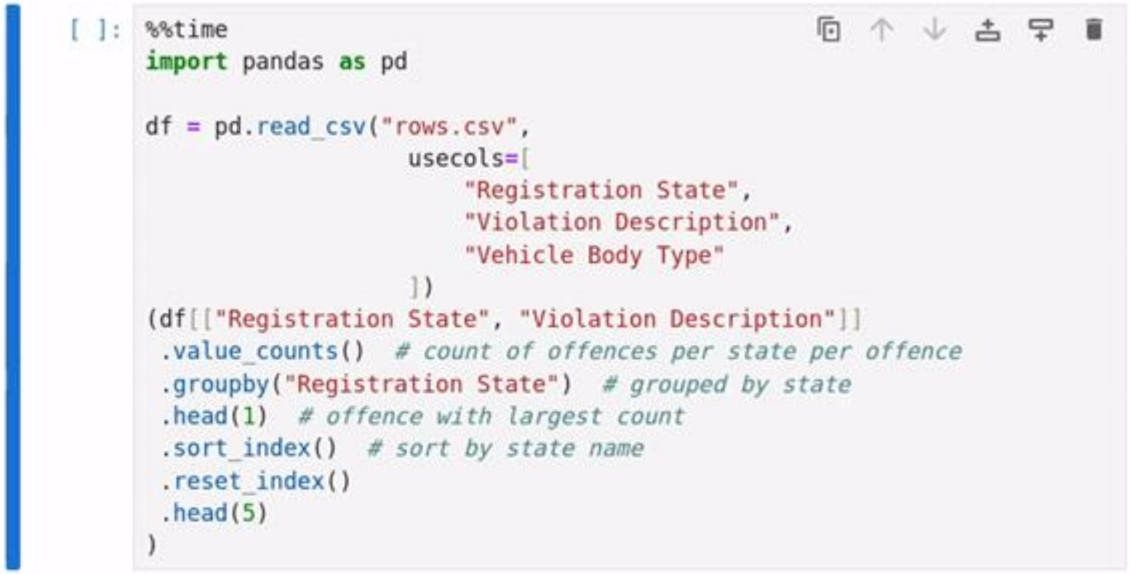
- Requires ***no changes*** to existing pandas code. Just
  - `%load_ext cudf.pandas`
  - `$ python –m cudf.pandas <script.py>`
- 100% of the pandas API
- Accelerates workflows up to 150x using the GPU
- Compatible with code that uses third-party libraries
- Falls back to using pandas on the CPU for unsupported functions and methods



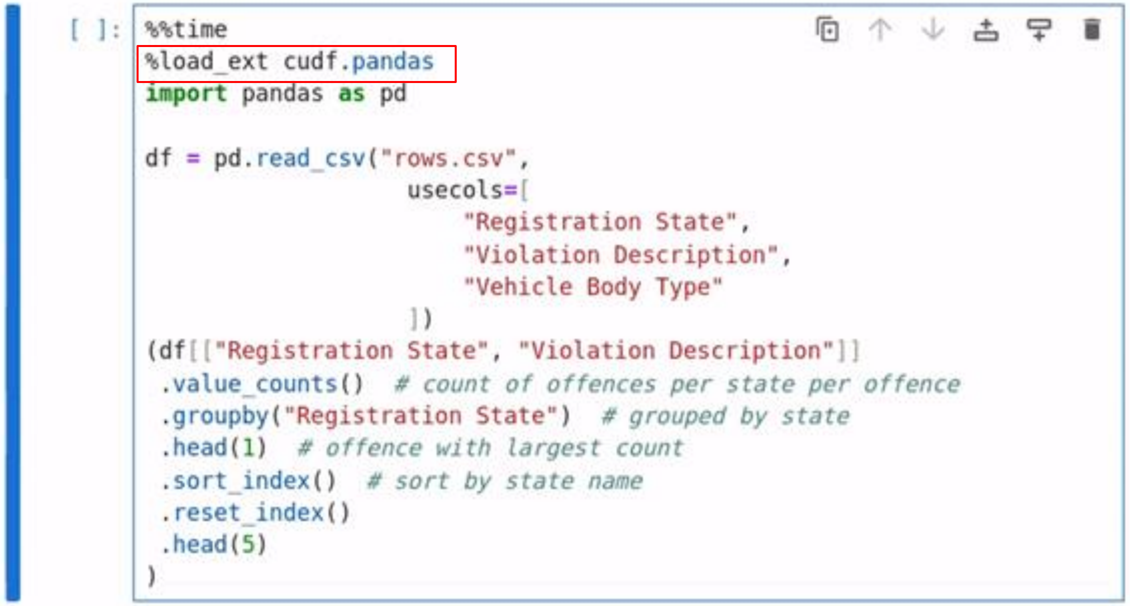
```python
import pandas as pd
import seaborn as sns
import matplotlib.pyplot as plt

data = pd.read_parquet("data.parquet")
subset = data.index.indexer_between_time("09:30", "16:00")
data = data.iloc[subset]
results = data.groupby(pd.Grouper(freq="1D")).mean()

sns.lineplot(results)
plt.xticks(rotation=30)
```


Load cudf.pandas
Module spoofing the pandas import
Your Code
Third-party Library Using Pandas
Call Pandas Function/Method
Use Equivalent cuDF Function/Method
If operation unsupported
Copy to CPU
Fallback to pandas
Copy to GPU
Result

# Pandas Accelerator Mode for cuDF (cudf.pandas)



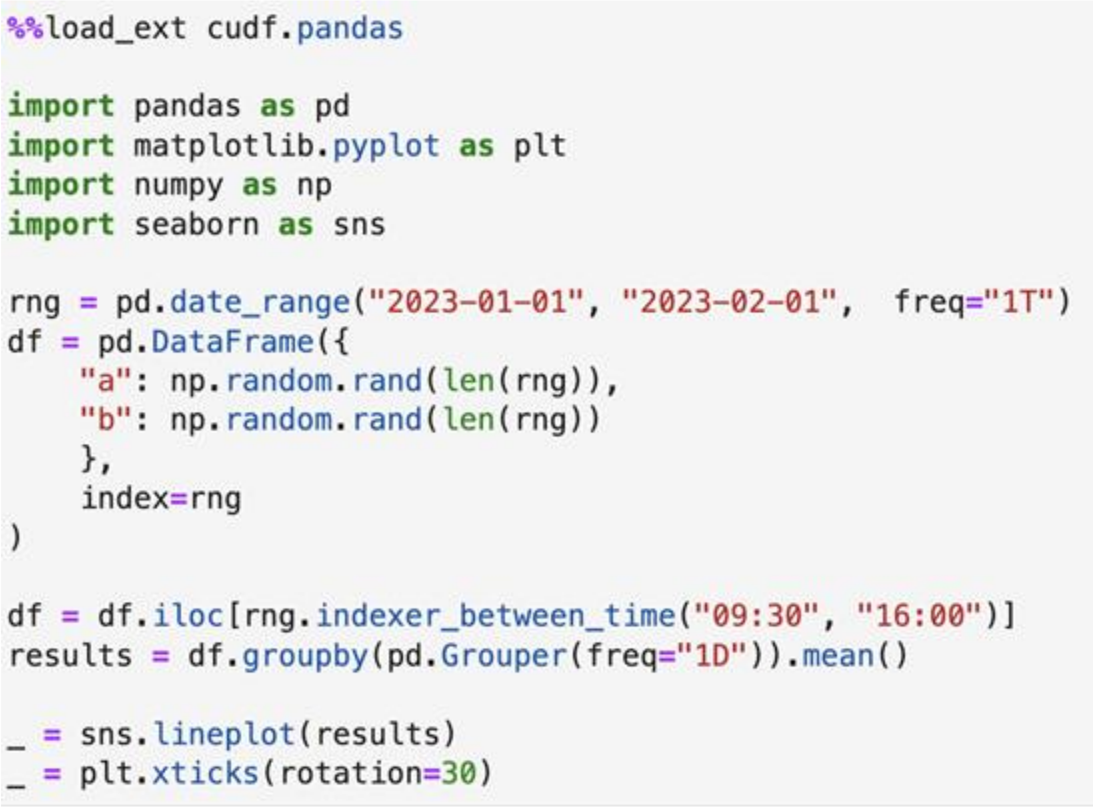
```
[ ]: %%time
     import pandas as pd

     df = pd.read_csv("rows.csv",
                        usecols=[
                            "Registration State",
                            "Violation Description",
                            "Vehicle Body Type"
                        ])
     (df[["Registration State", "Violation Description"]]
      .value_counts()  # count of offences per state per offence
      .groupby("Registration State")  # grouped by state
      .head(1)  # offence with largest count
      .sort_index()  # sort by state name
      .reset_index()
      .head(5)
     )
```



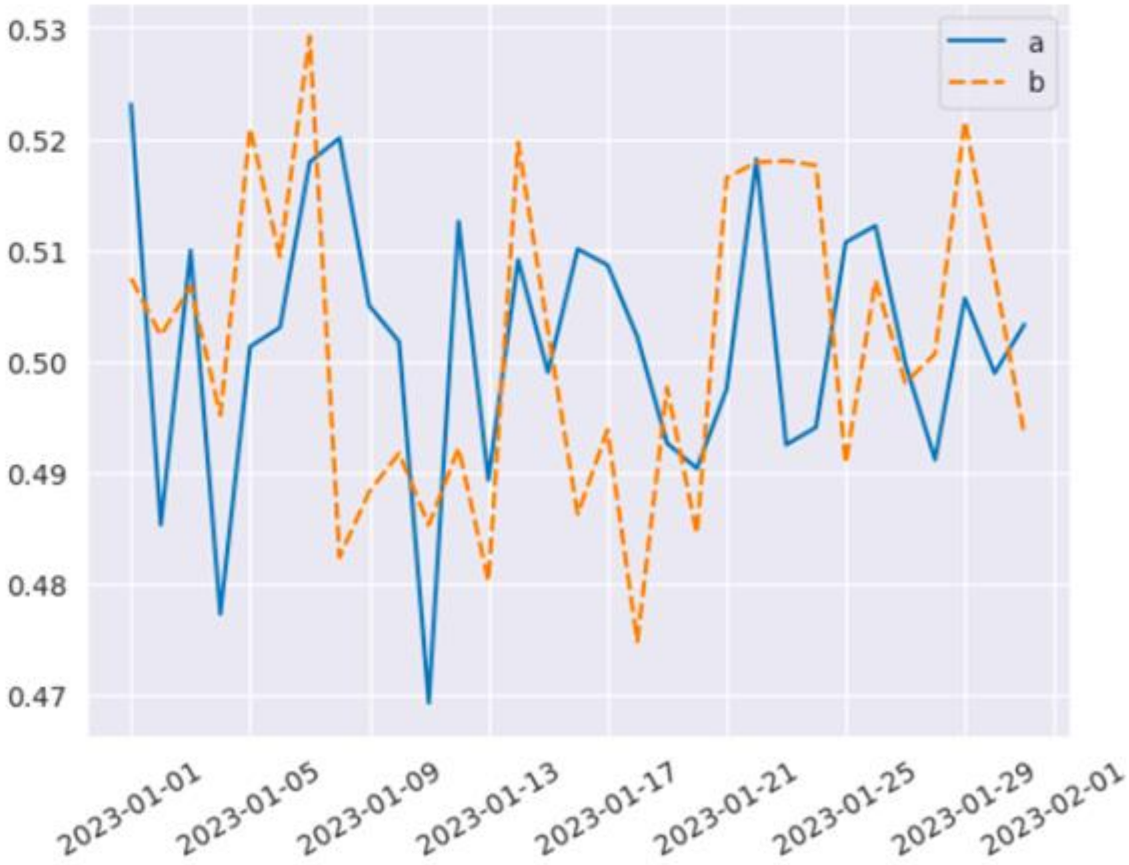
```
[ ]: %%time
     %load_ext cudf.pandas
     import pandas as pd

     df = pd.read_csv("rows.csv",
                        usecols=[
                            "Registration State",
                            "Violation Description",
                            "Vehicle Body Type"
                        ])
     (df[["Registration State", "Violation Description"]]
      .value_counts()  # count of offences per state per offence
      .groupby("Registration State")  # grouped by state
      .head(1)  # offence with largest count
      .sort_index()  # sort by state name
      .reset_index()
      .head(5)
     )
```

