Accelerated DataScience Tools Overview

On choosing the right tool between **Pandas**, Modin, Dask, CuDF, SQLite, Spark, **NumPy**, CuPy, **NetworkX**, CuGraph and RetworkX

--

By Ashot Vardanian
Founder @ Unum.Cloud

linkedin.com/in/ashvardanian
fb.com/ashvardanian
t.me/ashvardanian

Hardware

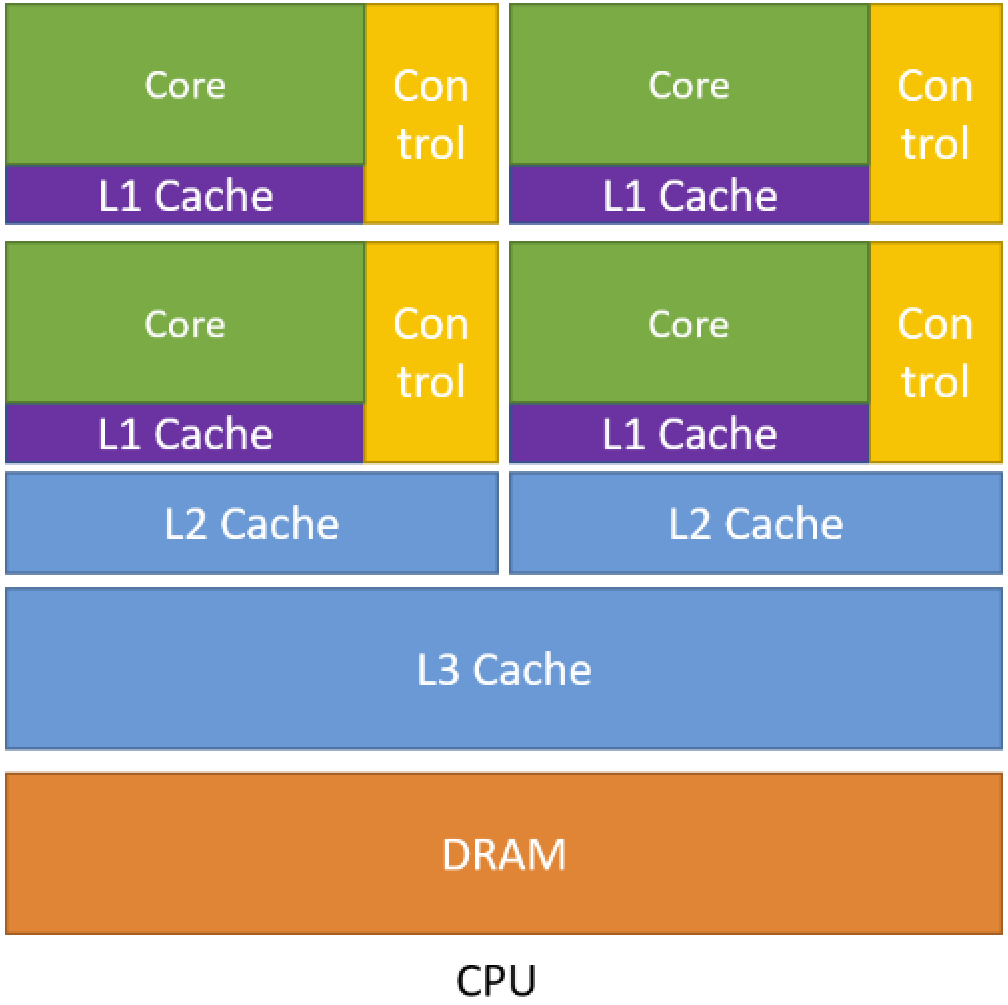
- Multi-core CPUs
- Highly-parallel GPUs

100 - 10'000 threads/device.

