NVIDIA

DEEP
LEARNING
INSTITUTE

FUNDAMENTALS OF ACCELERATED DATA SCIENCE WITH RAPIDS

COURSE GOALS

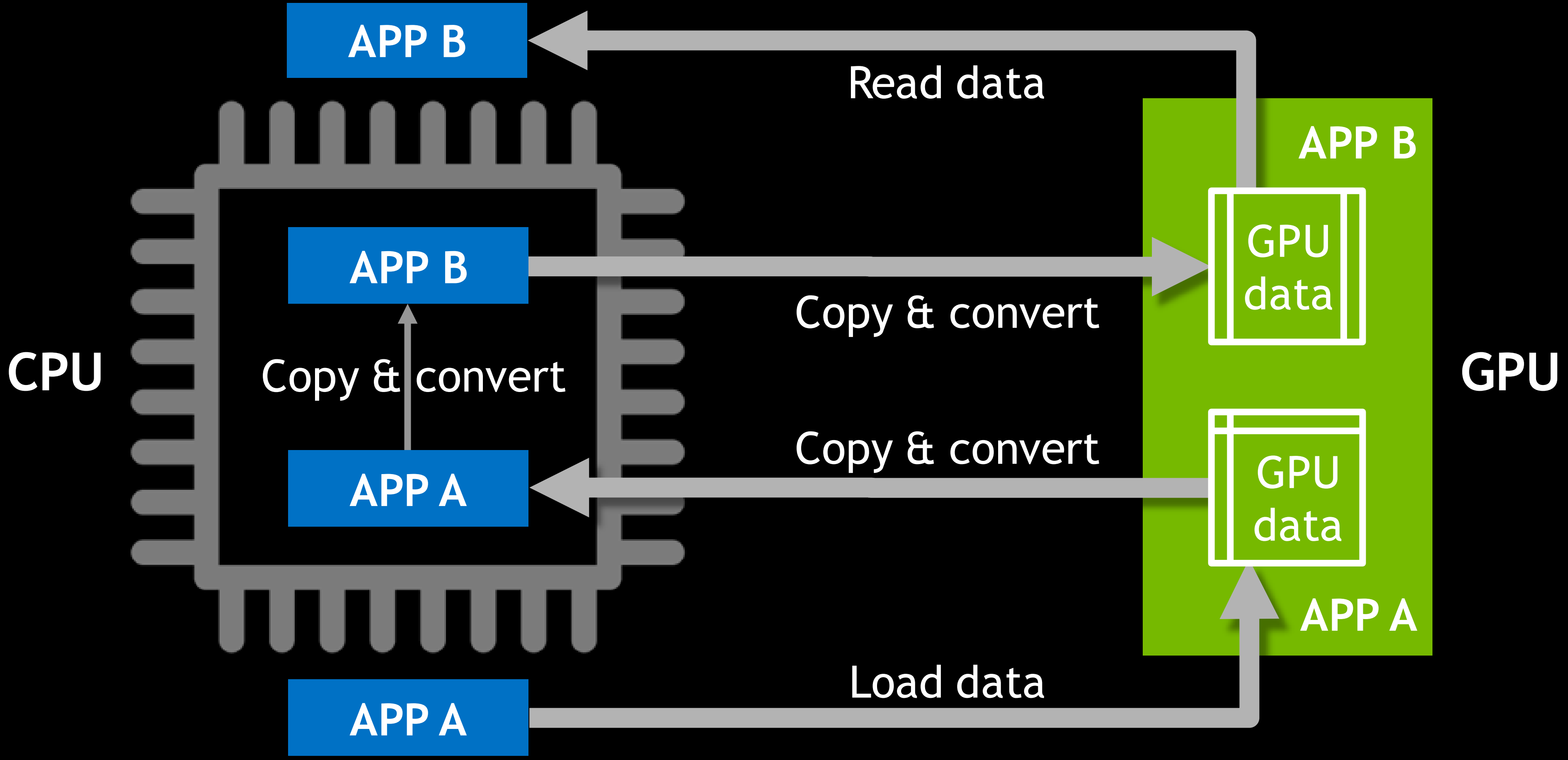
Learn the core tools to use RAPIDS for everyday data science