# cudf.pandas in Action

## A brief example

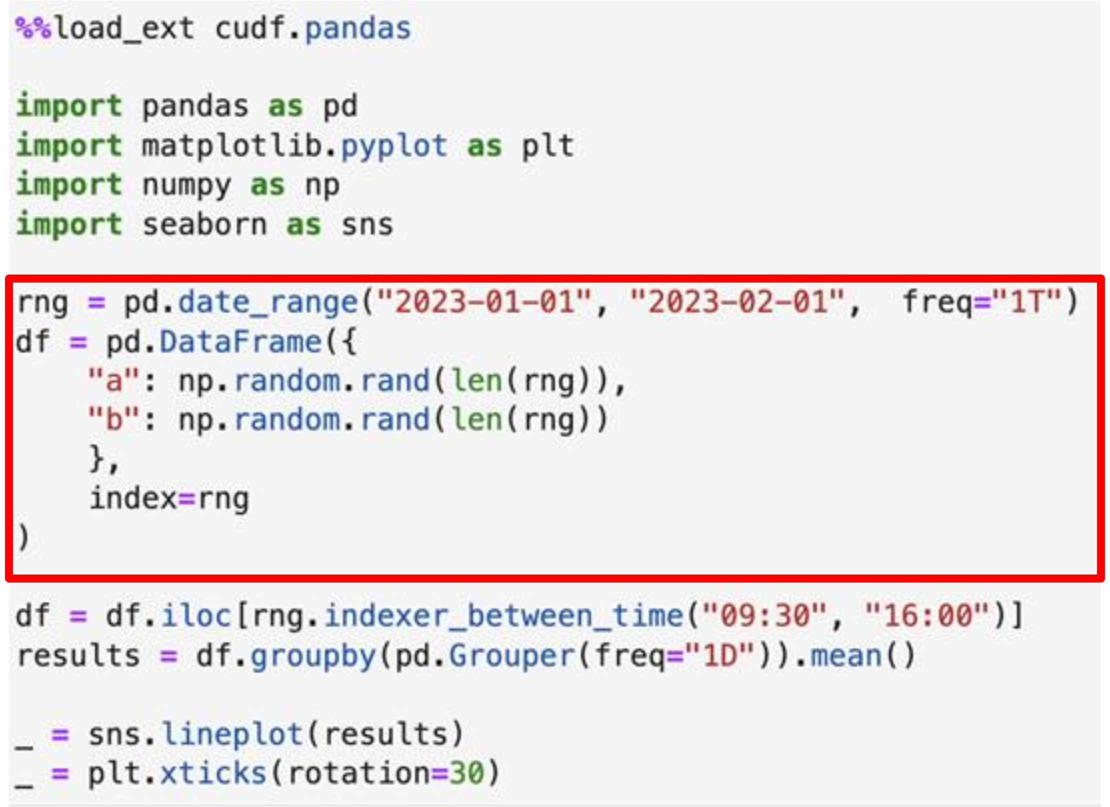


```
%%load_ext cudf.pandas

import pandas as pd
import matplotlib.pyplot as plt
import numpy as np
import seaborn as sns

rng = pd.date_range("2023-01-01", "2023-02-01",  freq="1T")
df = pd.DataFrame({
    "a": np.random.rand(len(rng)),
    "b": np.random.rand(len(rng))
    },
    index=rng
)

df = df.iloc[rng.indexer_between_time("09:30", "16:00")]
results = df.groupby(pd.Grouper(freq="1D")).mean()

_ = sns.lineplot(results)
_ = plt.xticks(rotation=30)
```



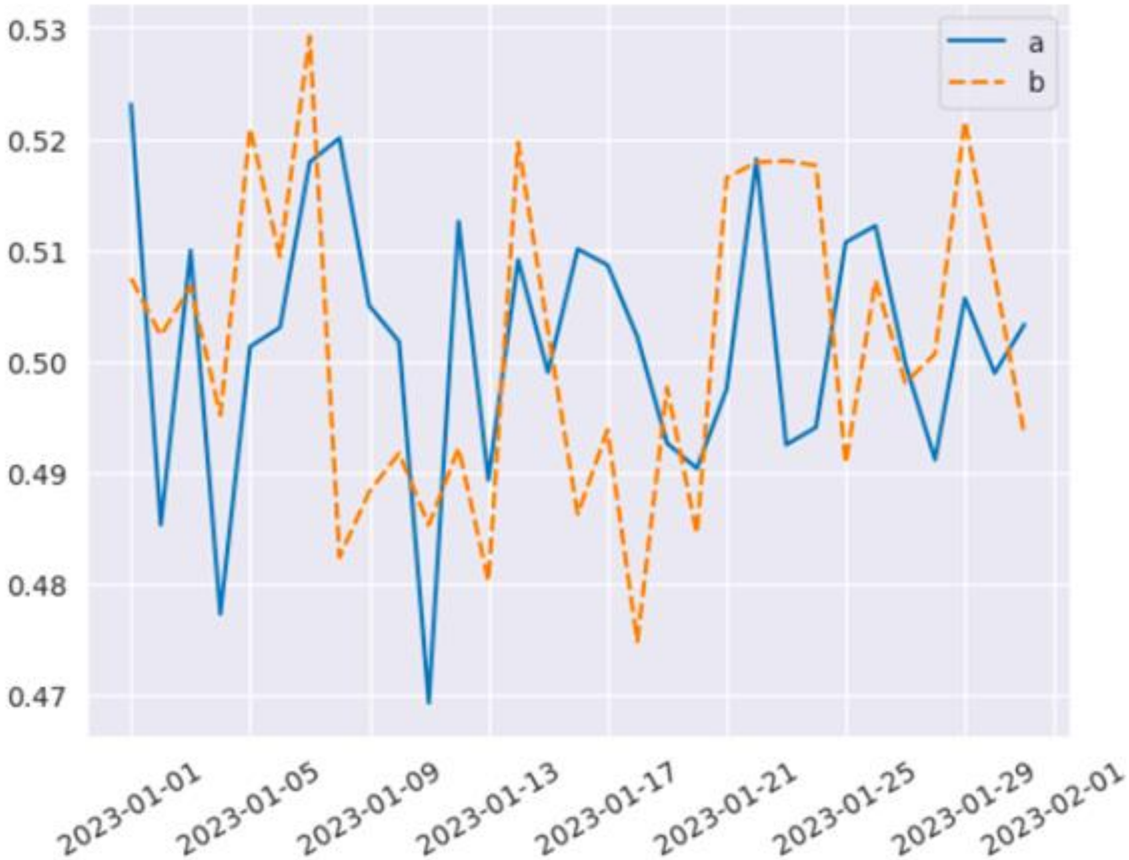
# `cudf.pandas` in Action

## A brief example



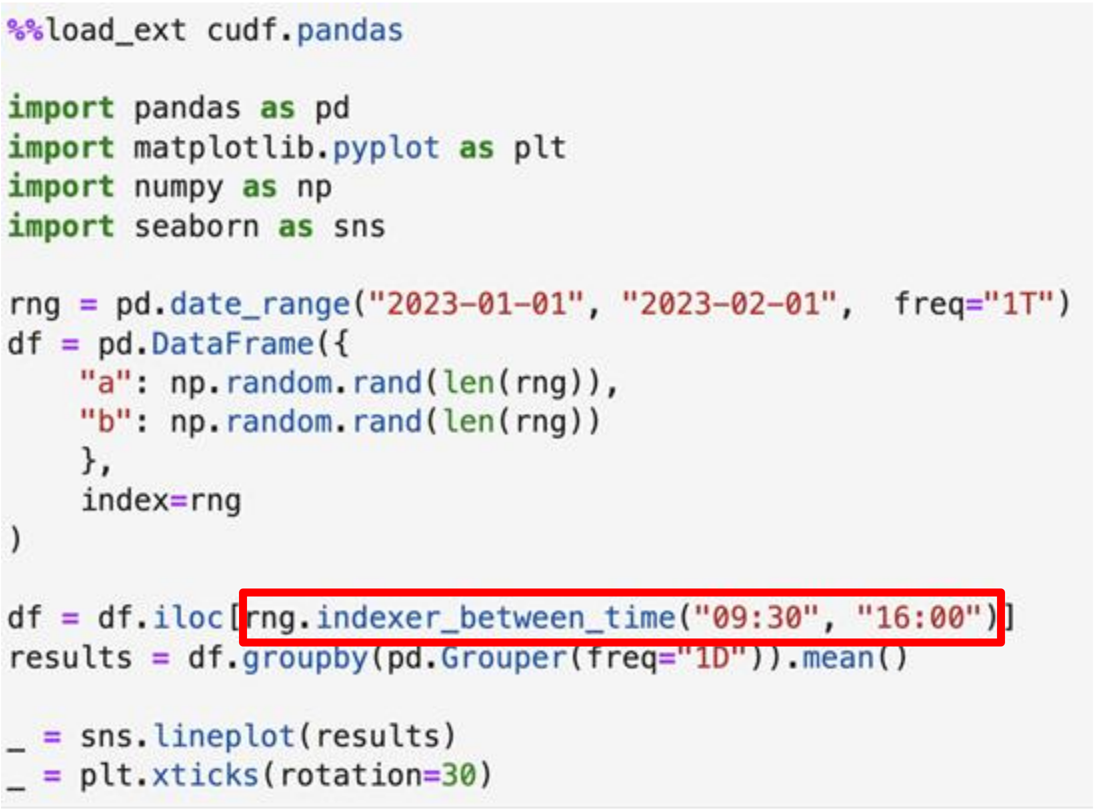
```
%%load_ext cudf.pandas

import pandas as pd
import matplotlib.pyplot as plt
import numpy as np
import seaborn as sns

rng = pd.date_range("2023-01-01", "2023-02-01",  freq="1T")
df = pd.DataFrame({
    "a": np.random.rand(len(rng)),
    "b": np.random.rand(len(rng))
    },
    index=rng
)

df = df.iloc[rng.indexer_between_time("09:30", "16:00")]
results = df.groupby(pd.Grouper(freq="1D")).mean()

_ = sns.lineplot(results)
_ = plt.xticks(rotation=30)
```

This part runs entirely on the GPU
cuDF supports all these operations



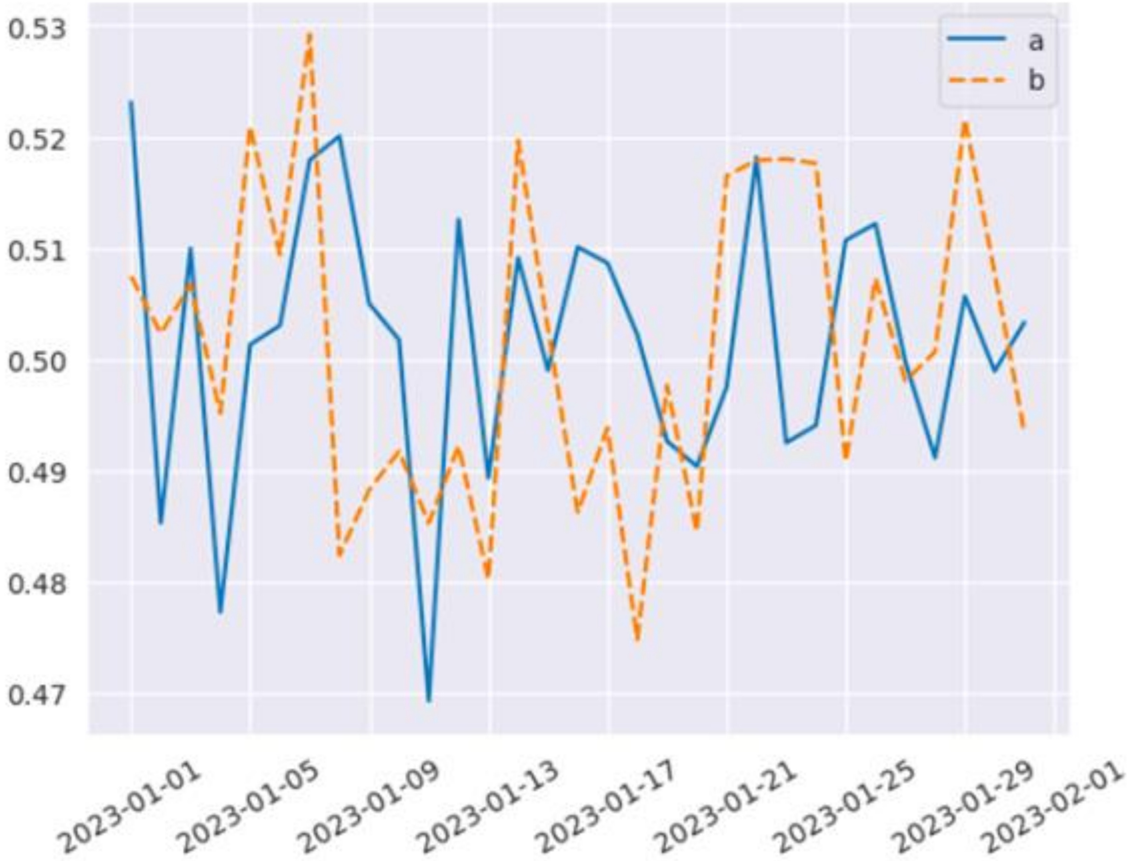
# cudf.pandas in Action

## A brief example



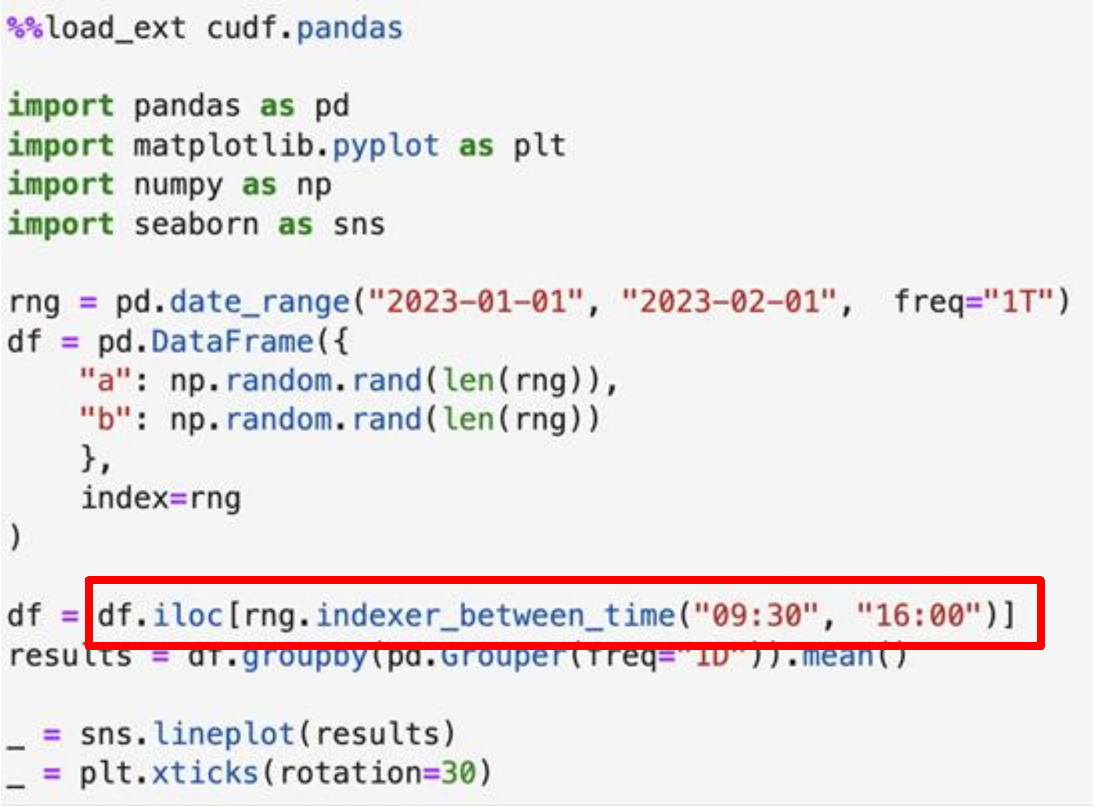
```
%%load_ext cudf.pandas

import pandas as pd
import matplotlib.pyplot as plt
import numpy as np
import seaborn as sns

rng = pd.date_range("2023-01-01", "2023-02-01",  freq="1T")
df = pd.DataFrame({
    "a": np.random.rand(len(rng)),
    "b": np.random.rand(len(rng))
    },
    index=rng
)

df = df.iloc[rng.indexer_between_time("09:30", "16:00")]
results = df.groupby(pd.Grouper(freq="1D")).mean()

_ = sns.lineplot(results)
_ = plt.xticks(rotation=30)
```