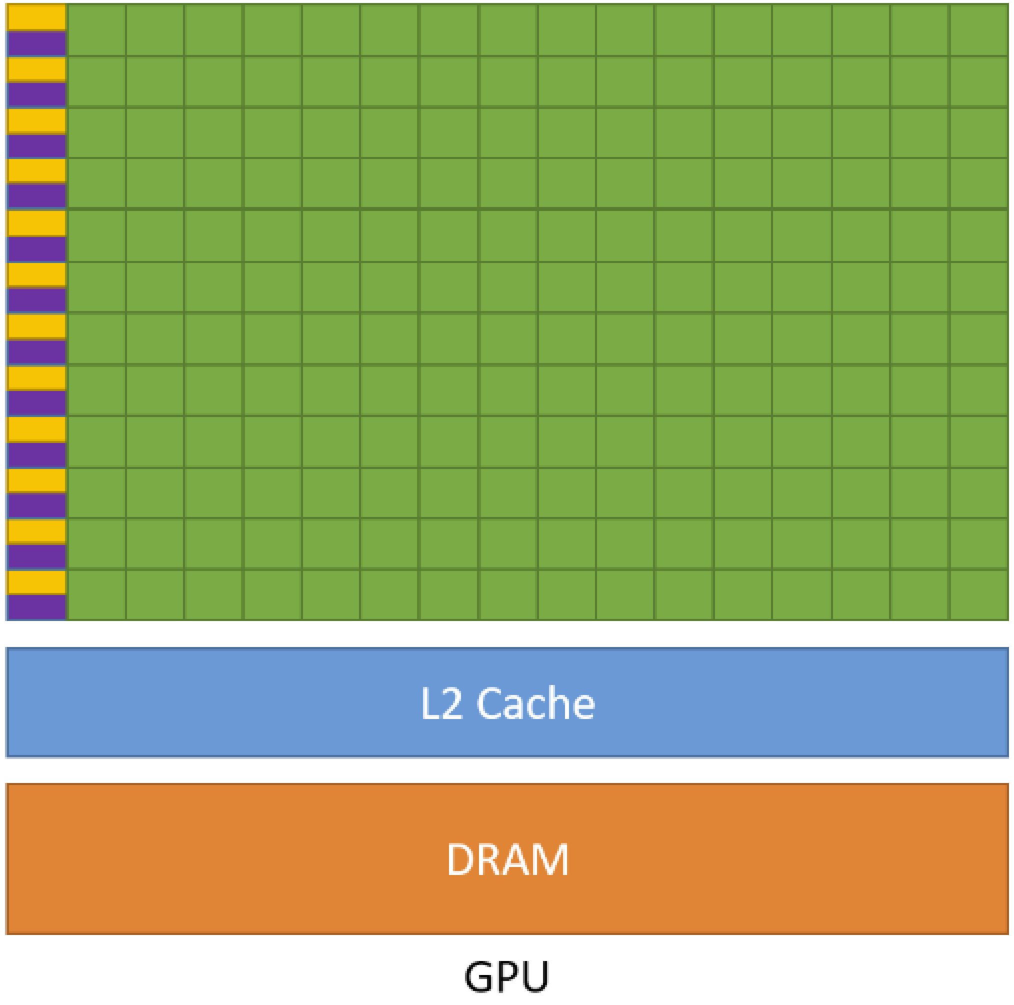
200+ Gbit networking.

Datasets 100x bigger than RAM.

