



No-Code-Change GPU Acceleration for Your Pandas and NetworkX Workflows

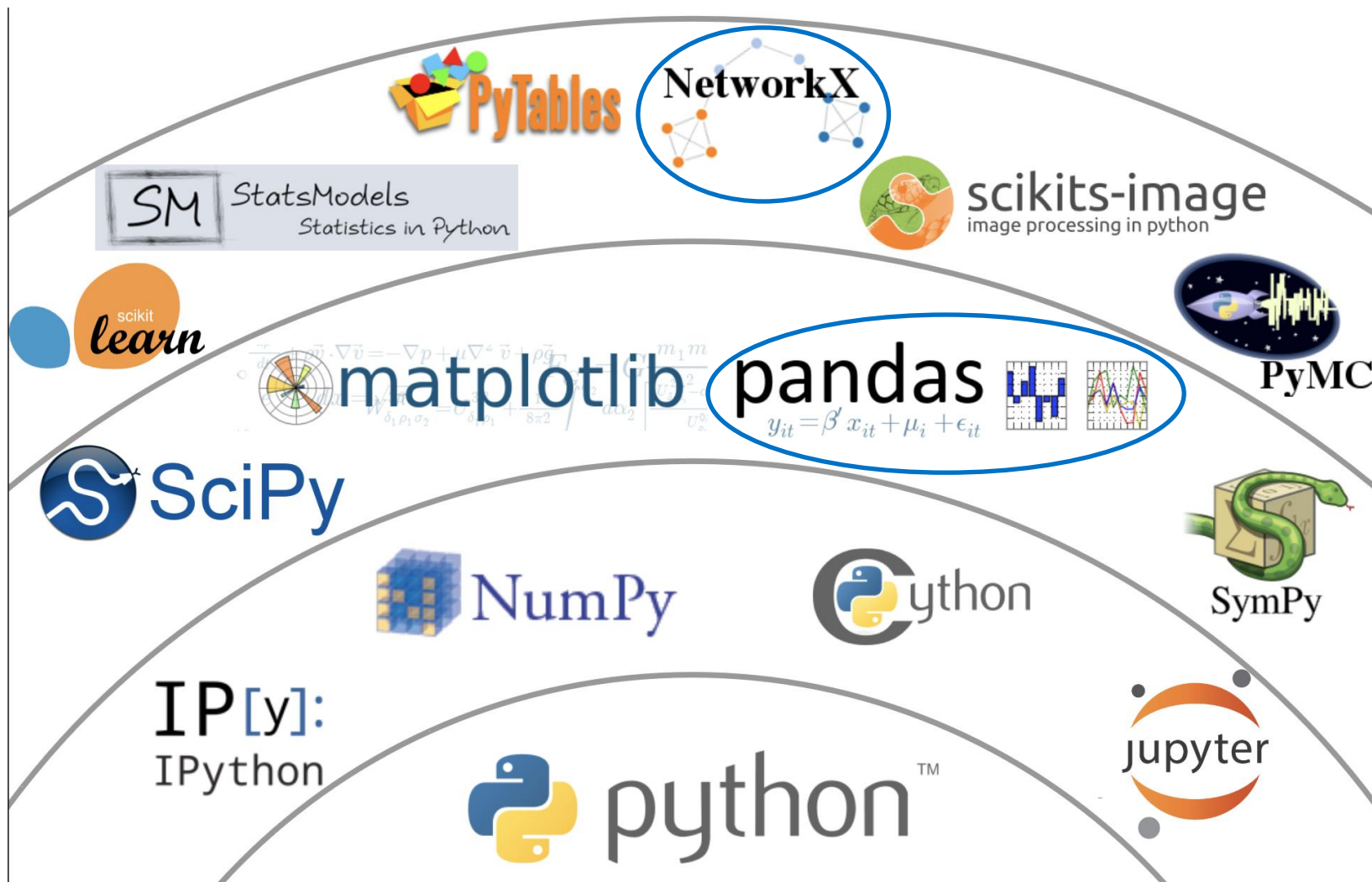
SciPy 2024
Wednesday, July 10, 4:00pm

Rick Ratzel – NVIDIA

Vyas Ramasubramani – NVIDIA

The Scientific Python Stack

Circa 2015



Credit: Jake Vanderplas, 2015 SciPy Keynote

A Typical Application Using DataFrames and Graph Analytics...

“Rank Wikipedia editors based on the ‘importance’ of their contributions”

<https://github.com/rlratzel/SciPy2024>

```
import os

import pandas as pd
import networkx as nx

nx.config.cache_converted_graphs = True # This is the default in NX 3.4
revisions_df = pd.read_csv(
    "halved_revisions.csv",
    sep="\t",
    names=["title", "editor"],
    dtype="str",
)
nodedata_df = pd.read_csv(
    "full_data.csv",
    sep="\t",
    names=["nodeid", "title"],
    dtype={"nodeid": "int32", "title": "str"},
)
node_revisions_df = nodedata_df.merge(revisions_df, on="title")

edgelist_df = pd.read_csv(
    "full_graph.csv",
    sep=" ",
    names=["src", "dst"],
    dtype="int32",
)
G = nx.from_pandas_edgelist(edgelist_df, "src", "dst", create_using=nx.DiGraph)
nx_pr_vals = nx.pagerank(G)

pagerank_df = pd.DataFrame({"nodeid": nx_pr_vals.keys(), "pagerank": nx_pr_vals.values()})

final_df = node_revisions_df.merge(pagerank_df, on="nodeid").drop("nodeid", axis=1)
influence = final_df[["editor", "pagerank"]].groupby("editor").sum().reset_index()
most_influential_human = influence[~influence["editor"].str.lower().str.contains("bot")]
print(most_influential_human.sort_values(by="pagerank").tail(10))
```

- ~10GB CSV data
- ~21M nodes
- ~315M edges

(scipy_demo) dgx05% python demo.py

Read the Wikipedia revision history from halved_revisions.csv...
Done in: 0:01:08.949760

Read the Wikipedia page metadata from full_data.csv...
Done in: 0:00:17.499024

Connect page editors to the page ids...
Done in: 0:01:04.894338

Read the Wikipedia connectivity information from full_graph.csv...
Done in: 0:00:37.812829

Create a NetworkX graph from the connectivity info...
Done in: 0:14:10.917641

Run NetworkX pagerank...
Done in: 0:32:10.346657

Create a DataFrame containing PageRank values...
Done in: 0:00:10.625677

Merge the PageRank scores onto the per-page information...
Done in: 0:01:00.995132

Compute the most influential editors...
Done in: 0:01:19.192866

Show the most influential human editors...

	editor	pagerank_sum
1121071	CommonsDelinker	0.068351
2679114	John of Reading	0.069264
1037544	Chris the speller	0.076814
5396511	Tom.Reding	0.080647
3406264	MaterialsScientist	0.081280
4489182	Rjwilmsi	0.082212
534689	BD2412	0.086898
825038	BrownHairedGirl	0.089414
4459803	Rich Farmbrough	0.090024
4768550	Ser Amantio di Nicolao	0.096206