`indexer_between_time` isn’t supported on the GPU — so it runs on the CPU

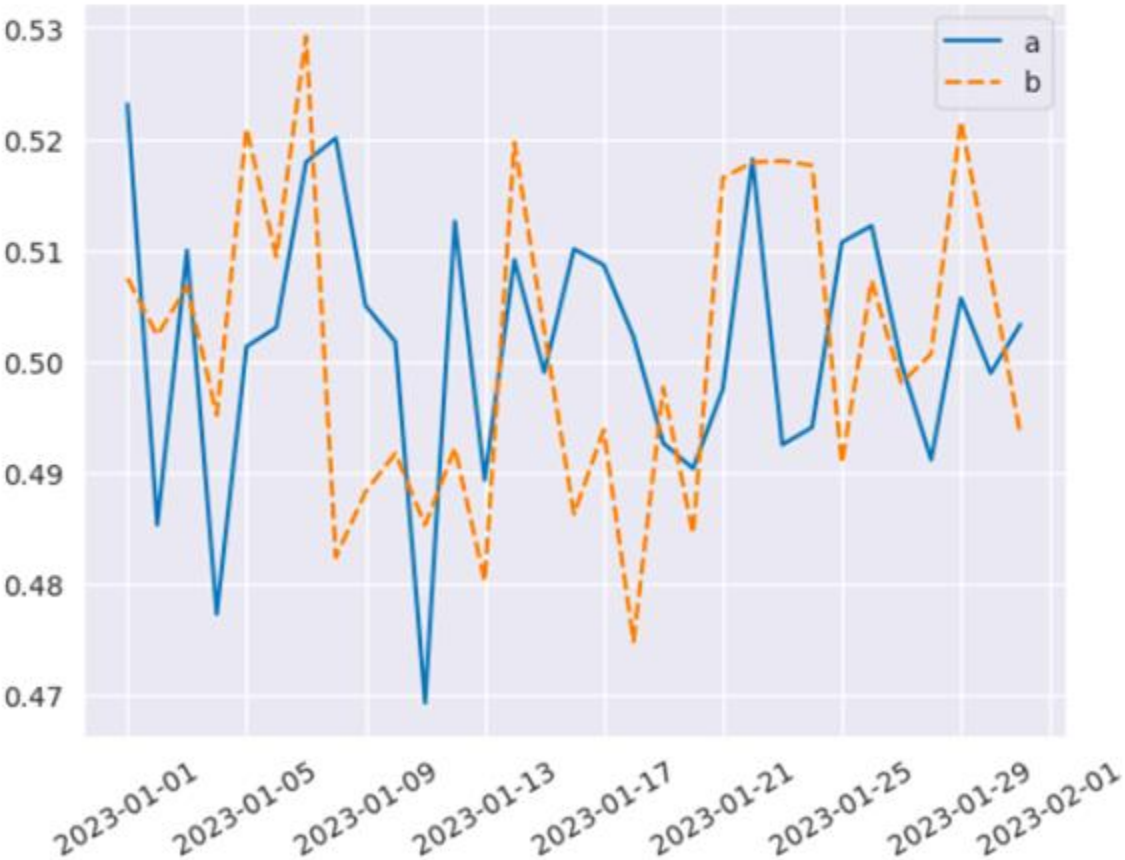


# `cudf.pandas` in Action

## A brief example



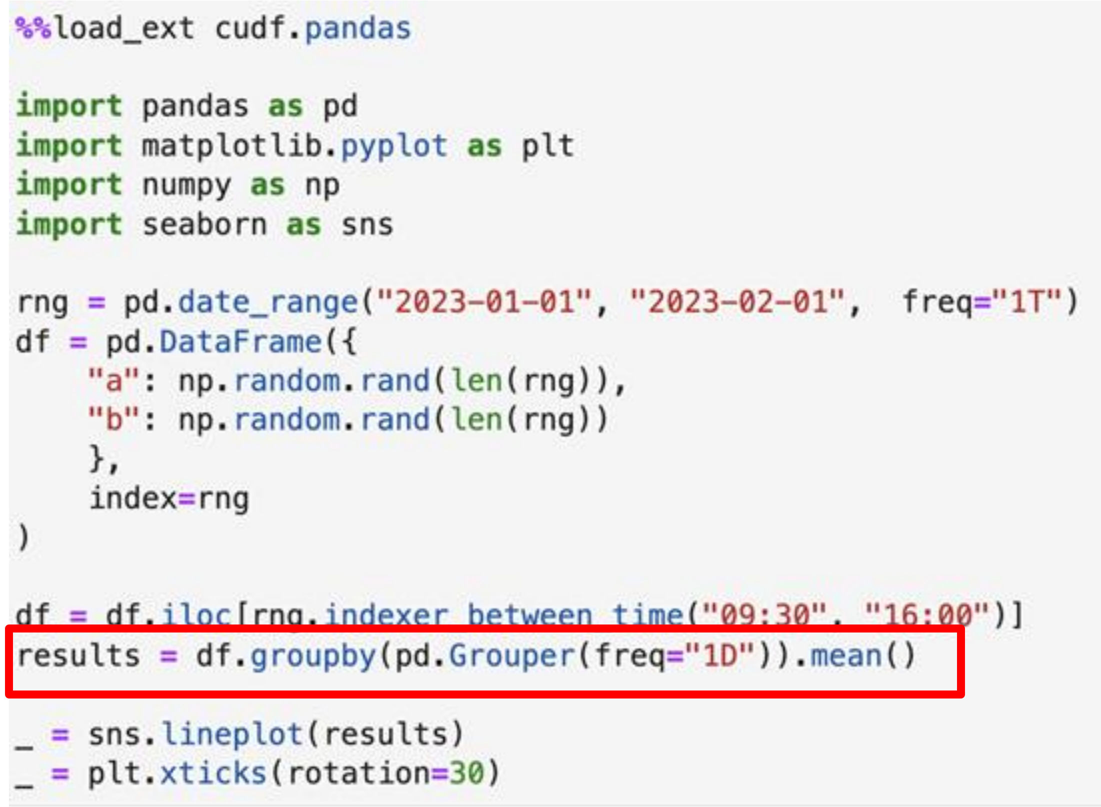
```
%%load_ext cudf.pandas

import pandas as pd
import matplotlib.pyplot as plt
import numpy as np
import seaborn as sns

rng = pd.date_range("2023-01-01", "2023-02-01",  freq="1T")
df = pd.DataFrame({
    "a": np.random.rand(len(rng)),
    "b": np.random.rand(len(rng))
    },
    index=rng
)

df = df.iloc[rng.indexer_between_time("09:30", "16:00")]
results = df.groupby(pd.Grouper(freq="1D")).mean()

_ = sns.lineplot(results)
_ = plt.xticks(rotation=30)
```



But this part happens on the GPU. The result of `indexer_between_time` is copied back from CPU to GPU

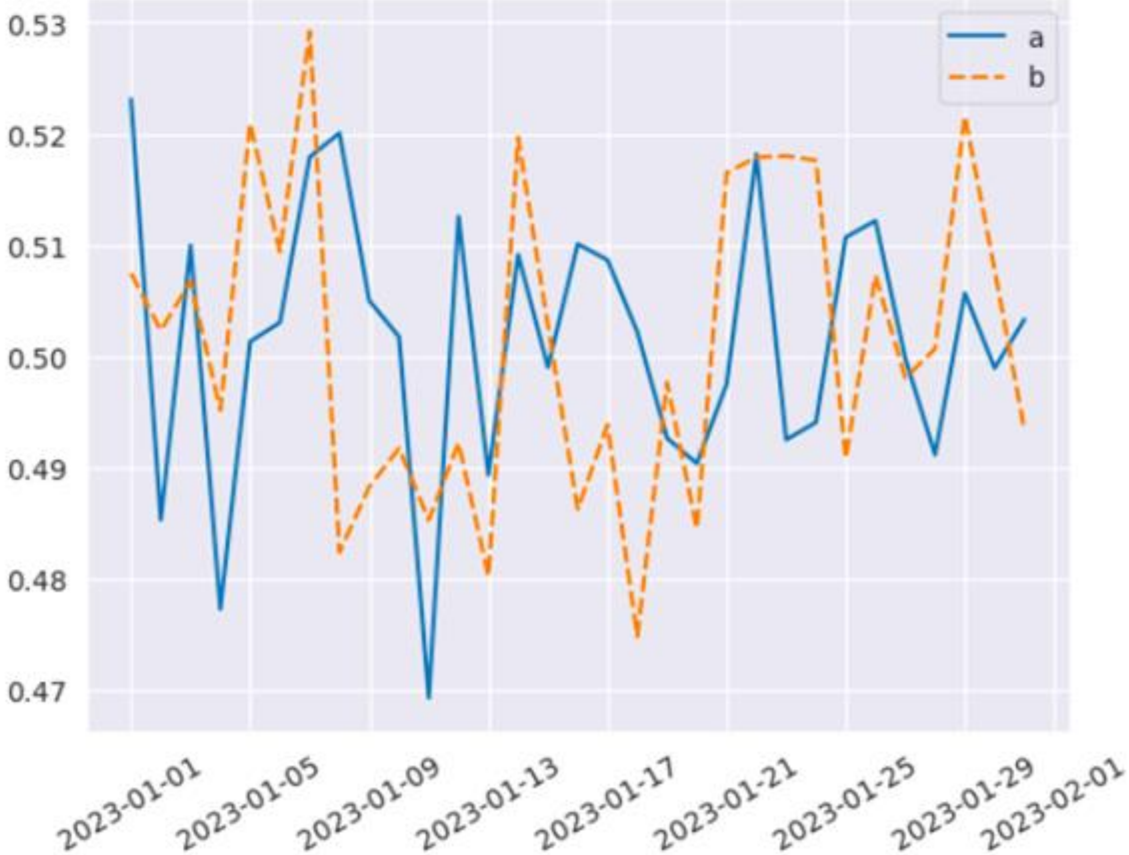
# cudf.pandas in Action

## A brief example



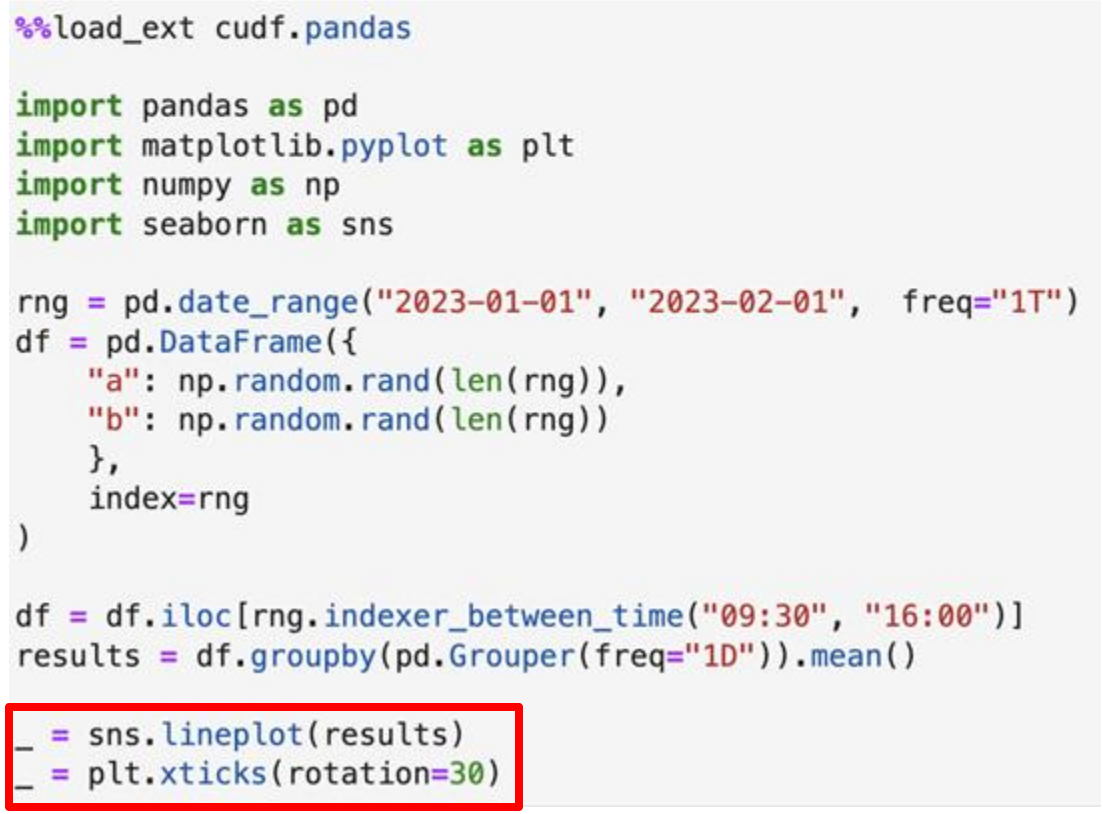
```
%%load_ext cudf.pandas

import pandas as pd
import matplotlib.pyplot as plt
import numpy as np
import seaborn as sns

rng = pd.date_range("2023-01-01", "2023-02-01",  freq="1T")
df = pd.DataFrame({
    "a": np.random.rand(len(rng)),
    "b": np.random.rand(len(rng))
    },
    index=rng
)

df = df.iloc[rng.indexer_between_time("09:30", "16:00")]
results = df.groupby(pd.Grouper(freq="1D")).mean()

_ = sns.lineplot(results)
_ = plt.xticks(rotation=30)
```