Understand RAPIDS’ scalability from workstation and cluster to cloud and HPC

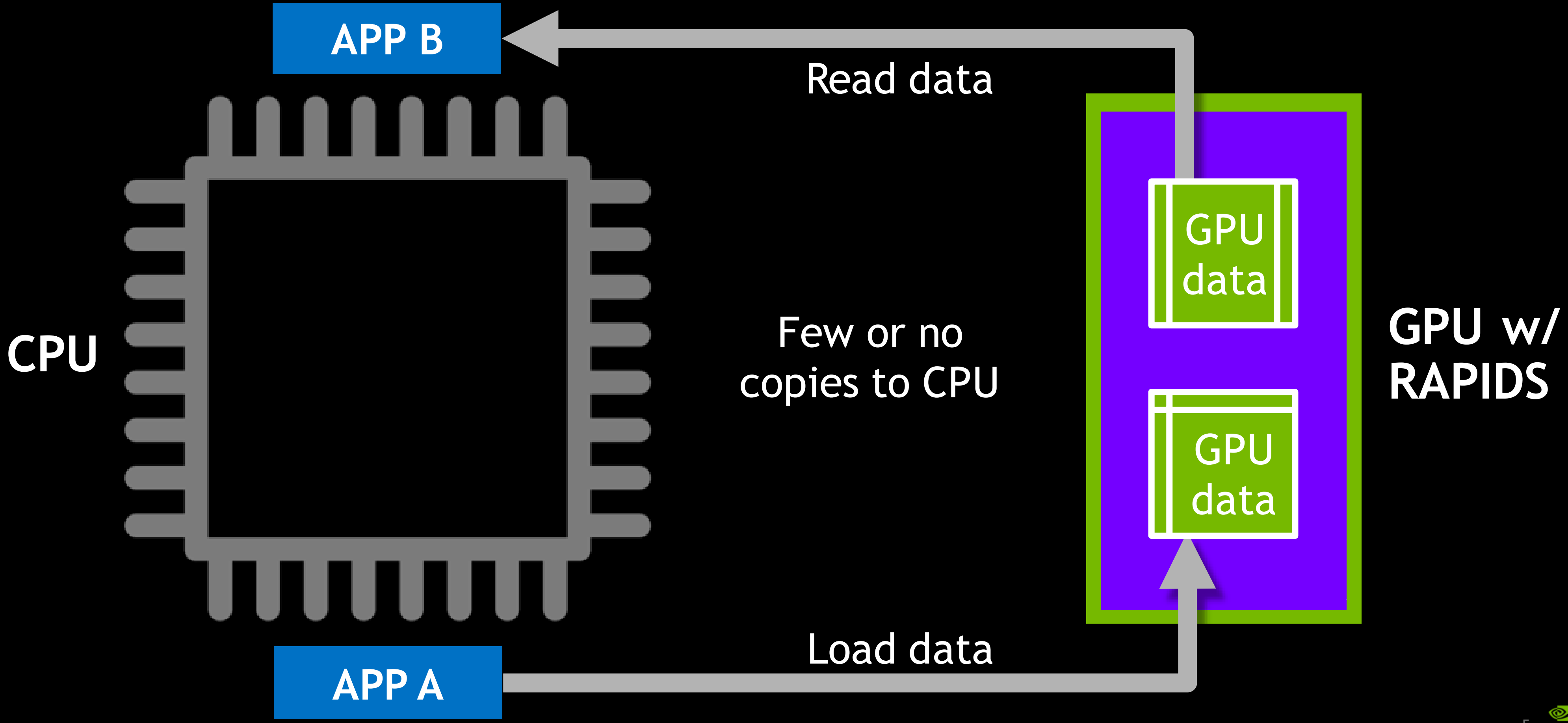
Build the foundations for you to learn RAPIDS capabilities now and in the future