Done in: 0:00:07.298137

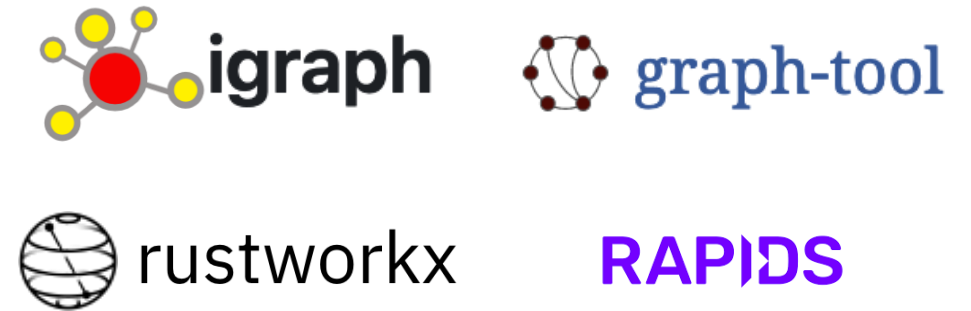
Total time:
52:08.53

Many Other Options Exist, But None Are As Popular

Python Data Processing Libraries



Python Graph Libraries



- Pandas and NetworkX have well-known performance limitations
- Despite this, their usage generally outstrips alternatives due to:
 - Familiarity
 - Availability of tooling
 - Alternatives requiring changes to preexisting code
- While different API choices can lead to improved performance, it can slow or even permanently hinder adoption

Even the Robots Know the Standards

Just ask ChatGPT...

How do I join two tables in Python?



Joining two tables in Python can be accomplished using the `pandas` library, which provides a powerful data manipulation and analysis toolset. Here is a step-by-step guide on how to join two tables (DataFrames) using `pandas`.

Step 1: Install `pandas`

If you haven't already installed `pandas`, you can do so using pip:



Step 4: Perform the Join

You can join two DataFrames using the `merge` function. Here are different types of joins you can perform:

Inner Join

An inner join returns only the rows that have matching values in both DataFrames.

python

Copy code

```
inner_join = pd.merge(df1, df2, on='ID', how='inner')
print("\nInner Join:")
print(inner_join)
```

How do I find the betweenness centrality values for each node in a graph?



To find the betweenness centrality values for each node in a graph, you can use the `networkx` library in Python. Betweenness centrality is a measure of the number of times a node acts as a bridge along the shortest path between two other nodes. Here's how you can calculate it:

Step 1: Install `networkx`

If you haven't already installed `networkx`, you can do so using pip:



Step 3: Calculate Betweenness Centrality

Use the `betweenness centrality` function provided by `networkx` to calculate the betweenness centrality for each node:

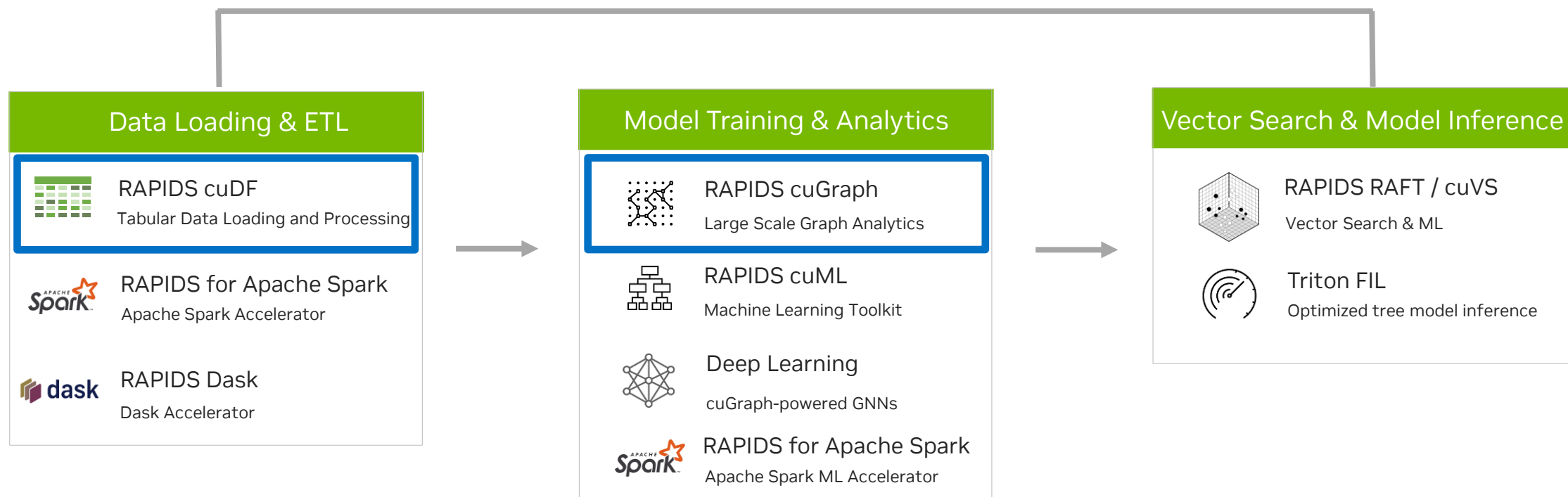
python

Copy code

```
# Calculate betweenness centrality for all nodes
betweenness = nx.betweenness centrality(G)

# Print the betweenness centrality for each node
print("\nBetweenness Centrality for each node:")
for node, centrality in betweenness.items():
    print(f"Node {node}: {centrality:.3f}")
```

RAPIDS Accelerates Data Science End-to-End



NVIDIA AI Enterprise

Development Tools | Cloud Native Management and Orchestration | Infrastructure Optimization