CPU vs GPU

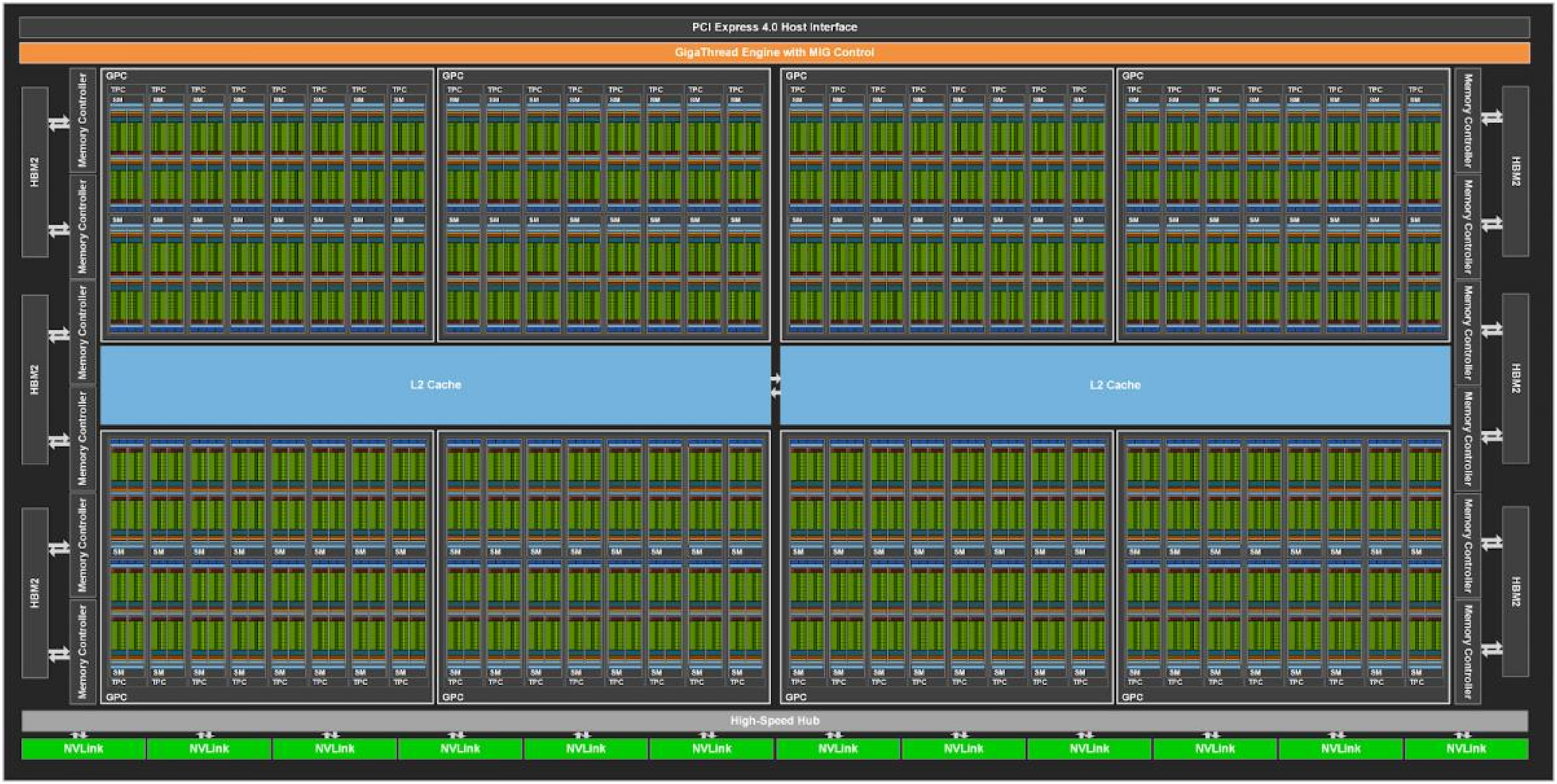


Core
Con trol
L1 Cache
Core
Con trol
L1 Cache
Core
Con trol
L1 Cache
Core
Con trol
L1 Cache
L2 Cache
L2 Cache
L3 Cache
DRAM
CPU



L2 Cache
DRAM
GPU

A100 Zoom In


PCI Express 4.0 Host Interface
GigaThread Engine with MIG Control
GPC
TPC
SM
Memory Controller
HBM2
L2 Cache
L2 Cache
High-Speed Hub
NVLink

How to sum some numbers?