This part runs entirely on the GPU

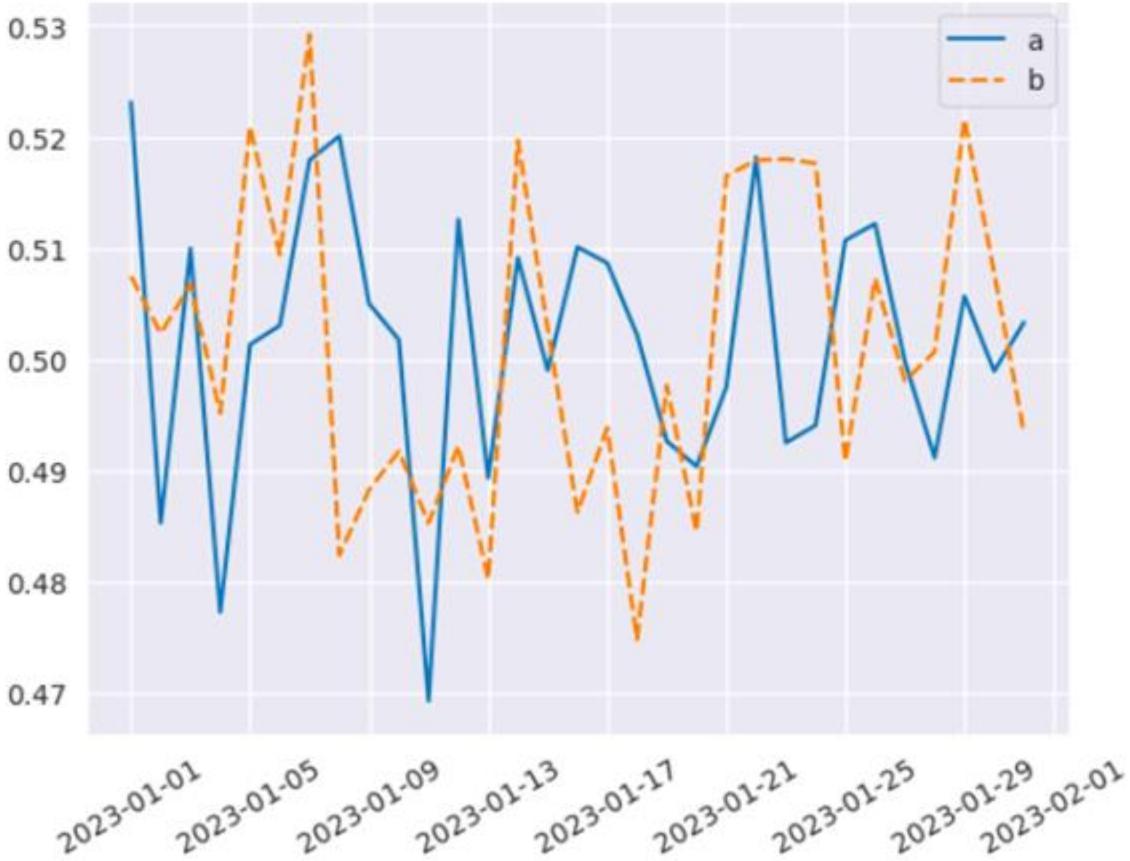


# cudf.pandas in Action

## A brief example



```
%%load_ext cudf.pandas

import pandas as pd
import matplotlib.pyplot as plt
import numpy as np
import seaborn as sns

rng = pd.date_range("2023-01-01", "2023-02-01",  freq="1T")
df = pd.DataFrame({
    "a": np.random.rand(len(rng)),
    "b": np.random.rand(len(rng))
    },
    index=rng
)

df = df.iloc[rng.indexer_between_time("09:30", "16:00")]
results = df.groupby(pd.Grouper(freq="1D")).mean()

_ = sns.lineplot(results)
_ = plt.xticks(rotation=30)
```



We can seamlessly interoperate with third-party libraries like Seaborn

# cudf.pandas summary

Provides **all** of the Pandas API

Uses the GPU (via cuDF) for operations supported by cuDF

Uses the CPU (via Pandas) for operations not supported by cuDF

Data movement is completely hidden from the user

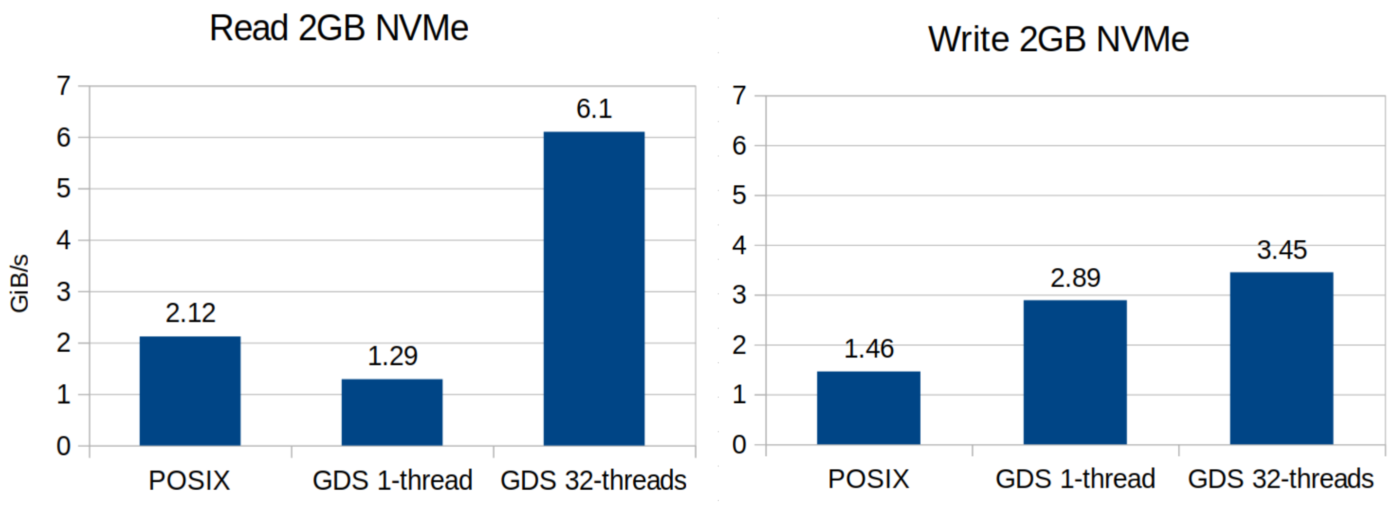
Zero code change: accelerates Pandas “in-place”

# RAPIDS KvikIO

KvikIO is a C++ and Python frontend for cuFile that provide features such as an object-oriented API, exception handling, RAII semantic, multithreading IO, fallback mode, and a Zarr backend.

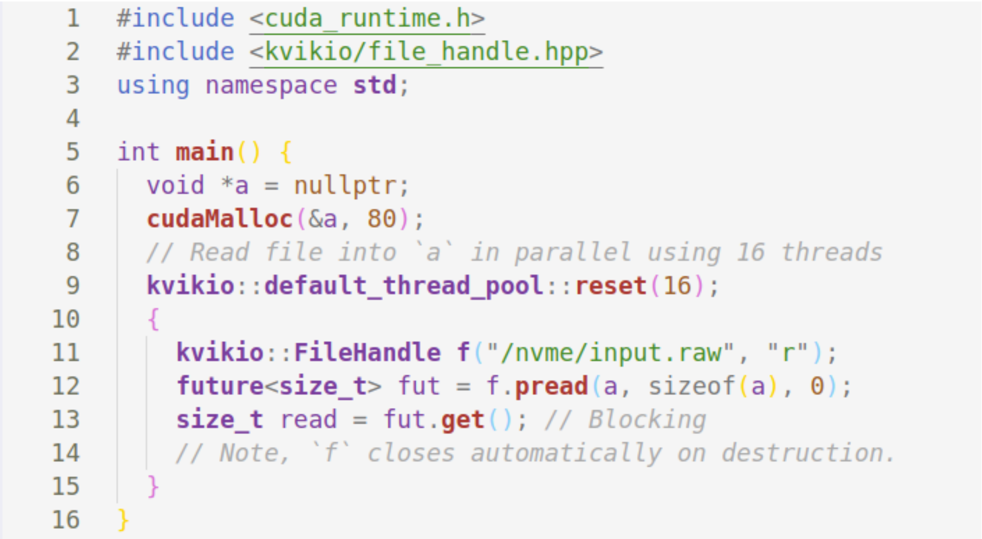
Using KvikIO should feel natural to C++ and Python developers.

Comparing KvikIO's Zarr backend versus manually copying between GPU and host memory before accessing the Zarr array using POSIX

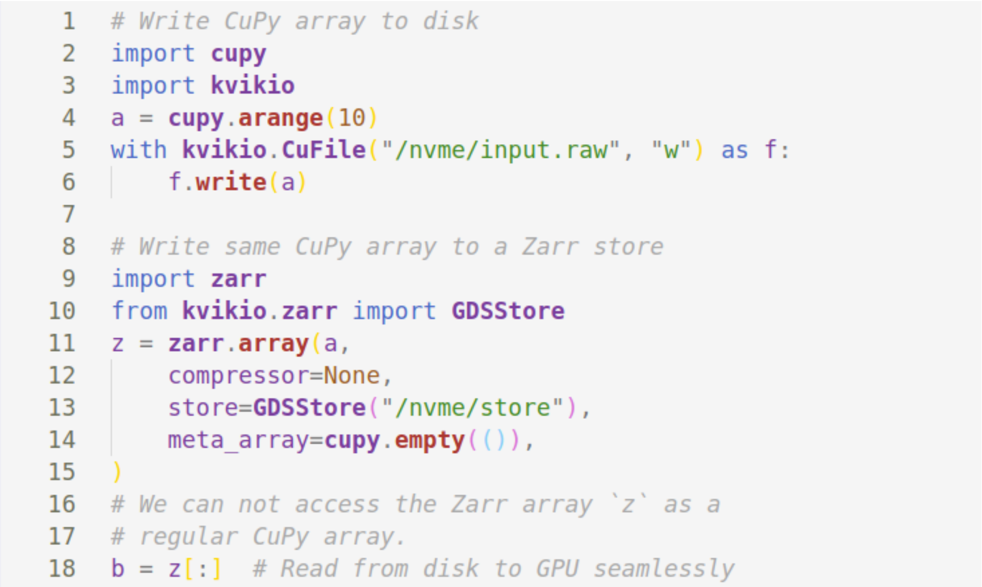


NVIDIA DGX A100 (using one of the GPUs)
2x AMD EPYC 7742 64-Core@3.4GHz (max boost)
1x NVMe Samsung PM1733 SSD (MZWLJ3T8HBLS-00007)

KvikIO: https://github.com/rapidsai/kvikio



```cpp
#include <cuda_runtime.h>
#include <kvikio/file_handle.hpp>
using namespace std;

int main() {
  void *a = nullptr;
  cudaMalloc(&a, 80);
  // Read file into `a` in parallel using 16 threads
  kvikio::default_thread_pool::reset(16);
  {
    kvikio::FileHandle f("/nvme/input.raw", "r");
    future<size_t> fut = f.pread(a, sizeof(a), 0);
    size_t read = fut.get(); // Blocking
    // Note, `f` closes automatically on destruction.
  }
}
```



```python
# Write CuPy array to disk
import cupy
import kvikio
a = cupy.arange(10)
with kvikio.CuFile("/nvme/input.raw", "w") as f:
    f.write(a)

# Write same CuPy array to a Zarr store
import zarr
from kvikio.zarr import GDSStore
z = zarr.array(a,
    compressor=None,
    store=GDSStore("/nvme/store"),
    meta_array=cupy.empty(()),
)
# We can not access the Zarr array `z` as a
# regular CuPy array.
b = z[:]  # Read from disk to GPU seamlessly
```