Cloud



Data Center



Edge

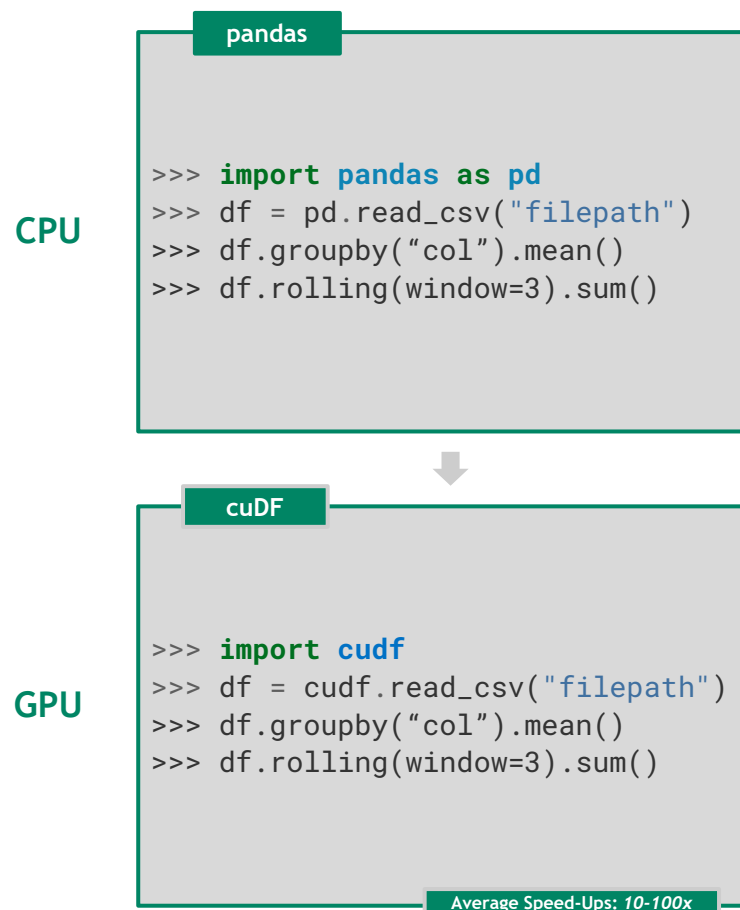


RTX Laptop

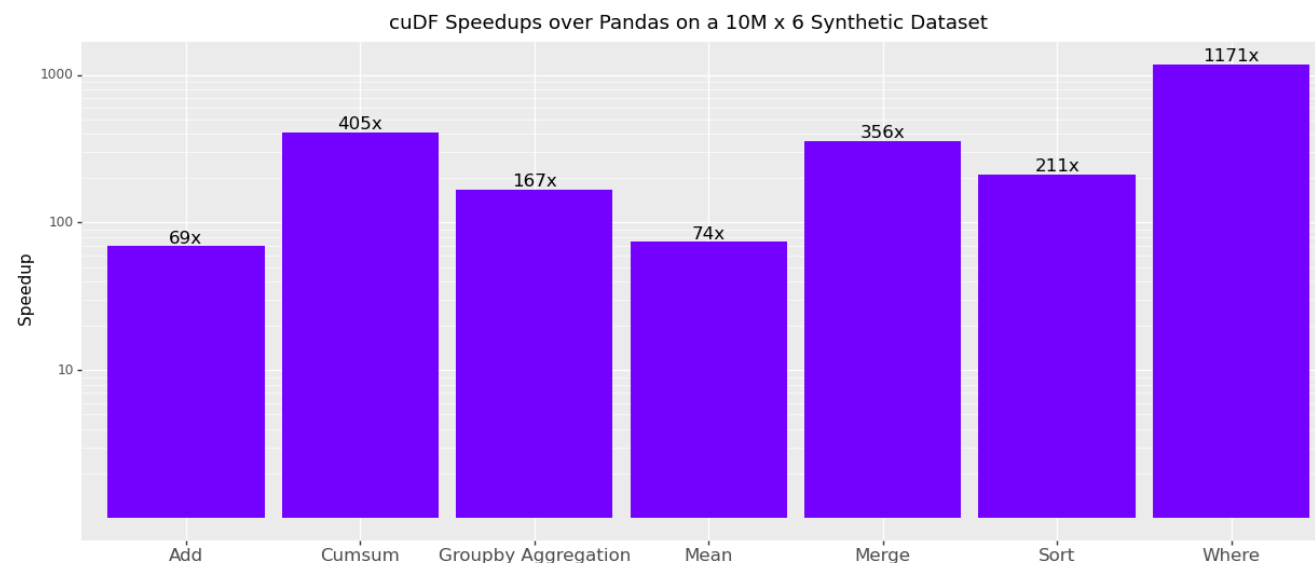
cuDF: CUDA DataFrames

GPU DataFrame library with a Pandas-like API

Pandas-like API on the GPU



Best-in-Class Performance



Groupby	Strings and Regex	UDFs	Nested Types	Time Series
Indexing	Missing Data	CuPy Interoperability	Rolling Windows	

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

cuGraph: GPU Accelerated Python Graph Analytics

GPU accelerated NetworkX-like python library

NetworkX-like API on the GPU

CPU

NetworkX

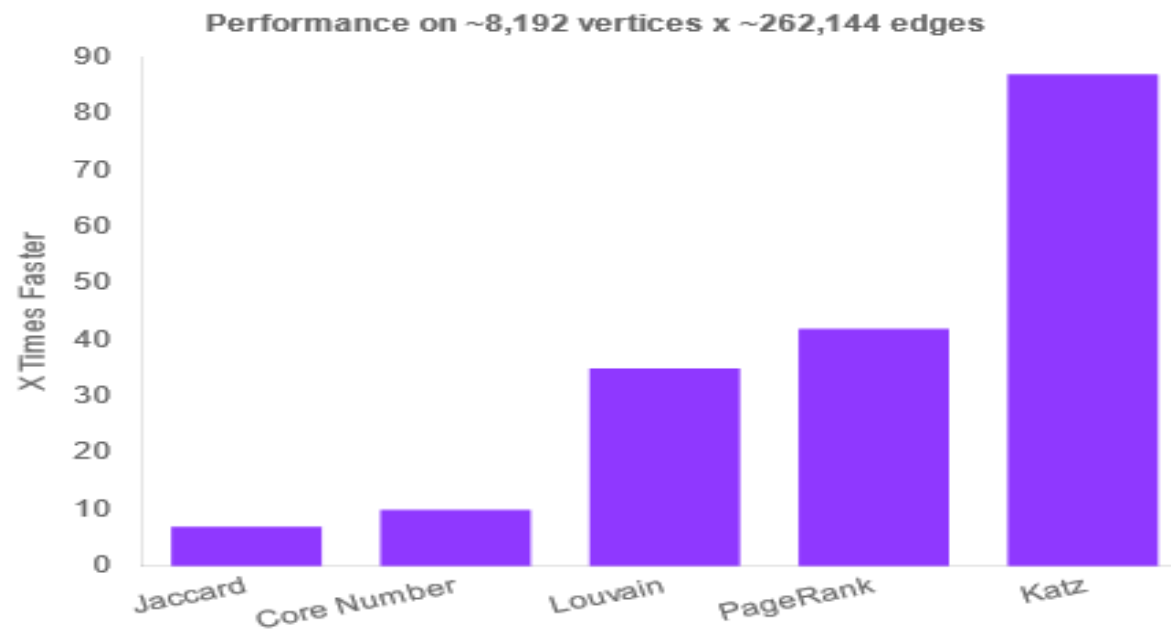
```
>>> import pandas as pd
>>> import networkx as nx
>>> df = pd.read_csv("filepath")
>>> G = nx.from_pandas_edgelist(df)
>>> nx.pagerank(G)
```