Python:

```
sum(x)
```

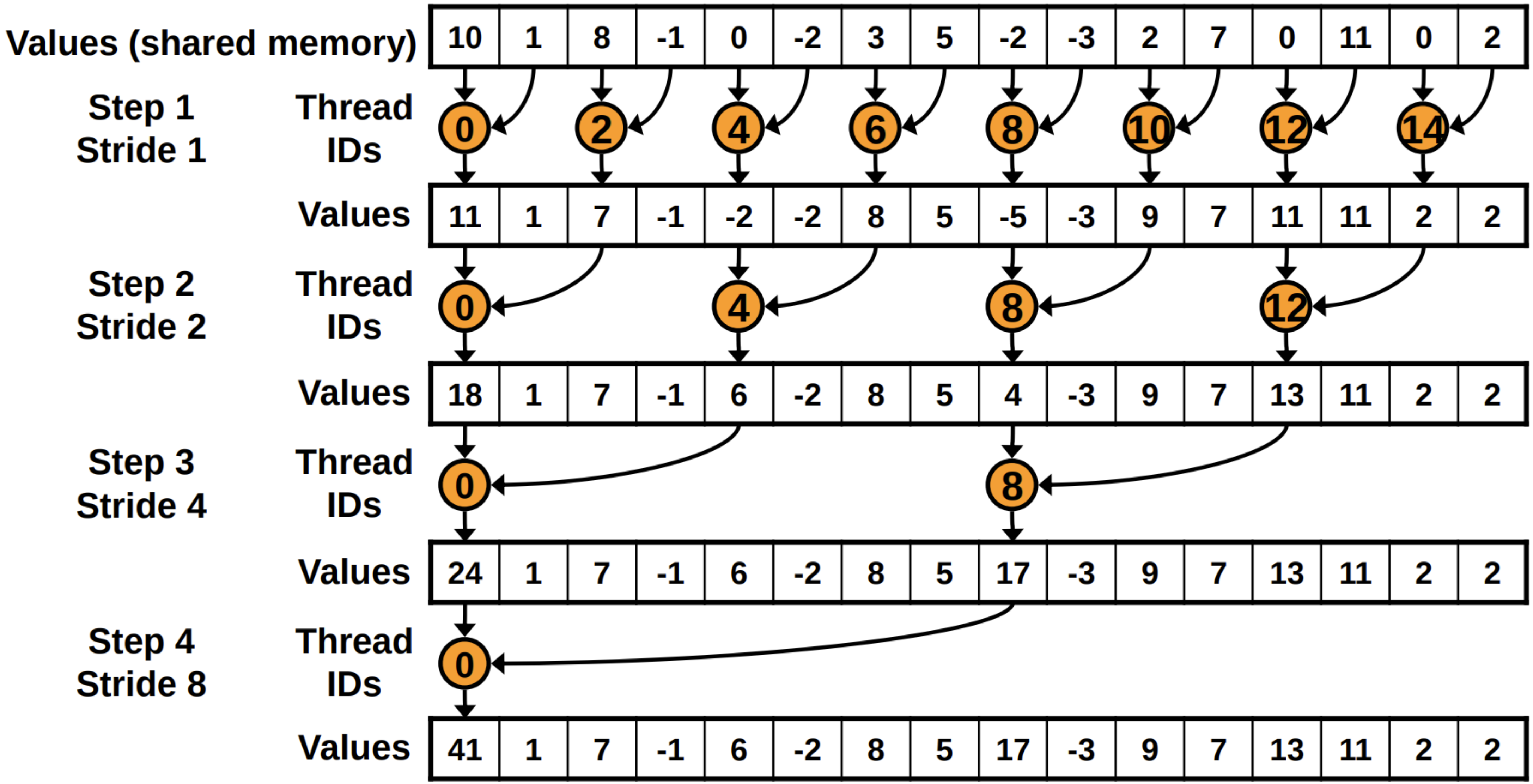
C++:

```
std::accumulate(x.begin(), x.end(), 0.f);
```