# RAPIDS ML and Graph Analytics

# cuML

Accelerated machine learning with a scikit-learn API

CPU

Scikit-learn

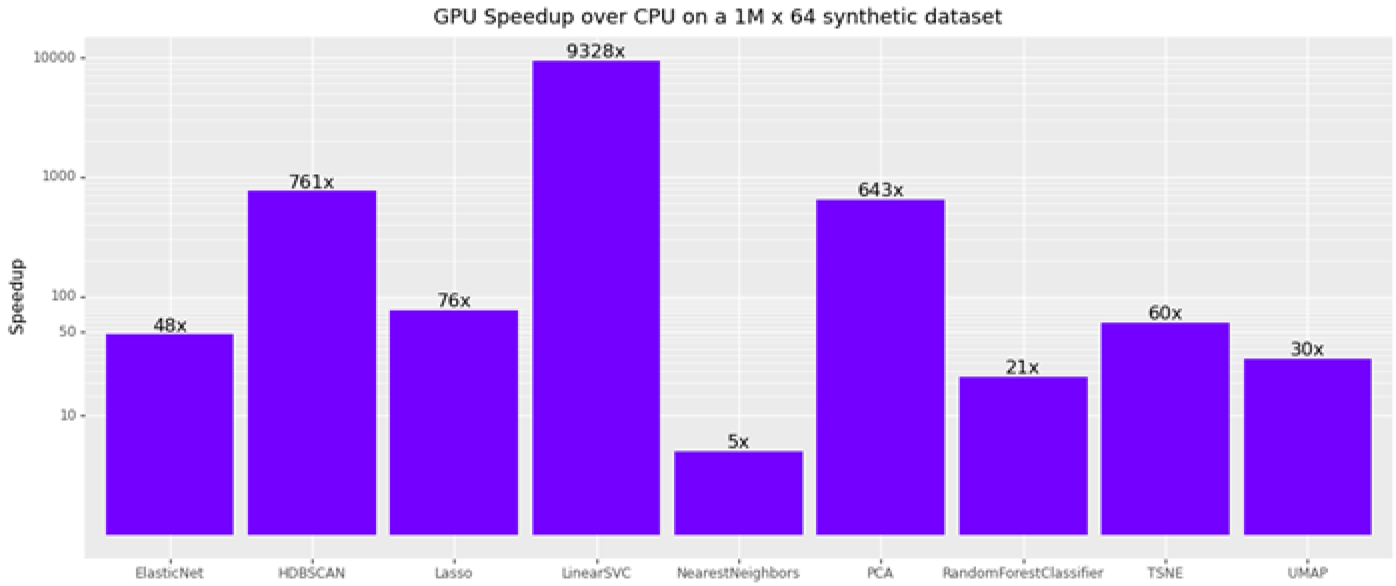
```
>>> from sklearn.ensemble import
RandomForestClassifier
>>> clf = RandomForestClassifier()
>>> clf.fit(x, y)
```

GPU

cuML

```
>>> from cuml.ensemble import
RandomForestClassifier
>>> clf = RandomForestClassifier()
>>> clf.fit(x, y)
```

## 50+ GPU-Accelerated Algorithms

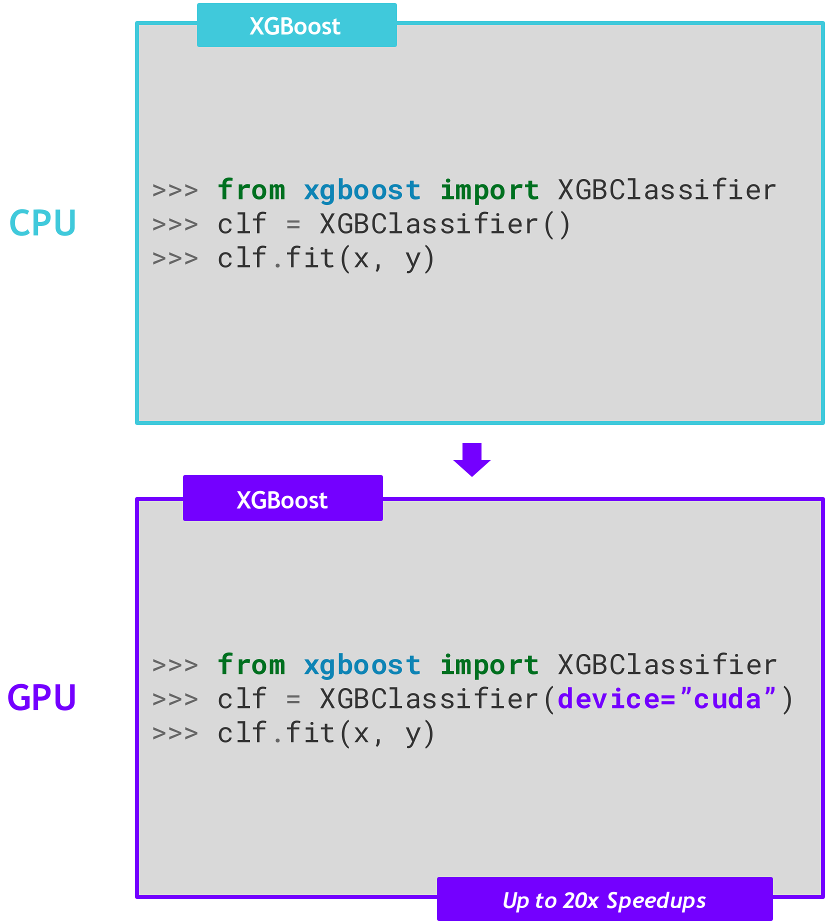


- Time Series
- Classification
- Regression
- Clustering
- Preprocessing
- Cross Validation
- Tree Models
- Dimensionality Reduction
- Explainability

A100 GPU vs. AMD EPYC 7642 (96 logical cores)
cuML 23.04, scikit-learn 1.2.2, umap-learn 0.5.3

# Accelerated XGBoost

“XGBoost is All You Need” – Bojan Tunguz, 4x Kaggle Grandmaster



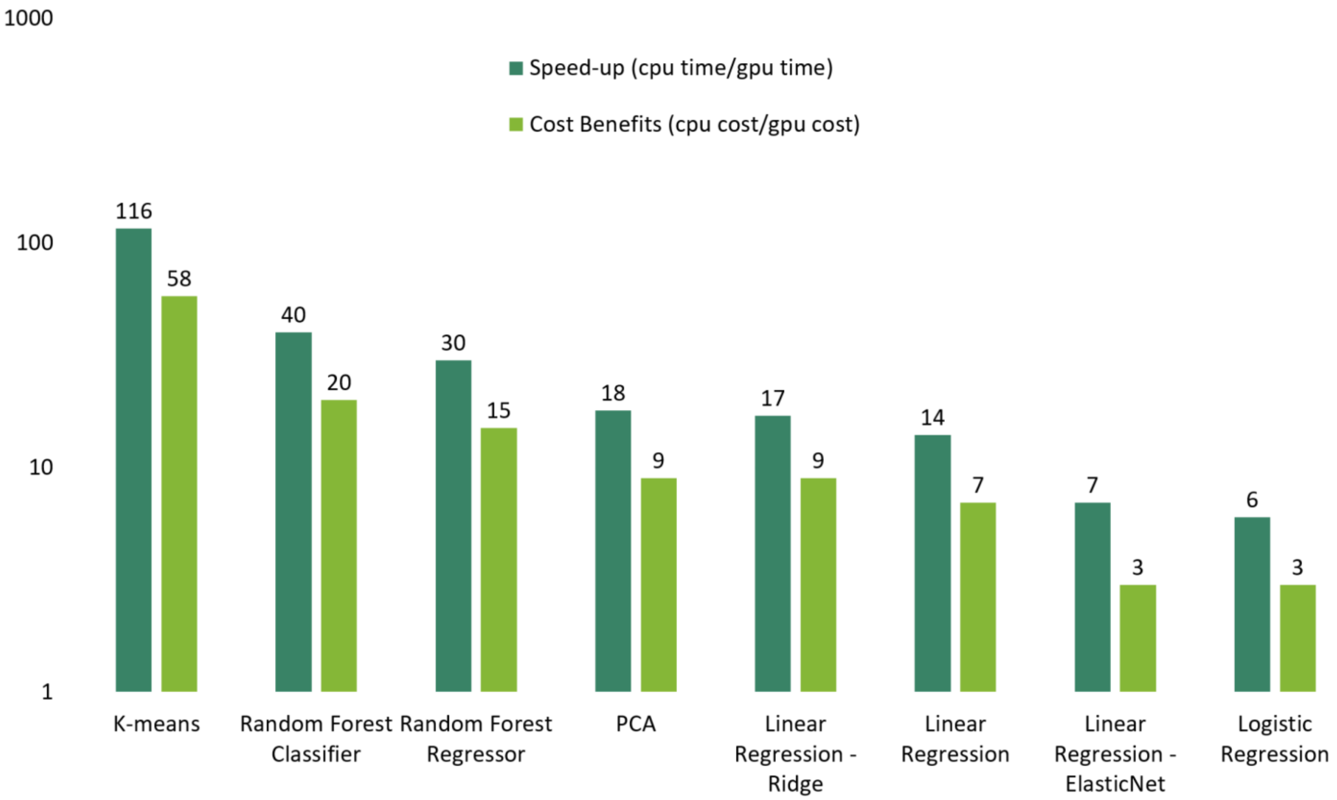
```
>>> from xgboost import XGBClassifier
>>> clf = XGBClassifier()
>>> clf.fit(x, y)
```

```
>>> from xgboost import XGBClassifier
>>> clf = XGBClassifier(device=”cuda”)
>>> clf.fit(x, y)
```

- One line of code change to unlock up to 20x speedups with GPUs
- Scalable to the world’s largest datasets with Dask and PySpark
- Built-in SHAP support for model explainability
- Deployable with Triton for lighting-fast inference in production
- RAPIDS helps maintain the XGBoost project

RAPIDS ❤ dmlc XGBoost

| Available Algorithms |
|---|
| K-Means |
| Linear Regression |
| Logistic Regression[1] |
| PCA |
| Random Forest Classifier |
| Random Forest Regressor |



## 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
and many more

Single CPU core
In-memory data

PyData

NumPy

scikit learn

pandas

$y_{it} = \beta' x_{it} + \mu_i + \epsilon_{it}$

### Dask

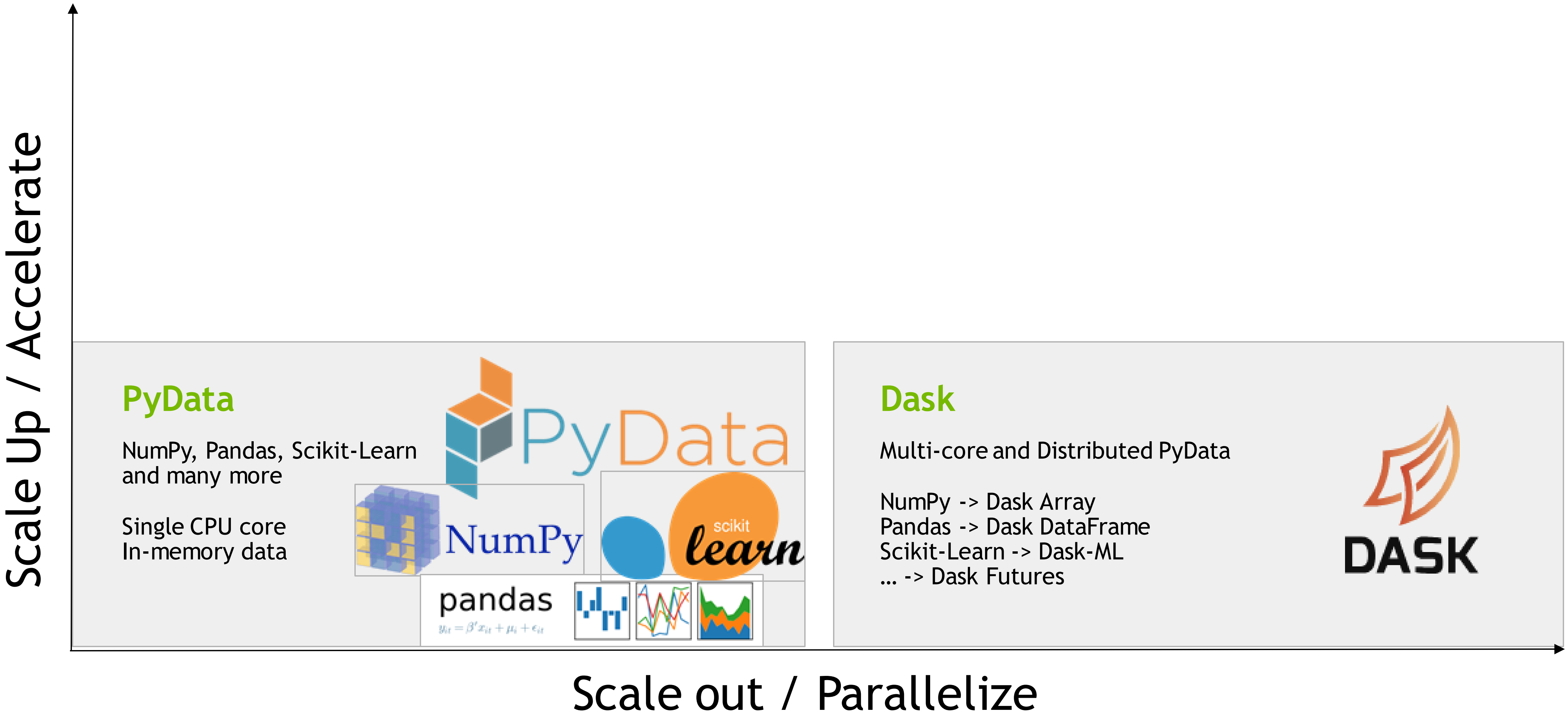
Multi-core and Distributed PyData

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

DASK

Scale out / Parallelize

# Scale up and out with RAPIDS and Dask



**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

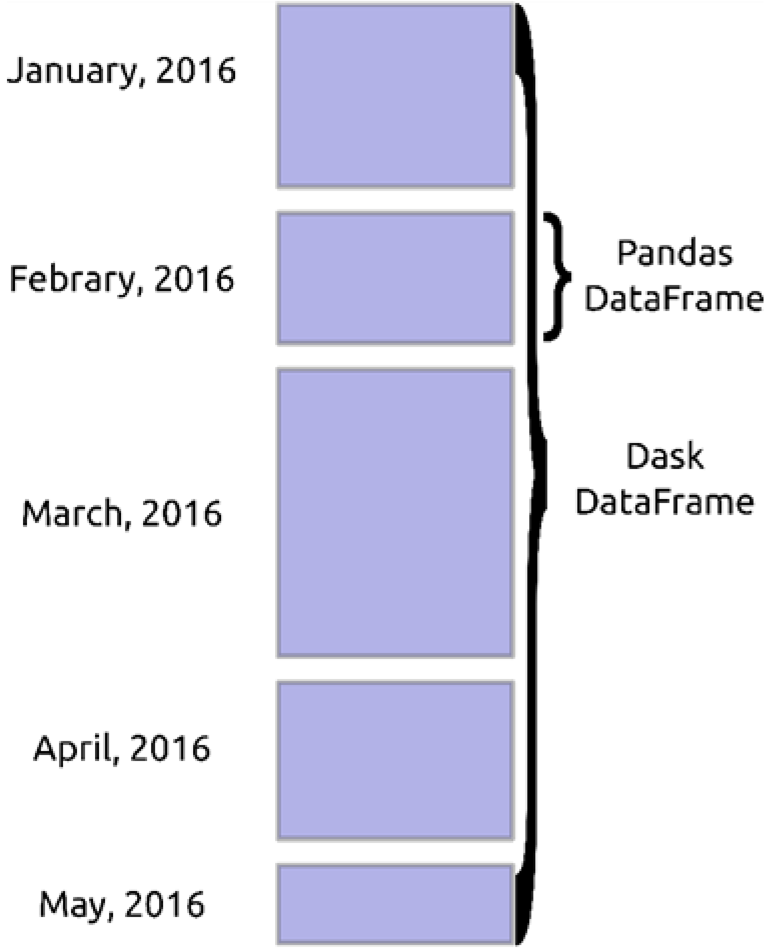
# Parallel Pandas
For ETL, time series, data munging