GPU

cuGraph

```
>>> import cudf
>>> import cugraph as cg
>>> df = cudf.read_csv("filepath")
>>> G = cg.from_cudf_edgelist(df)
>>> cg.pagerank(G)
```



Link Analysis

Community
Detection

Graph
Traversal

Sampling

Centrality

MultiGraphs

Connected
Components

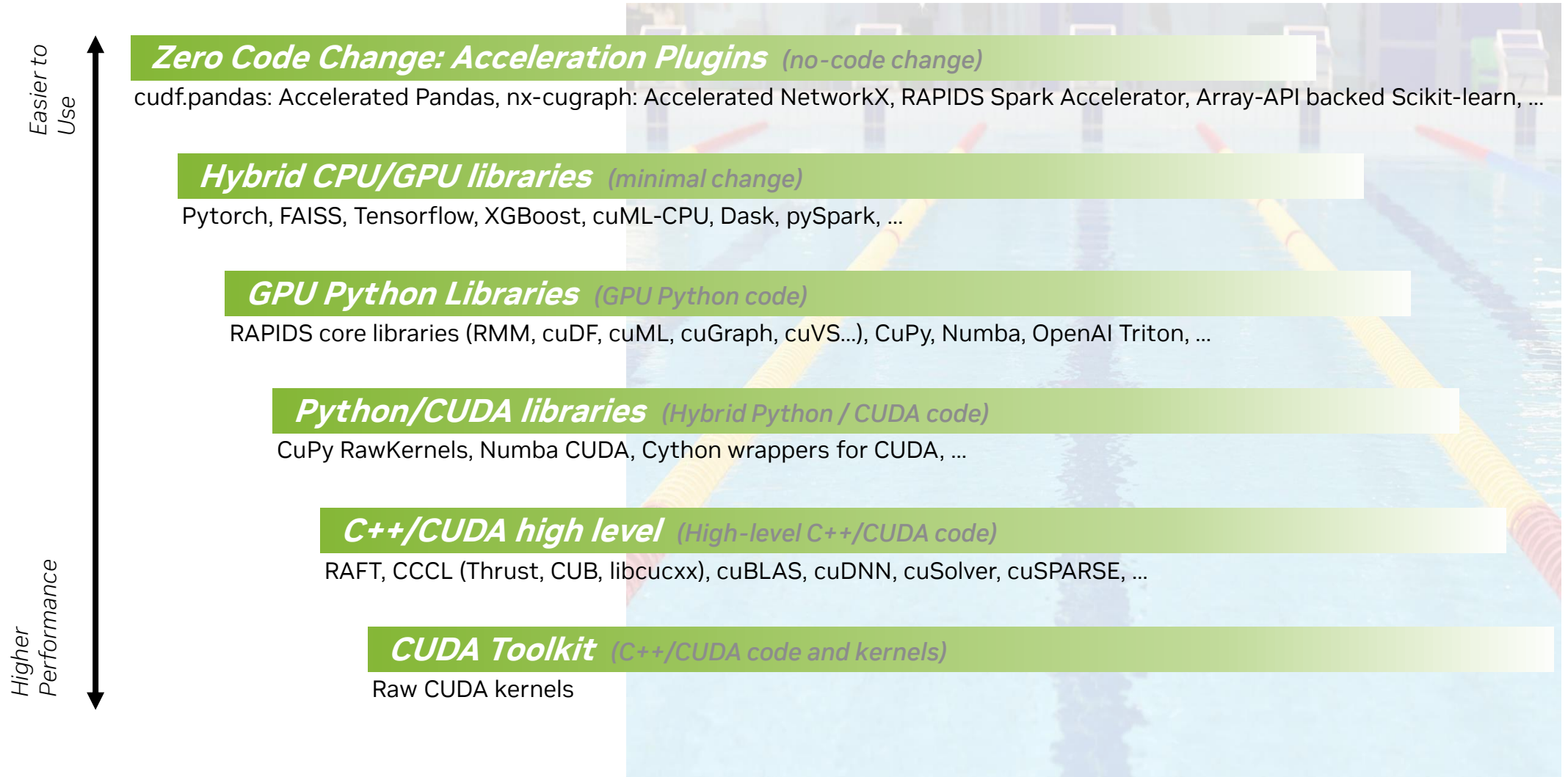
CuDF Interoperability

GNNs

NVIDIA A100 vs. AMD EPYC 7642 48-Core Processor
cuGraph Python vs. NetworkX

Evolution of Accelerated Computing

Finding the right niche for every kind of user



Accelerated Pandas

Coming soon:
cudf.polars!

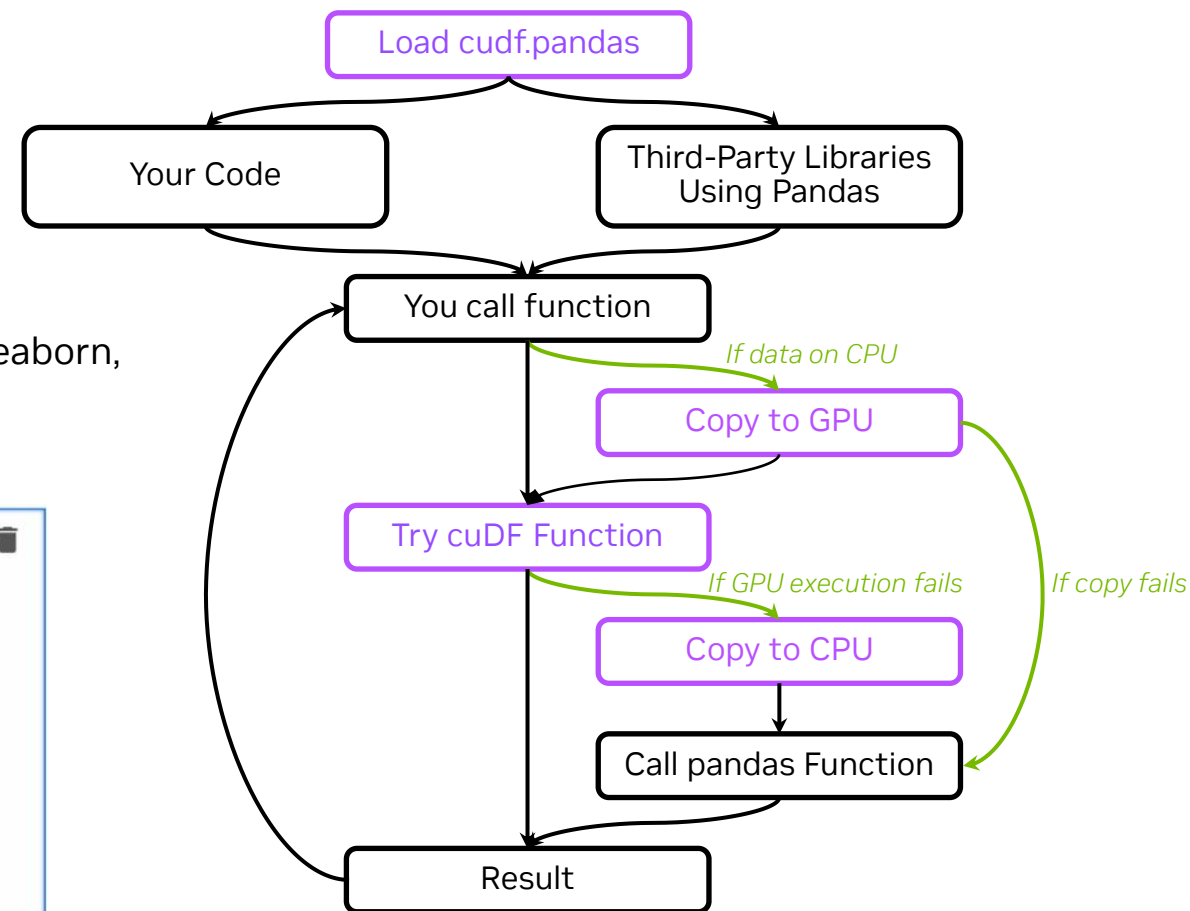
cudf.pandas: the zero-code-change GPU accelerator for Pandas built on cuDF