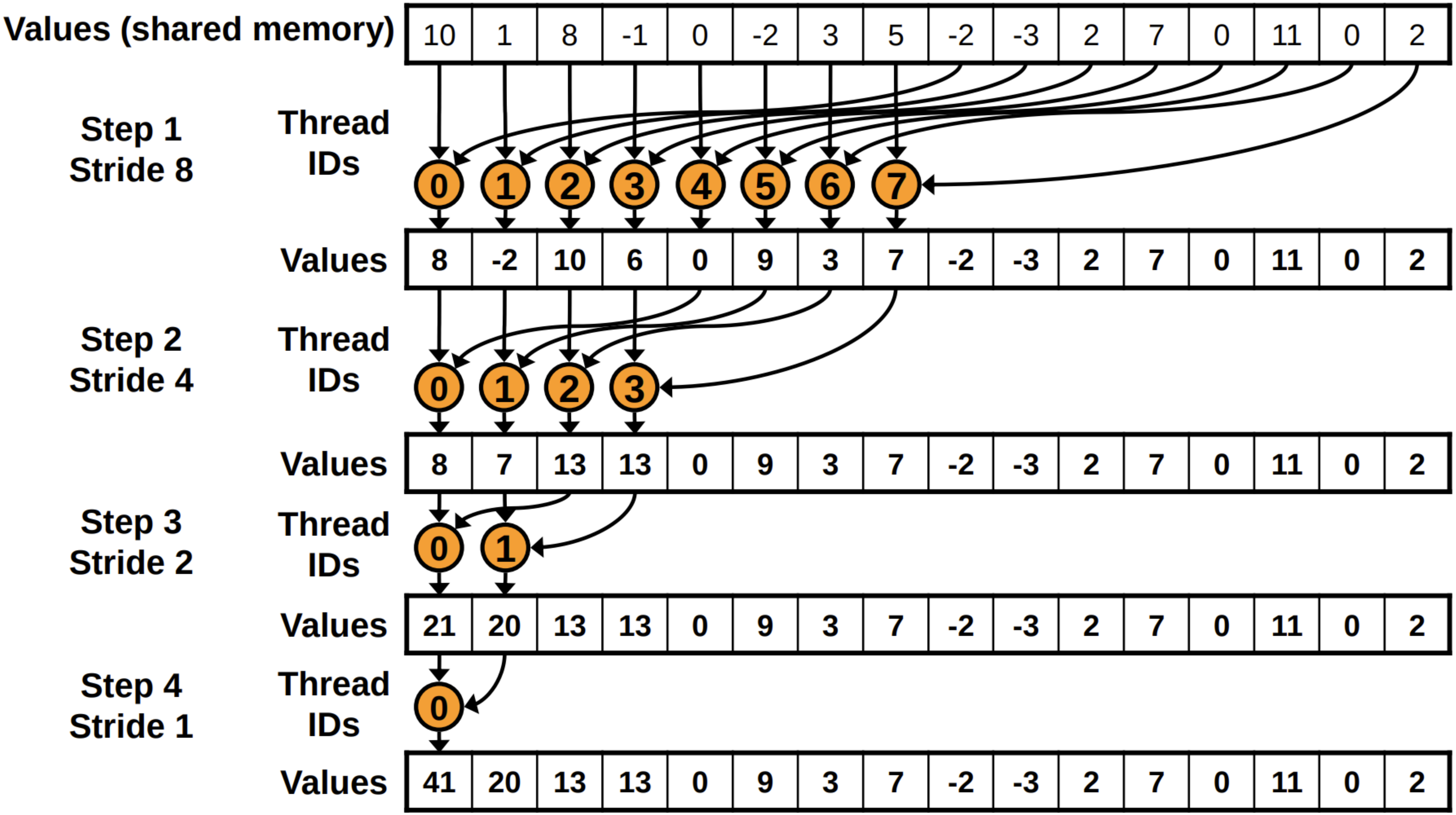
Accumulation, the hardest task!

```
__global__ void reduce_warps(float const *inputs, unsigned int input_size, float *outputs) {
    float sum = 0;
    for (unsigned int i = blockIdx.x * blockDim.x + threadIdx.x; i < input_size; i += blockDim.x * gridDim.x)
        sum += inputs[i];

    __shared__ float shared[32];
    unsigned int lane = threadIdx.x % warpSize;
    unsigned int wid = threadIdx.x / warpSize;

    sum = reduce_warp(sum); // Important
    if (lane == 0)
        shared[wid] = sum;
    __syncthreads();

    sum = (threadIdx.x < blockDim.x / warpSize) ? shared[lane] : 0;
    if (wid == 0)
        sum = reduce_warp(sum); // Important
    if (threadIdx.x == 0)
        outputs[blockIdx.x] = sum;
}
```

What's inside?



What's the alternative?



Why Suffer?

Python: **1 GB/s**

```
sum(x)
```

C++ 17: **87 GB/s**

```
std::reduce(std::execution::par_unseq, x.begin(), x.end(), 0.f);
```

CUDA: **789 GB/s**

Can Performance Be Usable?

Python:

```
sum(x)
```

C++:

```
std::accumulate(x.begin(), x.end(), 0.f);
```

CUDA + Thrust:

```
thrust::reduce(x.begin(), x.end(), 0.f);
```

If C++ can be readable, can Python be FAST?

- NumPy → CuPy
- NetworkX → CuGraph or RetworkX
- Pandas →
  - Modin is Multi-Threaded
  - Dask is Multi-Node
  - CuDF is on GPUs
  - Dask-CuDF is Multi-Node on GPUs

Change is ~~Hard~~ Easy

```
# import numpy as np
import cupy as np

np.matmul(mat, mat)
```

Yields us almost compatiable API!

```
# np.random.rand(100, 100).astype(np.float32)
cupy.random.rand(100, 100, dtype=np.float32)
cupy.cuda.stream.get_current_stream().synchronize()
```

Calm your Horses! CPUs have something to say...