- 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

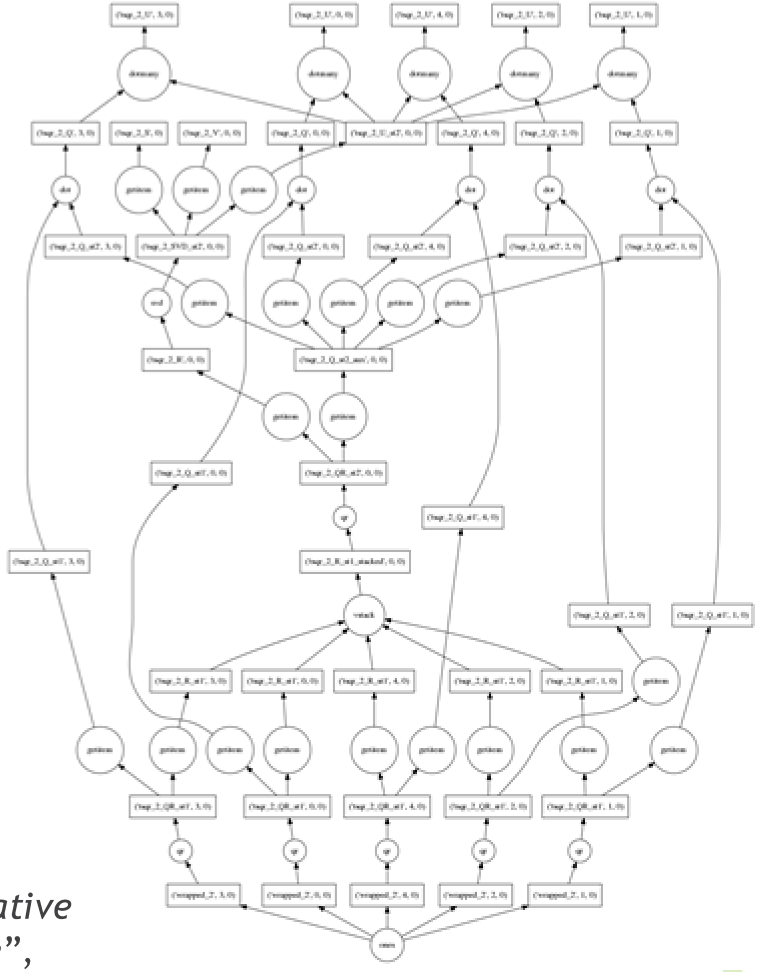
  Either lazily fetched from disk
  Or distributed throughout a cluster



# Parallel Python
## For custom systems, ML algorithms, workflow engines

- Parallelize existing codebases

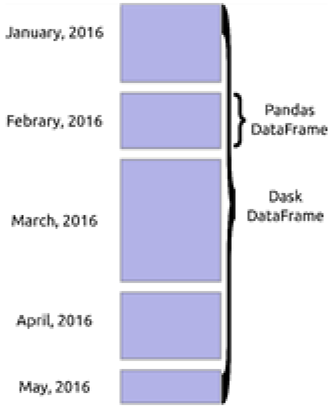
```
f = dask.delayed(f)
g = dask.delayed(g)

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)
```



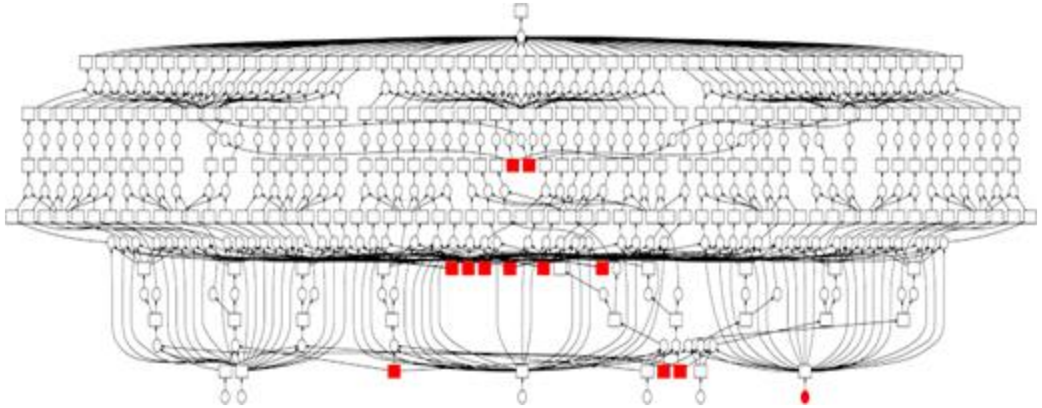
M Tepper, G Sapiro "*Compressed nonnegative matrix factorization is fast and accurate*", IEEE Transactions on Signal Processing, 2016

# Dask Connects Python users to Hardware

User



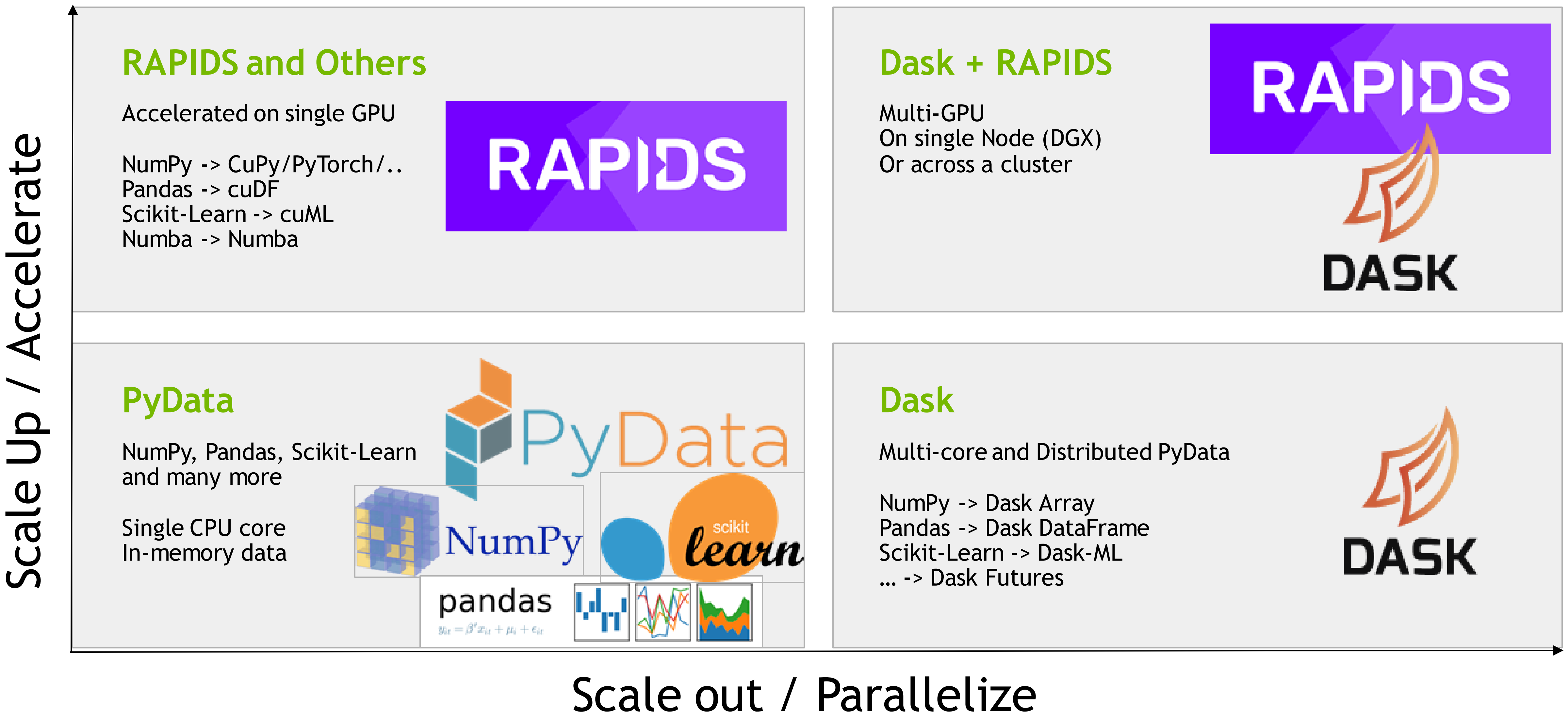
Writes high level code (NumPy/Pandas/Scikit-Learn)



Turns into a task graph

Execute on distributed hardware

## Scale up and out with RAPIDS and Dask



### 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

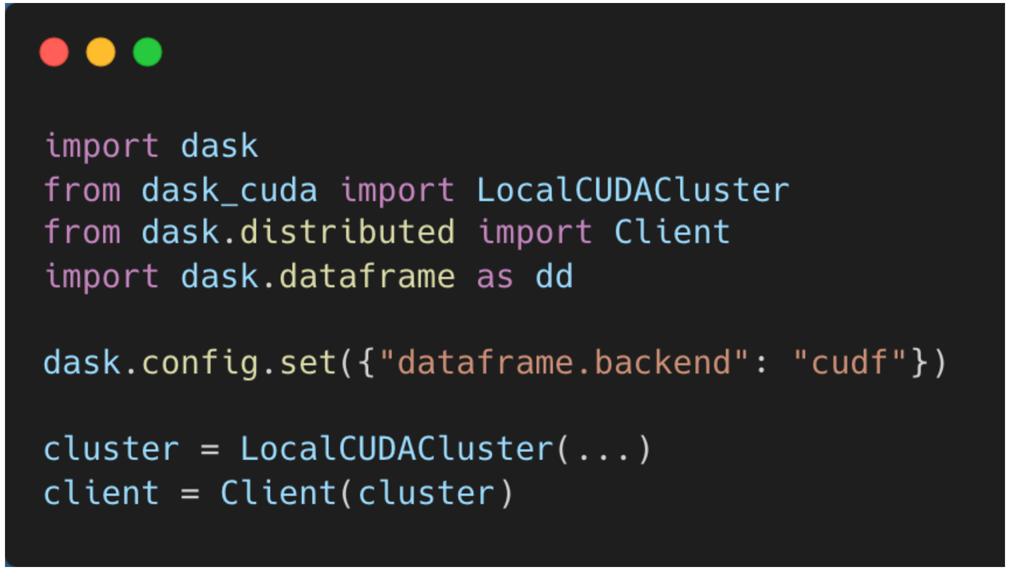
Scale Up / Accelerate

Scale out / Parallelize

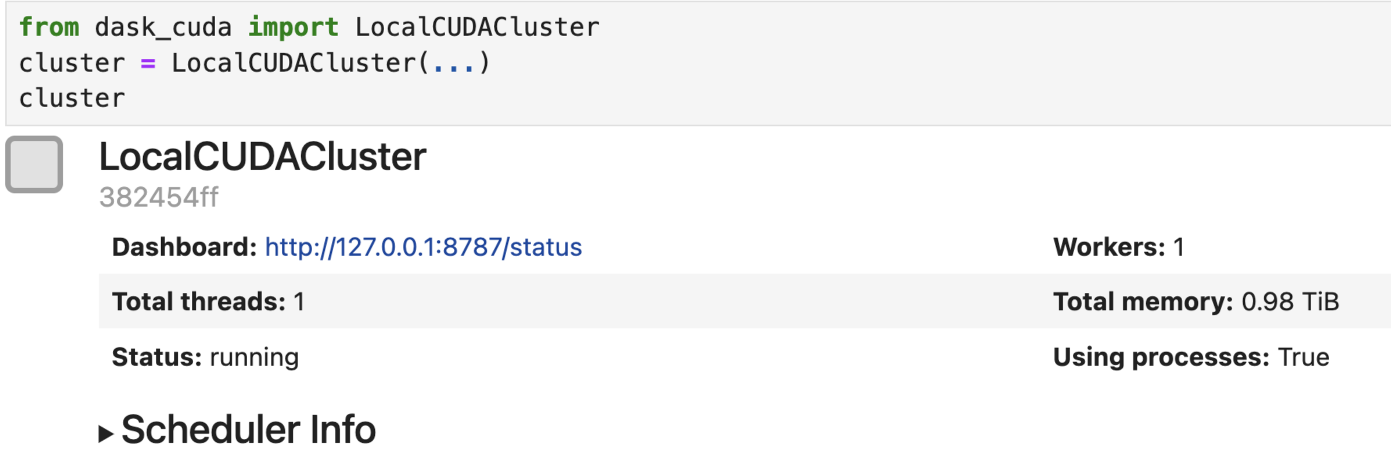
# Accelerated Dask

Just set “cudf” as the backend and use Dask-CUDA Workers

- Configurable Backend and GPU-Aware Workers
- Memory Spilling (GPU->CPU->Disk)
- Optimized Memory Management
- Accelerated RDMA and Networking (UCX)



```python
import dask
from dask_cuda import LocalCUDACluster
from dask.distributed import Client
import dask.dataframe as dd

dask.config.set({"dataframe.backend": "cudf"})

cluster = LocalCUDACluster(...)
client = Client(cluster)
```



```python
from dask_cuda import LocalCUDACluster
cluster = LocalCUDACluster(...)
cluster
```