- Requires **no changes** to existing pandas code. Just
 - `%load_ext cudf.pandas`
 - `$ python -m cudf.pandas <script.py>`
- Accelerates workflows up to 150x using the GPU
- Compatible with code that uses third-party libraries
 - Integration tested with SciPy, scikit-learn, XGBoost, Matplotlib, seaborn, HoloViews, PyTorch, TensorFlow, ...

```
[ ]:
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)
```



Easy to Use, Built-in Profiler!

- Use the `%%cudf.pandas.profile` cell magic in Jupyter, or import it directly:

```
from cudf.pandas import Profiler
```

```
with Profiler() as p:  
    # code goes here
```

```
p.print_per_function_stats()
```

- Shows which functions ran on the CPU and which ran on the GPU

```
%%cudf.pandas.profile
```

```
rng = pd.date_range("2023-01-01", "2023-02-01", freq="10ms")  
data = pd.DataFrame(  
    {  
        "a": np.random.rand(len(rng)),  
        "b": np.random.rand(len(rng))  
    },  
    index=rng  
)  
data = data.iloc[rng.indexer_between_time("09:30", "16:00")]  
results = data.groupby(pd.Grouper(freq="1D")).mean()  
results.head()
```

Total time elapsed: 12.855 seconds
11 GPU function calls in 1.322 seconds
1 CPU function calls in 4.416 seconds

Stats

Function	GPU ncalls	GPU cumtime	GPU percall	CPU ncalls	CPU cumtime	CPU percall
date_range	1	0.008	0.008	0	0.000	0.000
DatetimeIndex.__len__	2	0.000	0.000	0	0.000	0.000
DataFrame	2	0.873	0.436	0	0.000	0.000
DatetimeIndex.indexer_between...	0	0.000	0.000	1	4.416	4.416
DataFrameIlocIndexer.__geti...	1	0.127	0.127	0	0.000	0.000
Grouper	1	0.000	0.000	0	0.000	0.000
DataFrame.groupby	1	0.021	0.021	0	0.000	0.000
DataFrameResampler.mean	1	0.259	0.259	0	0.000	0.000
DataFrame.head	1	0.001	0.001	0	0.000	0.000
DataFrame.__repr__	1	0.033	0.033	0	0.000	0.000

Not all pandas operations ran on the GPU. The following functions required CPU fallback:

– `DatetimeIndex.indexer_between_time`

To request GPU support for any of these functions, please file a Github issue here:
<https://github.com/rapidsai/cudf/issues/new/choose>.

Spoofing Pandas and Its Contents

Modules

- What happens when you `import pd`?
- Normally, checks various built-ins, PYTHONPATH, etc
- But! We can insert a custom **finder** that runs first
- `cudf.pandas` implements a finder, the `ModuleAccelerator`, which returns proxy modules

```
In [1]: %load_ext cudf.pandas
In [2]: import pandas as pd
In [3]: pd
Out[3]: <module 'pandas'
(ModuleAccelerator(fast=cudf, slow=pandas))>

In [4]: import pandas.plotting as plt
In [5]: plt
Out[5]: <module 'pandas.plotting'
(ModuleAccelerator(fast=cudf, slow=pandas))>
```

Module Contents

- What happens when you access attributes (free functions, classes, class methods)?
- `cudf.pandas` produces **proxy objects**
- Proxies masquerade as pandas objects

```
In [6]: pd.DataFrame
Out[6]: pandas.core.frame.DataFrame
In [7]: type(pd.DataFrame())
Out[7]: pandas.core.frame.DataFrame
```

- But if you look more closely...

```
In [7]: type(pd.DataFrame)
Out[8]: cudf.pandas.fast_slow_proxy._FastSlowProxyMeta
```

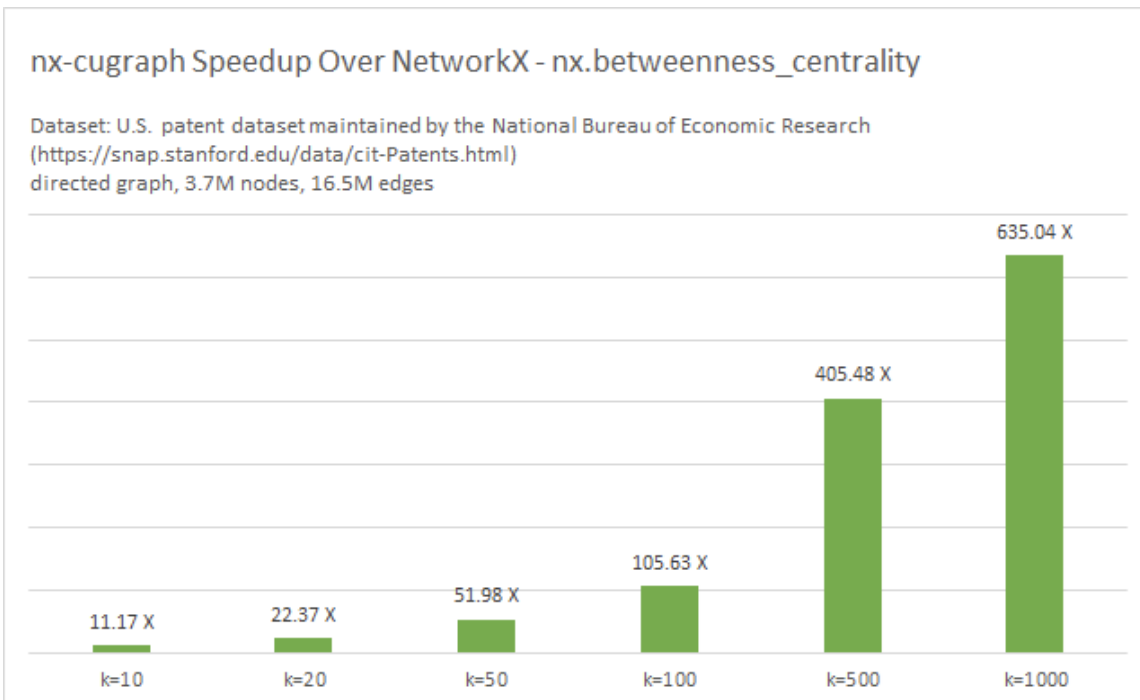
- Fundamental limitations (numpy C API calls)
- Hacking import isn't ideal