Let's check our configs:

```yaml
name: benchmark
channels:
  - conda-forge
  - defaults
dependencies:
  - numpy
```

Do you know what you are getting?

The Preceise Way

```yaml
dependencies:
  - 'blas=*=mkl'
  - numpy
```

or:

```yaml
dependencies:
  - 'blas=*=openblas'
  - numpy
```

What Have We Achieved?

In short, up to 1000x performance improvements!

Speedups	512^2	1024^2	2048^2	4096^2	8192^2	16384^2
SVD	0.8x	0.7x	0.6x	0.5x	0.5x	0.6x
Pearson Corr.	2.5x	2.0x	1.4x	1.1x	1.5x	1.4x
GEMM	8.3x	17.9x	25.1x	21.0x	19.9x	23.4x
Moving Average	10.9x	19.9x	49.0x	59.3x	59.4x	53.9x
Medians	11.2x	30.3x	58.8x	72.2x	99.4x	83.5x
Sorting	87.7x	274.4x	547.3x	788.8x	920.5x	1008.5x

Tell us more! What's up with Graphs?

- NetworkX = Python
- RetworkX = Rust 🤮
- CuGraph = CUDA 🔥

How close are they?

```
networkx.weakly_connected_components(g)
```

```
retworkx.weakly_connected_components(g)
```

```
cugraph.components.connectivity.weakly_connected_components(g)
```

How close are they? Reality

```
networkx.pagerank(g)
```

```
raise NotImplemented()
```

```
cugraph.pagerank(g)
```

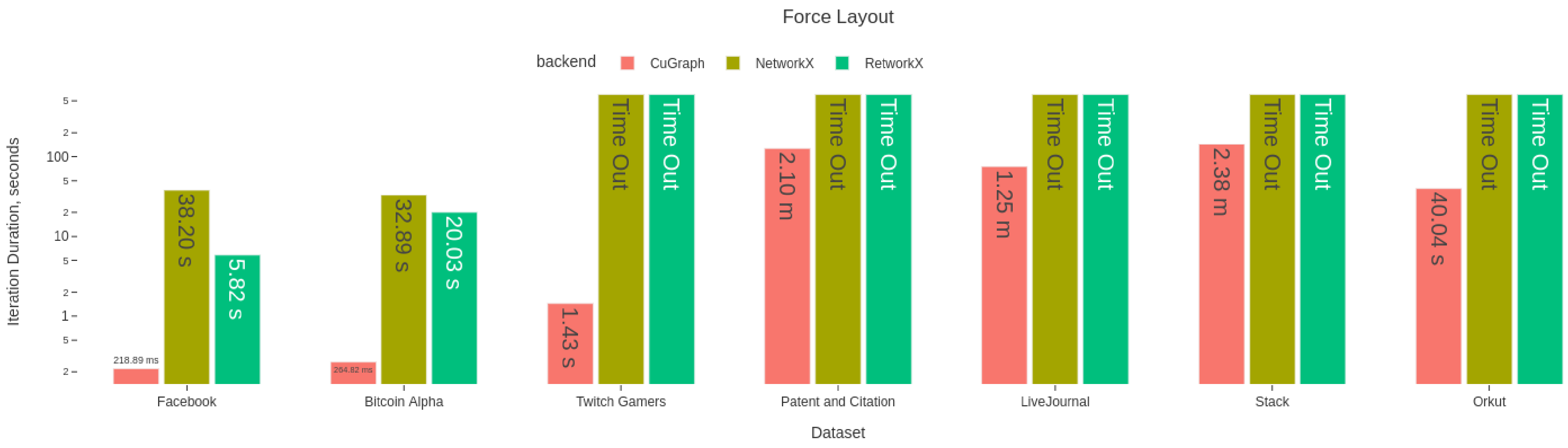
How close are they? Algorithm Mismatch

```
networkx.spring_layout(g)
```

```
retworkx.spring_layout(g)
```