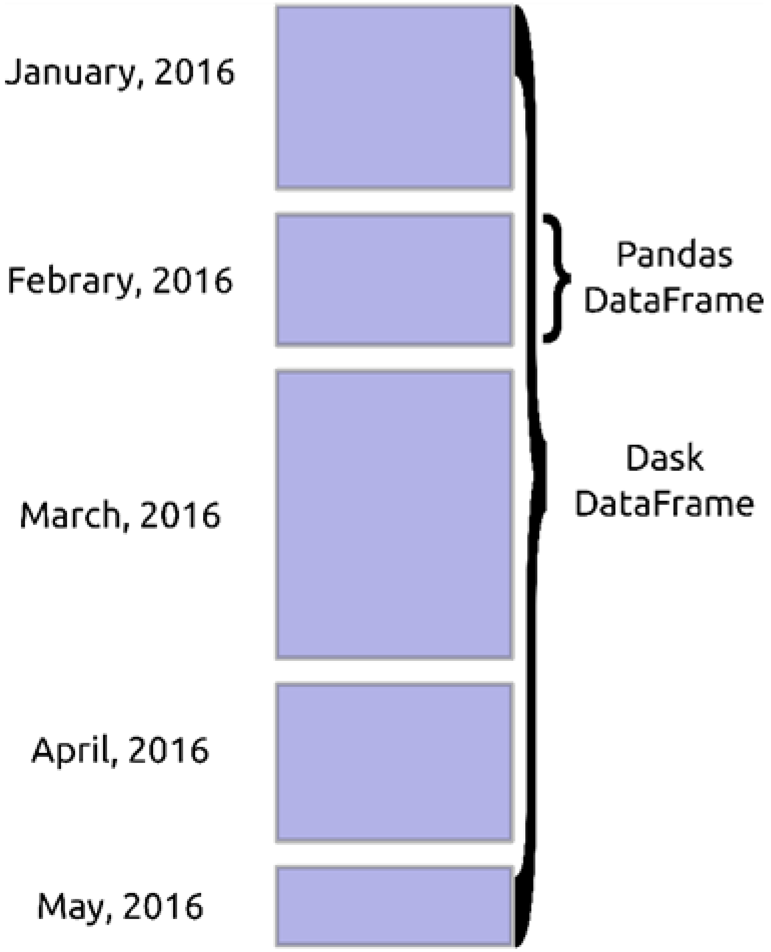
LocalCUDACluster

382454ff

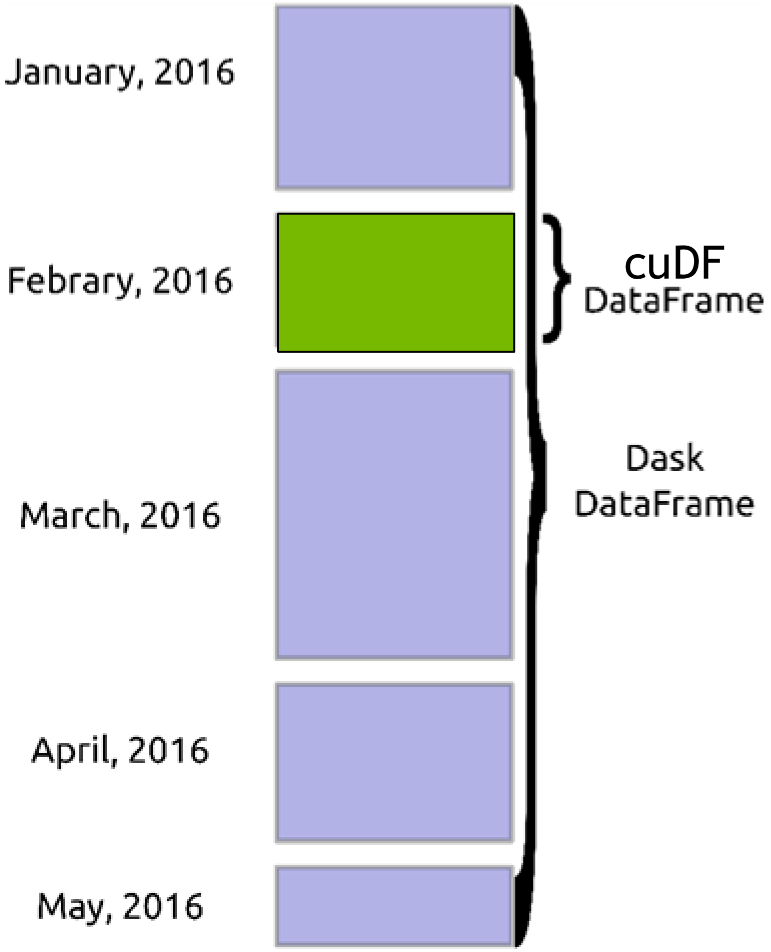
| | |
|---|---|
| **Dashboard:** http://127.0.0.1:8787/status | **Workers:** 1 |
| **Total threads:** 1 | **Total memory:** 0.98 TiB |
| **Status:** running | **Using processes:** True |

▸ Scheduler Info

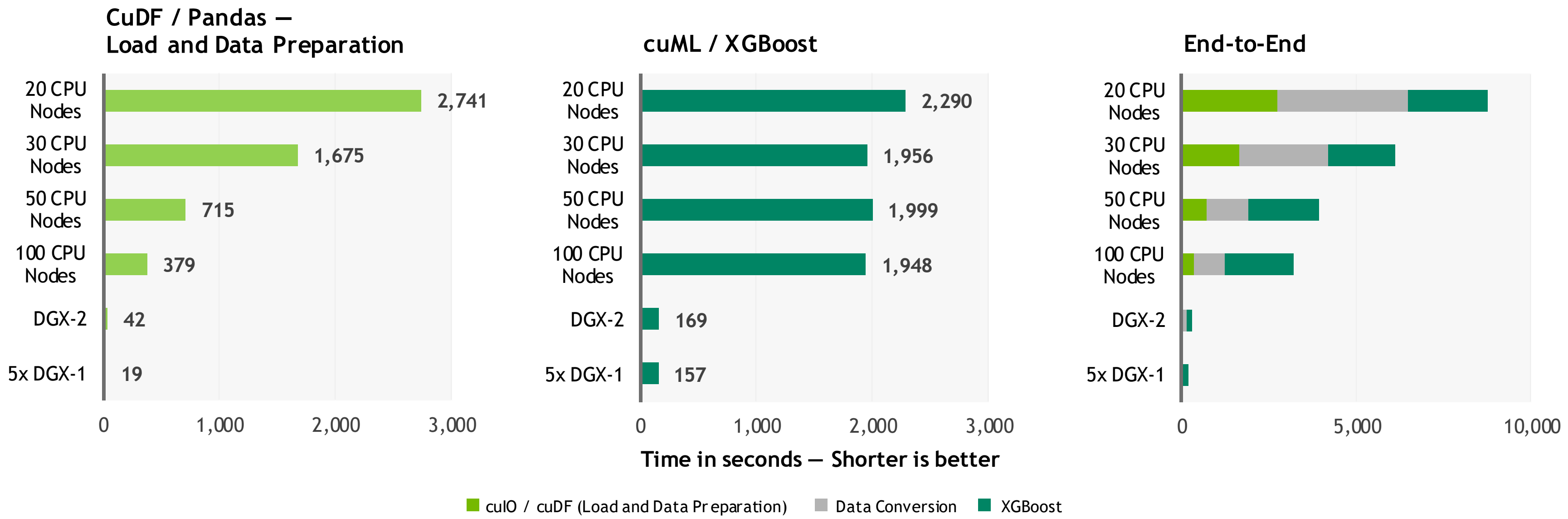
# Combine Dask with cuDF
## Many GPU DataFrames form a distributed DataFrame



## Combine Dask with cuDF
## Many GPU DataFrames form a distributed DataFrame



# 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

# Accelerated Apache Spark

## Zero code change acceleration for Spark DataFrames and SQL

CPU Spark

```
spark.sql("""
select
    order
    count(*) as order_count
from
    orders"""
)
```

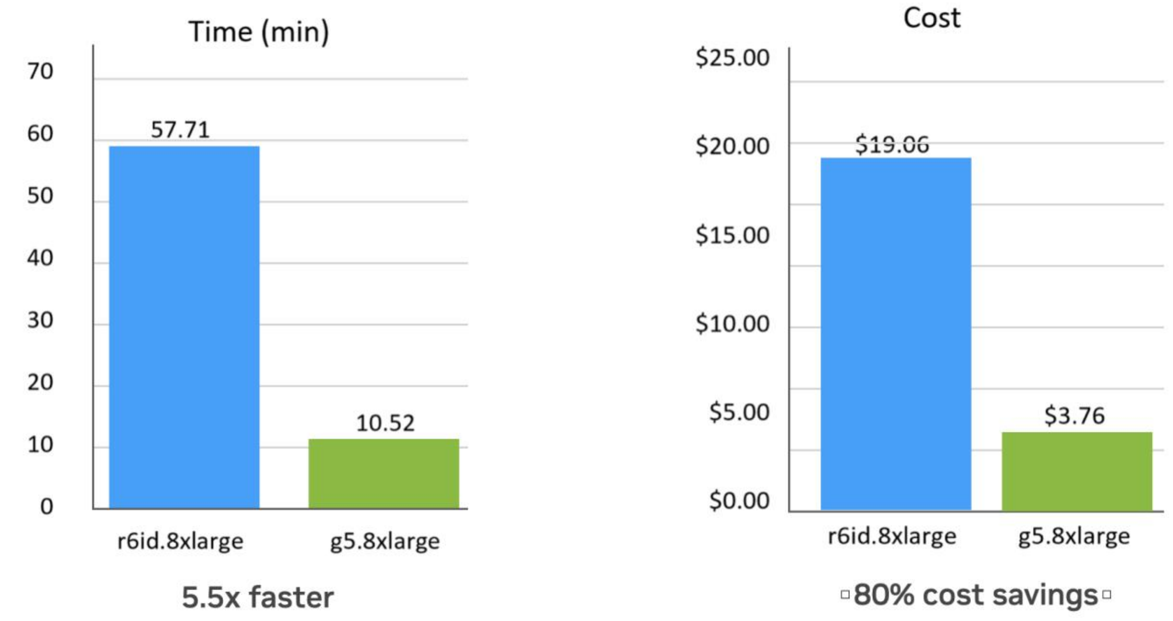
GPU Spark

```
spark.conf.set("spark.plugins",
"com.nvidia.spark.SQLPlugin")

spark.sql("""
select
    order
    count(*) as order_count
from
    orders"""
)
```

Average Speed-Ups: >5x

- RAPIDS operates as a software plugin to the popular Apache Spark platform
- Automatically accelerates supported operations (with CPU fallback if needed)
- Requires no code changes
- Works with Spark standalone, YARN clusters, Kubernetes clusters

NVIDIA Decision Support Benchmark 3TB (Public Cloud)



Apache Spark 3.4.1, RAPIDS Spark release 24.04
See GTC session S62257 for details