<https://docs.python.org/3/reference/import.html>

Accelerated NetworkX

nx-cugraph: zero-code-change acceleration for NetworkX, powered by cuGraph

- Zero-code-change GPU-acceleration for NetworkX code
- Accelerates up to 600x depending on algorithm and graph size
- Support for 60 popular graph algorithms and growing
- Fallback to CPU for any unsupported algorithms



```
import pandas as pd
import networkx as nx

url = "https://data.rapids.ai/cugraph/datasets/cit-Patents.csv"
df = pd.read_csv(url, sep=" ", names=["src", "dst"], dtype="int32")
G = nx.from_pandas_edgelist(df, source="src", target="dst")

%time result = nx.betweenness centrality(G, k=10)
```

```
user@machine:/# ipython bc_demo.ipynb
CPU times: user 7min 38s, sys: 5.6 s, total: 7min 44s
Wall time: 7min 44s

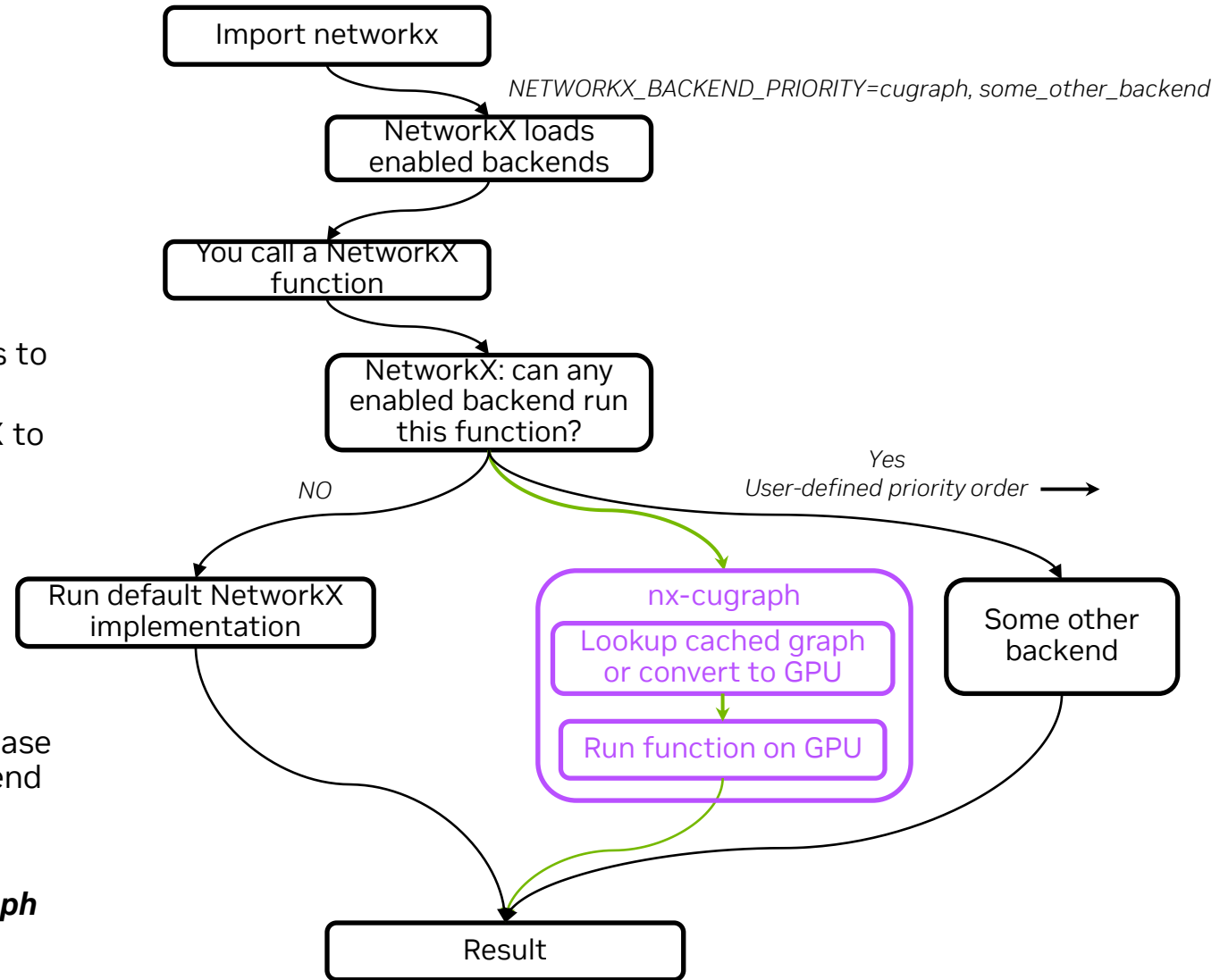
user@machine:/# NETWORKX_BACKEND_PRIORITY=cugraph ipython bc_demo.ipynb
CPU times: user 18.4 s, sys: 1.44 s, total: 19.9 s
Wall time: 20 s
```

NetworkX 3.2. CPU: Intel(R) Xeon(R) Platinum 8480CL 2TB. GPU: NVIDIA H100 80GB

nx-cugraph

A GPU-accelerated NetworkX backend

- nx-cugraph is a NetworkX **backend**
- What's a NetworkX backend?
 - NetworkX added the ability to **dispatch** various function calls to third-party backends, starting in NetworkX 3.0
 - Backends provide an alternate implementation for NetworkX to call
 - Allows users to run implementations optimized for their environment without changing their code – the NetworkX “frontend” remains the same
- Multiple backends can be used together:
 - Ex. Access a graph in a remote graph database using a database backend, run algorithms on GPU using the nx-cugraph backend
 - Learn more about about NetworkX dispatching and other NetworkX backends at the poster session: **Fast and Easy Graph Analytics with the NetworkX Ecosystem of Backends**



A Typical Application, Revisited...