RAPIDS FUNDAMENTALS

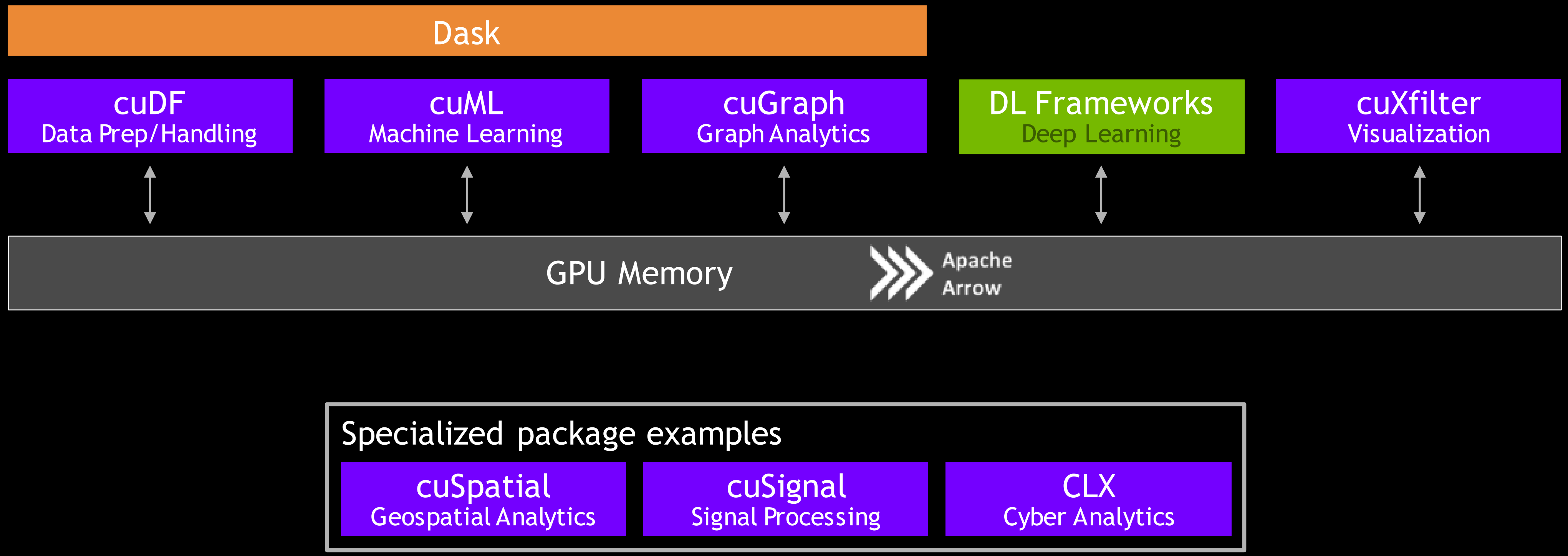
TRADITIONAL MODEL



RAPIDS MODEL



RAPIDS PLATFORM



Dask

cuDF
Data Prep/Handling

cuML
Machine Learning

cuGraph
Graph Analytics

DL Frameworks
Deep Learning

cuXfilter
Visualization

GPU Memory

Apache
Arrow

Specialized package examples

cuSpatial
Geospatial Analytics

cuSignal
Signal Processing

CLX
Cyber Analytics

DATA SCIENCE TOOLSETS

	CPU	GPU/RAPIDS
Data handling	pandas	cuDF
Machine learning	scikit-learn	cuML
Graph analytics	NetworkX	cuGraph

	CPU	GPU/RAPIDS
Viz	Bokeh/ Datashader	cuXfilter
Geospatial	GeoPandas/ SciPy.spatial	cuSpatial
Signals	SciPy.signal	cuSignal
Cyber	cyberpandas	CLX

REQUIREMENTS

Appropriate OS: Ubuntu 16.04/18.04/20.04, CentOS/RHEL 7, Windows with WSL (preview)

NVIDIA Pascal™ GPU architecture or newer

CUDA 10.1.2/10.2/11.x, drivers, etc. (see rapids.ai)