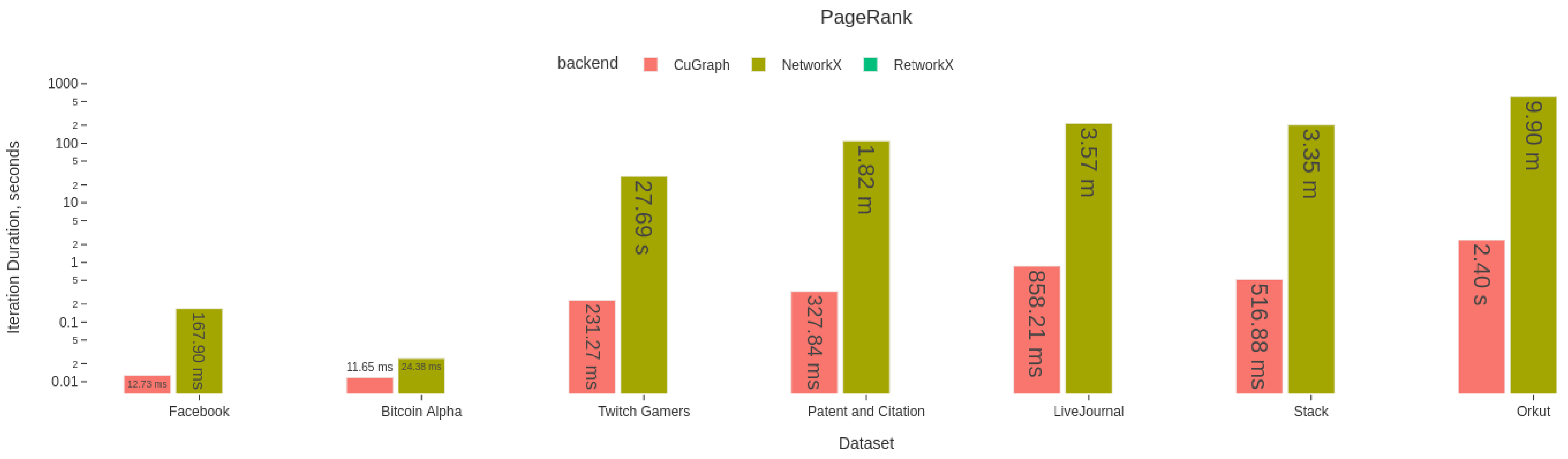
```
cugraph.force_atlas2(g)
```

What Are We Fighting For? Speed!



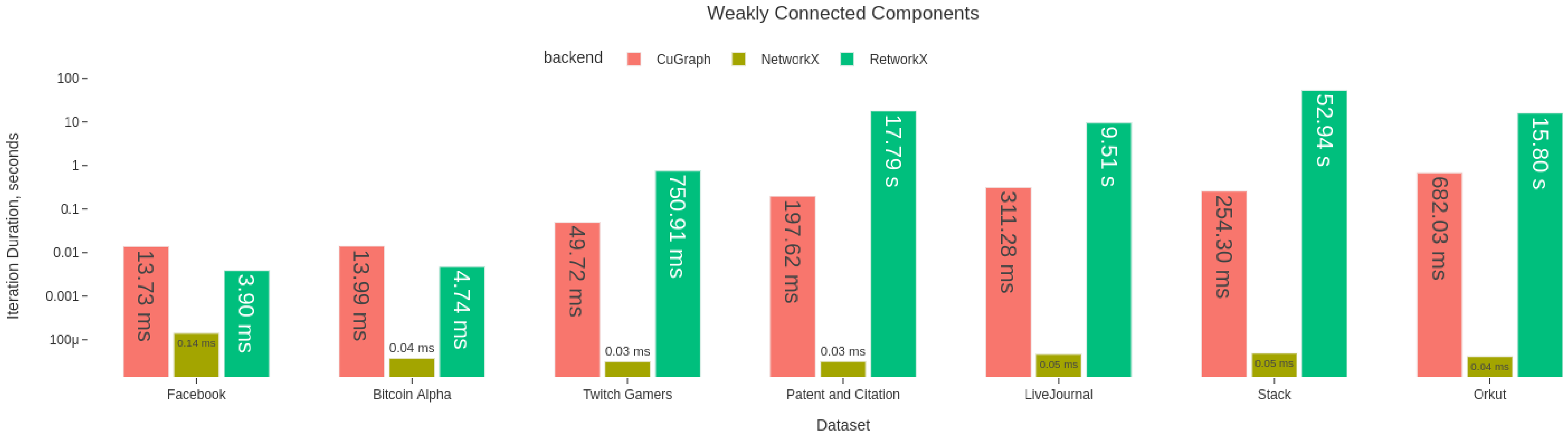
For Bitcoin Graph: **124x** improvement!

PageRank



On big graphs: **247x** improvement!