- No code changes! Simply enable both cudf.pandas and nx-cugraph:
 - Set environment variable NETWORKX_BACKEND_PRIORITY=cugraph
 - Run with the cudf.pandas module
 - Before:
 - `python demo.py`
 - After:
 - `NETWORKX_BACKEND_PRIORITY=cugraph python -m cudf.pandas demo.py`
- Total speedup: 52 min -> 22 min = 2.5x
 - Why not more?
- cudf.pandas:
 - CSV reads: ~20x speedup
 - Merges: ~130x speedup
 - Groupby-apply: ~200x speedup
 - Select+filter: ~3x speedup
- nx-cugraph:
 - Pagerank: ~10x speedup
 - Graph creation: 0.7x speedup (slower!)
- At 18 mins, graph creation dominates runtime!

```
(scipy_demo) dgx05% NETWORKX_BACKEND_PRIORITY="cugraph" python -m
cudf.pandas demo.py

Read the Wikipedia revision history from halved_revisions.csv...
Done in: 0:00:04.479977

Read the Wikipedia page metadata from full_data.csv...
Done in: 0:00:00.452238

Connect page editors to the page ids...
Done in: 0:00:01.134292

Read the Wikipedia connectivity information from full_graph.csv...
Done in: 0:00:03.843927

Create a NetworkX graph from the connectivity info...
Done in: 0:18:21.004385

Run NetworkX pagerank...
Done in: 0:03:21.999969

Run again using the cached graph conversion...
... # cugraph prints an informative message about caching here
Done in: 0:00:10.242561

Create a DataFrame containing PageRank values...
Done in: 0:00:05.711783

Merge the PageRank scores onto the per-page information...
Done in: 0:00:00.301918

Compute the most influential editors...
Done in: 0:00:00.431072

Show the most influential human editors...
editor pagerank_sum
1121010 CommonsDelinker 0.068355
2678970 John of Reading 0.069278
1037484 Chris the speller 0.076830
5396241 Tom.Reding 0.080654
3406082 MaterialsScientist 0.081262
4488962 Rjwilmsi 0.082204
534633 BD2412 0.086900
824982 BrownHairedGirl 0.089404
4459584 Rich Farmbrough 0.090030
4768324 Ser Amantio di Nicolao 0.096223
Done in: 0:00:02.381004
```

Total time:
22:11.98

unaccelerated:
52:08.53
2.5X speedup

A Typical Application, Revisited...

Why not even faster?

- cudf.pandas has a high memory footprint
 - Only using half the Wikipedia revision history
 - Processing ~10 Gb (4 + 1 + 5) of data
 - Reducing OOMs is ongoing work
- cudf.pandas → nx-cugraph handoff is not seamless
 - Graph creation is not accelerated because NetworkX acts like it's operating on a Pandas object
 - A python-based NetworkX Graph is created, not a GPU graph
- First algorithm call triggers conversion to that backend's graph type
 - For nx-cugraph: host->device data transfer
 - This conversion is cached
 - Subsequent algos reuse the GPU graph (*if the original was not modified*)
 - All other pagerank calls: **32:10 → 0:10 = ~190x speedup!**

```
(scipy_demo) dgx05% NETWORKX_BACKEND_PRIORITY="cugraph" python -m
cudf.pandas demo.py

Read the Wikipedia revision history from halved_revisions.csv...
Done in: 0:00:04.479977

Read the Wikipedia page metadata from full_data.csv...
Done in: 0:00:00.452238

Connect page editors to the page ids...
Done in: 0:00:01.134292

Read the Wikipedia connectivity information from full_graph.csv...
Done in: 0:00:03.843927

Create a NetworkX graph from the connectivity info...
Done in: 0:18:21.004385

Run NetworkX pagerank...
Done in: 0:03:21.999969

Run again using the cached graph conversion...
... # cugraph prints an informative message about caching here
Done in: 0:00:10.242561

Create a DataFrame containing PageRank values...
Done in: 0:00:05.711783

Merge the PageRank scores onto the per-page information...
Done in: 0:00:00.301918

Compute the most influential editors...
Done in: 0:00:00.431072

Show the most influential human editors...

```

	editor	pagerank_sum
1121010	CommonsDelinker	0.068355
2678970	John of Reading	0.069278
1037484	Chris the speller	0.076830
5396241	Tom.Reding	0.080654
3406082	Materials scientist	0.081262
4488962	Rjwilmsi	0.082204
534633	BD2412	0.086900
824982	BrownHairedGirl	0.089404
4459584	Rich Farmbrough	0.090030
4768324	Ser Amantio di Nicolao	0.096223

```
Done in: 0:00:02.381004
```

A Low-Code Change Approach

If you are willing to make small changes, you can go even faster

```
import cudf
import networkx as nx

revisions_df = cudf.read_csv(
    "halved_revisions.csv",
    sep="\t",
    names=["title", "editor"],
    dtype="str",
)
nodedata_df = cudf.read_csv(
    "full_data.csv",
    sep="\t",
    names=["nodeid", "title"],
    dtype={"nodeid": "int32", "title": "str"},
)
node_revisions_df = nodedata_df.merge(revisions_df, on="title")

edgelist_df = cudf.read_csv(
    "full_graph.csv",
    sep=" ",
    names=["src", "dst"],
    dtype="int32",
)

# Create an nx_cugraph (not NetworkX) Graph compatible only with nx_cugraph algorithms
G = nx.from_pandas_edgelist(
    edgelist_df,
    source="src",
    target="dst",
    create_using=nx.DiGraph,
    backend="cugraph"
)
nx_pr_vals = nx.pagerank(G)

pagerank_df = cudf.DataFrame({"nodeid": nx_pr_vals.keys(), "pagerank": nx_pr_vals.values()})
final_df = node_revisions_df.merge(pagerank_df, on="nodeid").drop("nodeid", axis=1)
influence = final_df[["editor", "pagerank"]].groupby("editor").sum().reset_index()
most_influent_human = influence[~influence["editor"].str.lower().str.contains("bot")]
print(most_influent_human.sort_values(by="pagerank").tail(10))
```

Read the Wikipedia revision history from halved_revisions.csv...
Done in: 0:00:05.226320

Read the Wikipedia page metadata from full_data.csv...
Done in: 0:00:00.457513

Connect page editors to the page ids...
Done in: 0:00:00.299906

Read the Wikipedia connectivity information from full_graph.csv...
Done in: 0:00:03.864327

Create a NetworkX graph from the connectivity info...
Done in: 0:00:09.624684

Run NetworkX pagerank...
Done in: 0:00:06.452435

Create a DataFrame containing PageRank values...
Done in: 0:00:04.281305

Merge the PageRank scores onto the per-page information...
Done in: 0:00:00.190582

Compute the most influential editors...
Done in: 0:00:00.293617

Show the most influential human editors...

	editor	pagerank
5767097	CommonsDelinker	0.070213
1536890	John of Reading	0.070812
5330010	Chris the speller	0.078867
3676022	Tom.Reding	0.081731
4843142	MaterialsScientist	0.083336
4298520	Rjwilmsi	0.084033
3835004	BD2412	0.088707
1419682	BrownHairedGirl	0.091291
1303378	Rich Farmbrough	0.092024
2516853	Ser Amantio di Nicolao	0.098005

Done in: 0:00:01.393367

Total time:
0:32.08

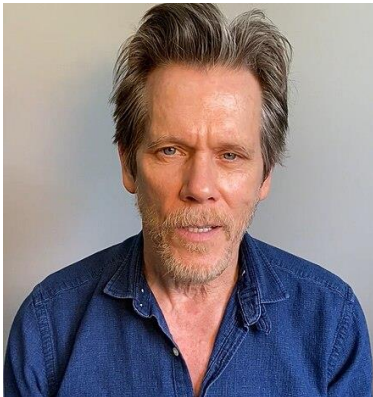
unaccelerated:
52:08.53

98X speedup

Further Exploration of the Data...