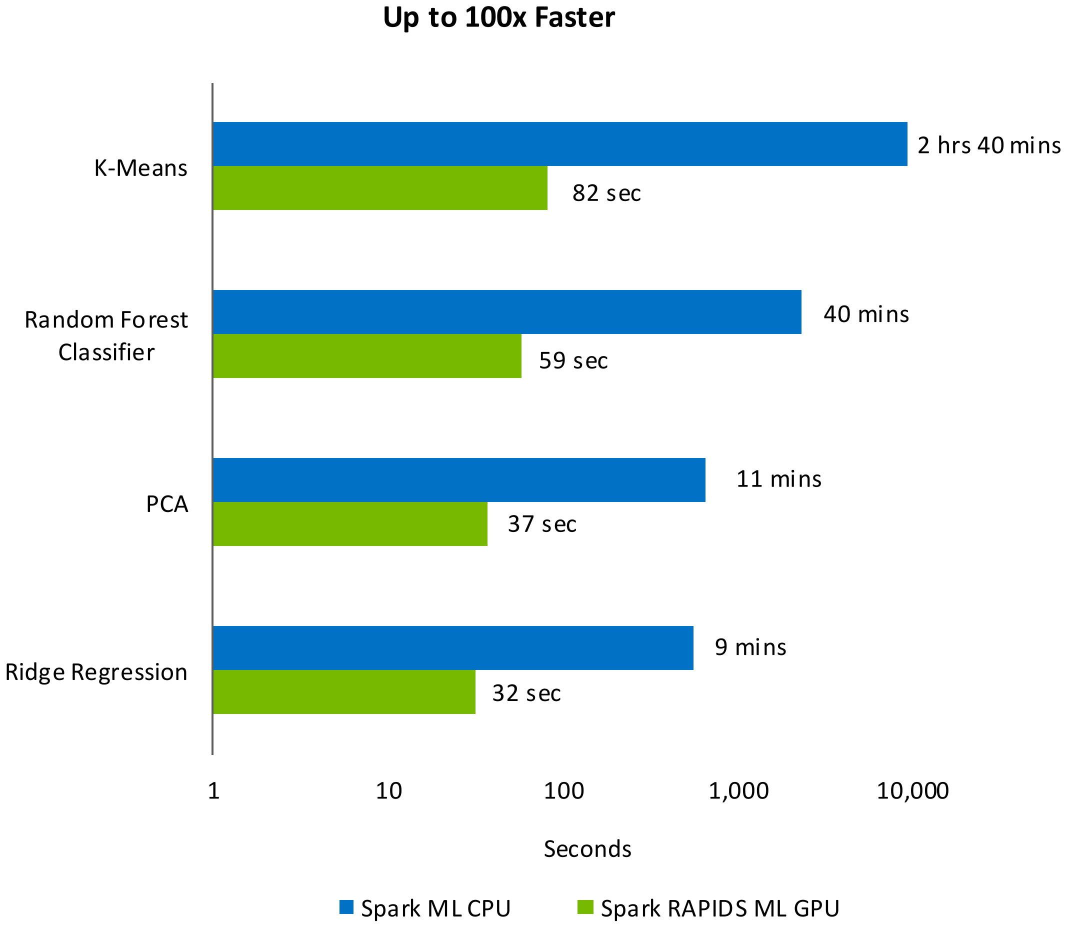
# Accelerated Apache Spark ML

Bringing GPU-accelerated machine learning to every Apache Spark user

Apache Spark™ MLlib

+

RAPIDS

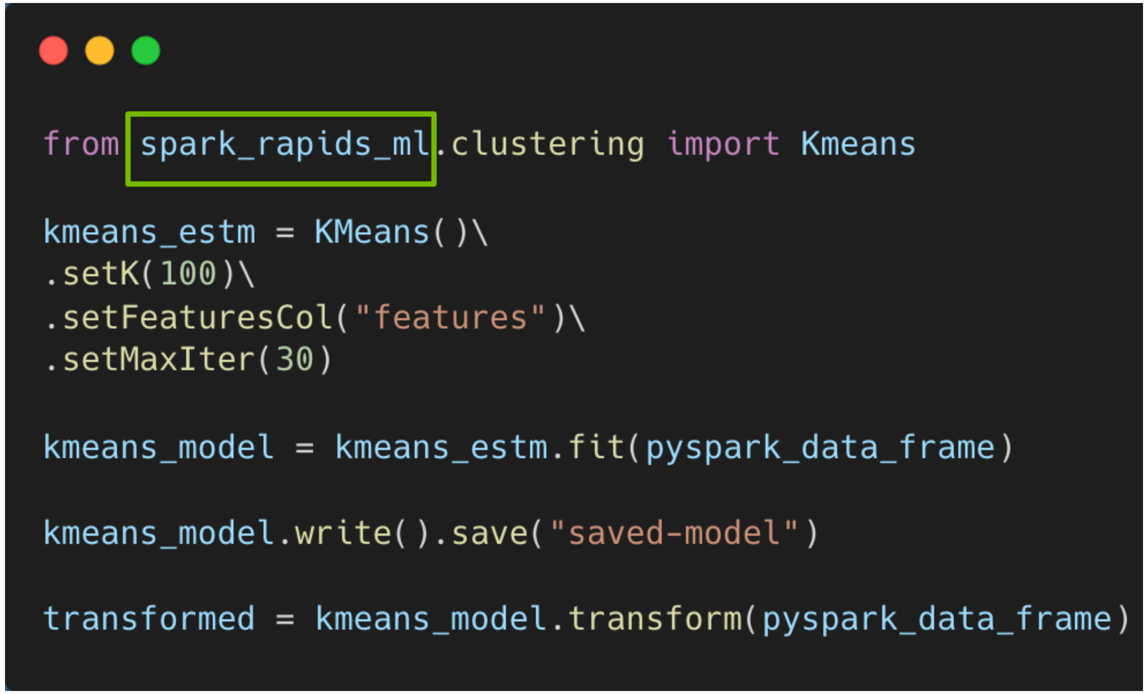


CPU Cluster: Intel Xeon Platinum 8000 series, 32GB RAM
GPU Cluster: NVIDIA A10 24GB, Dataset: 12GB Synthetic Dataset

*Hybrid CPU/GPU libraries*

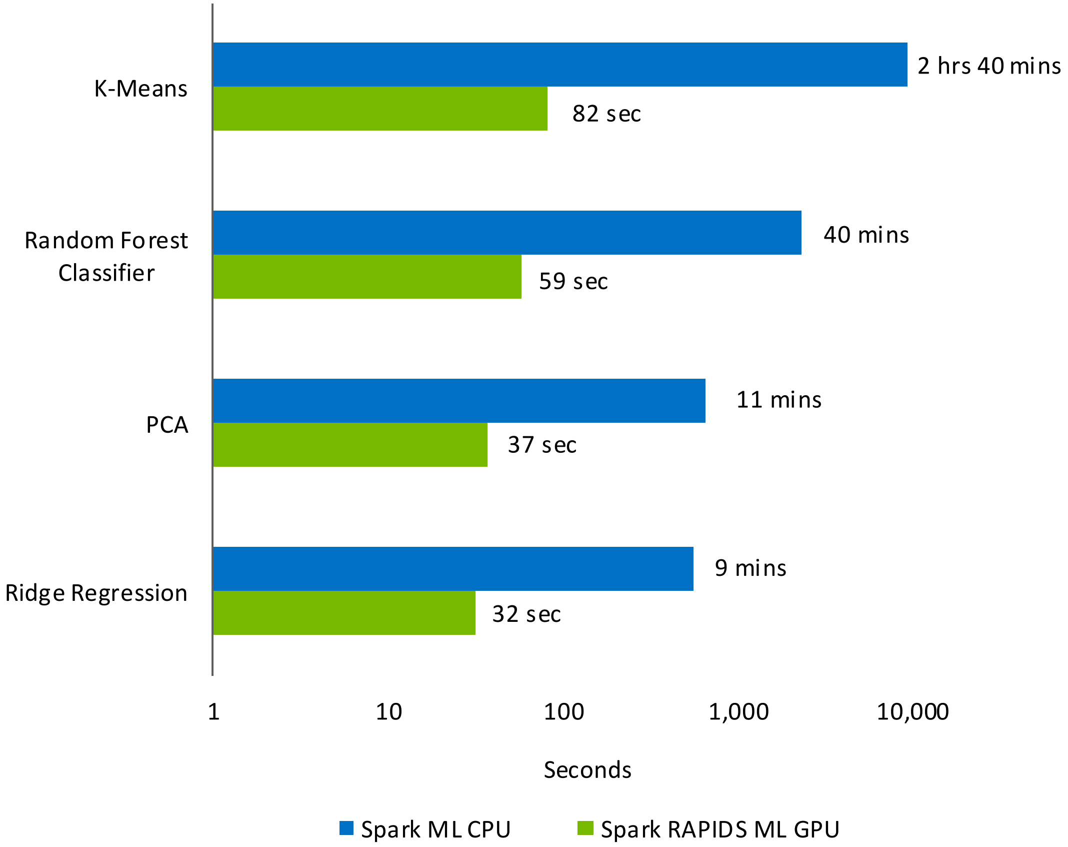
# Accelerated Apache Spark ML

Bringing GPU-accelerated machine learning to every Apache Spark user



```
from spark_rapids_ml.clustering import Kmeans

kmeans_estm = KMeans()\
.setK(100)\
.setFeaturesCol("features")\
.setMaxIter(30)

kmeans_model = kmeans_estm.fit(pyspark_data_frame)

kmeans_model.write().save("saved-model")

transformed = kmeans_model.transform(pyspark_data_frame)
```

**Up to 100x Faster**

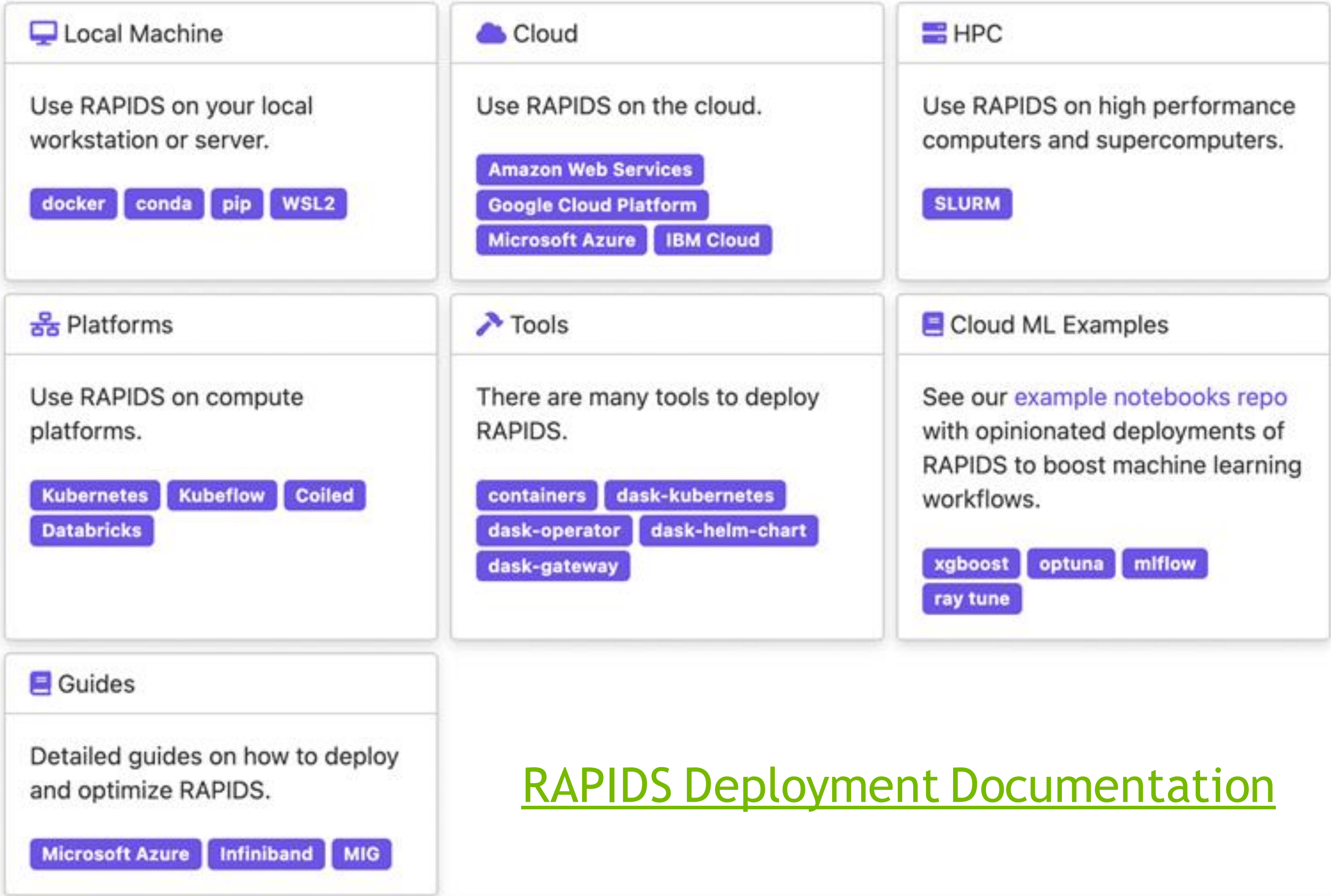


CPU Cluster: Intel Xeon Platinum 8000 series, 32GB RAM
GPU Cluster: NVIDIA A10 24GB, Dataset: 12GB Synthetic Dataset

# Getting Started and Learning More

# Deploying RAPIDS

Documentation to get you and up and running RAPIDS anywhere



### Local Machine

Use RAPIDS on your local workstation or server.

docker | conda | pip | WSL2

### Cloud

Use RAPIDS on the cloud.

Amazon Web Services | Google Cloud Platform | Microsoft Azure | IBM Cloud

### HPC

Use RAPIDS on high performance computers and supercomputers.

SLURM

### Platforms

Use RAPIDS on compute platforms.

Kubernetes | Kubeflow | Coiled | Databricks

### Tools

There are many tools to deploy RAPIDS.

containers | dask-kubernetes | dask-operator | dask-helm-chart | dask-gateway

### Cloud ML Examples

See our example notebooks repo with opinionated deployments of RAPIDS to boost machine learning workflows.

xgboost | optuna | mlflow | ray tune

### Guides

Detailed guides on how to deploy and optimize RAPIDS.

Microsoft Azure | Infiniband | MIG

RAPIDS Deployment Documentation

# How to Get Started with RAPIDS

A Variety of Ways to Get Up & Running

## More about RAPIDS

- Learn more at RAPIDS.ai
- Read the API docs
- Check out the RAPIDS blog
- Read the NVIDIA DevBlog

## Self-Start Resources

- Get started with RAPIDS
- Deploy on the Cloud today
- Start with Google Colab
- Look at the cheat sheets

## Discussion & Support

- Check the RAPIDS GitHub
- Use the NVIDIA Forums
- Reach out on Slack
- Talk to NVIDIA Services

## Get Engaged

@RAPIDSai

https://github.com/rapidsai

https://rapids.ai/slack-invite/

https://rapids.ai

NVIDIA®