No Guarantees



Stack: 1.6 GB.

Orkut: 1.7 GB.

What about Tabular Data?

Let's take the Taxi Rides Dataset!

```
aws s3 ls --recursive s3://ursa-labs-taxi-data/ --recursive --human-readable --summarize
aws s3 sync s3://ursa-labs-taxi-data/ ADSB
```

Or in R:

```
arrow::copy_files("s3://ursa-labs-taxi-data", "nyc-taxi")
```

Producing 40 GB in clean Parquet files.

What will we do? SQL time!

Query 1 in SQL:

```sql
SELECT cab_type,
       count(*)
FROM trips
GROUP BY 1;
```

In Pandas:

```python
selected_df = trips[['cab_type']]
grouped_df = selected_df.groupby('cab_type')
final_df = grouped_df.size().reset_index(name='counts')
```

Query 2: Average by Group

```sql
SELECT passenger_count,
       avg(total_amount)
FROM trips
GROUP BY 1;
```

In Pandas:

```python
selected_df = trips[['passenger_count', 'total_amount']]
grouped_df = selected_df.groupby('passenger_count')
final_df = grouped_df.mean().reset_index()
```

Query 3: Transform & Histogram

```sql
SELECT passenger_count,
       extract(year from pickup_datetime),
       count(*)
FROM trips
GROUP BY 1,
         2;
```

Our dataset contains dates in the following format: "2020-01-01 00:35:39".

```python
selected_df = trips[['passenger_count', 'pickup_datetime']]
selected_df['year'] = pd.to_datetime(
    selected_df.pop('pickup_datetime'),
    format='%Y-%m-%d %H:%M:%S'
).dt.year
grouped_df = selected_df.groupby(['passenger_count', 'year'])
final_df = grouped_df.size().reset_index(name='counts')
```

Query 4: All Together

```sql
SELECT passenger_count,
       extract(year from pickup_datetime),
       round(trip_distance),
       count(*)
FROM trips
GROUP BY 1,
         2,
         3
ORDER BY 2,
         4 desc;
```

```python
selected_df = trips[['passenger_count', 'pickup_datetime', 'trip_distance']]
selected_df['trip_distance'] = selected_df['trip_distance'].round().astype(int)
selected_df['year'] = pd.to_datetime(selected_df.pop('pickup_datetime'), format='%Y-%m-%d %H:%M:%S').dt.year
grouped_df = selected_df.groupby(['passenger_count', 'year', 'trip_distance'])
final_df = grouped_df.size().reset_index(name='counts')
final_df = final_df.sort_values(['year', 'counts'], ascending=[True, False])
```

Porting to Pandas and beyond!

- Pandas supports `reset_index(name='')` on series, but not on frames. Other libraries mostly don't have that so we rename afterwards for higher compatiability.
- In queries 3 and 4 we could have fetched/converted data from the main source in just a single run, but to allow lazy evaluation of `WHERE`-like sampling queries, we split it into two step.
- Major problem in Dask is the lack of compatiable constructors, the most essential function of any class. You are generally expected to start with Pandas and cuDF and later convert those.

Results: Parsing

Pandas compatiability: CuDF ✅, Modin ✅

Results: Query 1

Pandas compatiability: CuDF ✅, Modin ✅

Results: Query 2

Pandas compatiability: CuDF ✅, Modin ✔️

Results: Query 3

Pandas compatiability: CuDF ✅, Modin ✔️

Results: Query 4

Pandas compatiability: CuDF ✅, Modin ✔️

What's next?

- Extending NumPy comparisons: + JAX, + ATen.
- Publishing more tabular results: Dask, Spark.
- Machine Learning benchmarks: PT, TF, JAX.

General Recommendations

- Always provide `dtype`, don't use `float`.
- Power-of-two array sizes.
- Prefer symmetrical tensors.
- Structure-of-Arrays instead of Array-of-Structures.

Known Pitfalls

- Multi-GPU.
- Unified Memory Latencies.
- NV-Link vs NUMA nodes and AMD MI200.
- Synchronization of CUDA streams and graphs.

Where we apply?

- Processing 50 GB/s on a single machine.
- Rapid experimnatation with datasets between 100 MB and 4 GB.
- Fast experimentation with dataset above 4 GB.

All at Unum.cloud!

--

linkedin.com/in/ashvardanian
fb.com/ashvardanian
t.me/ashvardanian