Six Degrees of SciPy!

```
shortest_paths = nx.shortest_path(G, source=scipy_nodeid)
```



```
Find the shortest path between the SciPy article and all articles...  
Done in: 0:02:28.838333
```

```
Print the shortest paths...
```

7:33 unaccelerated,
3X speedup

```
Find the shortest path between SciPy and Orange juice...
```

```
SciPy  
Python (programming language)  
Blender (software)  
Orange (fruit)  
Orange juice
```

```
Find the shortest path between SciPy and Lake Leon (Florida)...
```

```
SciPy  
Python (programming language)  
Monty Python  
Dave Chappelle  
Xenia, Ohio  
Dean Chenoweth  
Tom Brown Park  
Lake Leon (Florida)
```

```
Find the shortest path between SciPy and Kevin Bacon...
```

```
SciPy  
Python (programming language)  
Industrial Light & Magic  
Ron Howard  
Kevin Bacon  
Done in: 0:00:00.360897
```



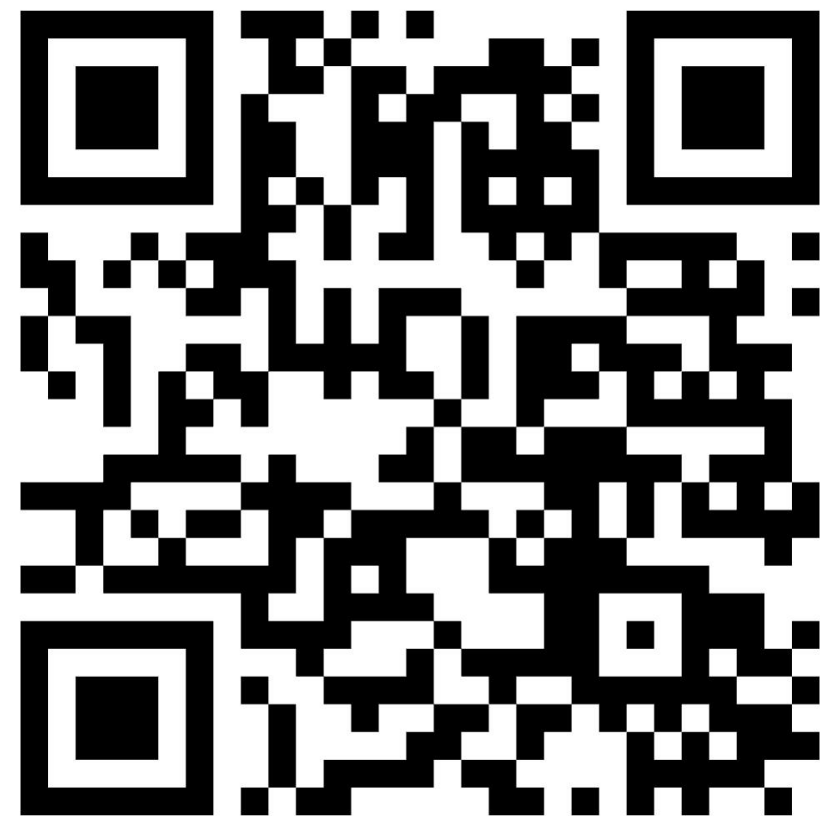
Interested in talking to us?
Fill out this 2-minute-long survey

Relevant Resources

- cuDF Github - <https://github.com/rapidsai/cudf>
- cuGraph Github - <https://github.com/rapidsai/cugraph>
- RAPIDS website - <https://rapids.ai>
- Code from this talk: <https://github.com/rlratzel/SciPy2024>
- `pip install cudf-cu12 nx-cugraph-cu12 --extra-index-url https://pypi.nvidia.com`
- `conda install -c rapidsai -c conda-forge -c nvidia cudf nx-cugraph`

Find us at SciPy

- BoF: Accelerated Python
- Poster Session: *Fast and Easy Graph Analytics with the NetworkX Ecosystem of Backends*





Extras

What about duck typing?

Check for behavior, not for inheritance

```
# this function is duck-typing friendly, and will work
# for any DataFrame-like object:
def function_one(df: pd.DataFrame) -> pd.Series:
    return df.groupby("a").max()

# this function is *not* duck-typing friendly. It will
# raise for anything that's not a pandas DataFrame:
def function_two(df: pd.DataFrame) -> pd.DataFrame:
    if not isinstance(df, pd.DataFrame):
        raise TypeError("Not a pandas DataFrame!")
    return pd.concat([df, df])
```

Under the hood

Deep import customization to hijack pandas imports

```
# a custom importer for "pandas" that gives you a module
# containing our proxy DataFrame instead of the real pandas
class PandasImporter(importlib.abc.MetaPathFinder, importlib.abc.Loader):
    def find_spec(self, fullname, path, target=None):
        if fullname == "pandas":
            return importlib.machinery.ModuleSpec(
                fullname, self
            )
        return None

    def exec_module(self, module: ModuleType):
        module.DataFrame = DataFrame
        return module

sys.meta_path.insert(0, PandasImporter())
```


Under the hood

Proxy objects that dispatch to cudf or pandas

```
class DataFrame:
    def __init__(self, *args, **kwargs):
        try:
            self._wrapped = cudf.DataFrame(*args, **kwargs)
        except Exception:
            self._wrapped = pd.DataFrame(*args, **kwargs)

    def count(self, *args, **kwargs):
        """Count the number of non-null elements along the given axis"""
        try:
            return self._wrapped.count(*args, **kwargs)
        except Exception:
            print("falling back to pandas!")
            result = self._wrapped.to_pandas().count(*args, **kwargs)
            return cudf.from_pandas(result)
```

Under the hood

Transparent fallback via proxied module

```
>>> df = DataFrame({'a': [1, 2, 3], 'b': [None, 3, 4]})
>>> df.count(axis=0)
a      3
b      2
dtype: int64
>>> df.count(axis=1)
falling back to pandas!
0      1
1      2
2      2
dtype: int64
```