Open source/flexible mindset

- Using v20.02 in this class
- New versions released regularly

RAPIDS

Source code on GitHub

https://github.com/rapidsai

GitHub

Containers on NGC & Docker Hub

https://ngc.nvidia.com

NVIDIA. NGC

docker

Conda packages

https://anaconda.org/rapidsai

CONDA

On-premises

rapids.ai

In the cloud

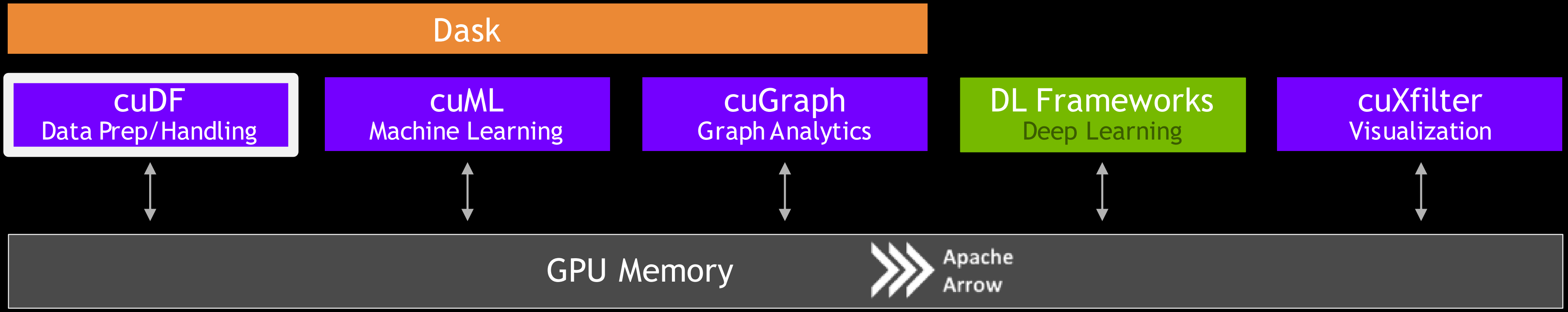
EXERCISE DATA

Fused and simulated from several sources

- Population data
  - Simulated from UK Census data on England and Wales, both from details (age, sex, given name, county) and aggregate statistics (geographic coordinates, employment)
- Road network data
  - Nodes (endpoints/junctions) and edges of the entire road network of Great Britain
- Epidemic data
  - Detailed hospital/clinic data from the UK National Health Service
  - Spread modeled on academic research on Ebolavirus risk factors

SECTION 1
01 - 04

RAPIDS PLATFORM



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CUDF DATAFRAMES

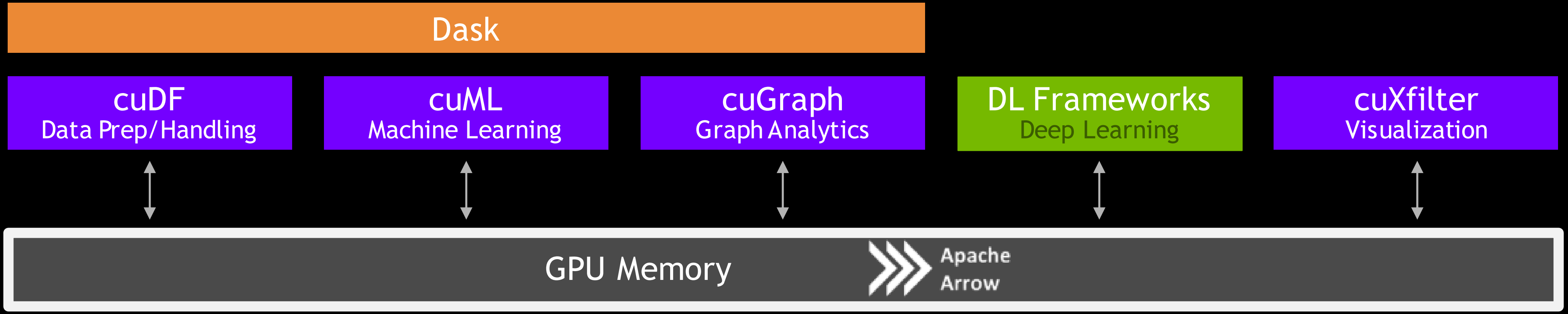
Pandas model: observations/records (rows) of features (columns)

Each feature/column has a single datatype

Simple, flexible interface to complex, performant datastructure

Special emphasis on columnar structure

RAPIDS PLATFORM



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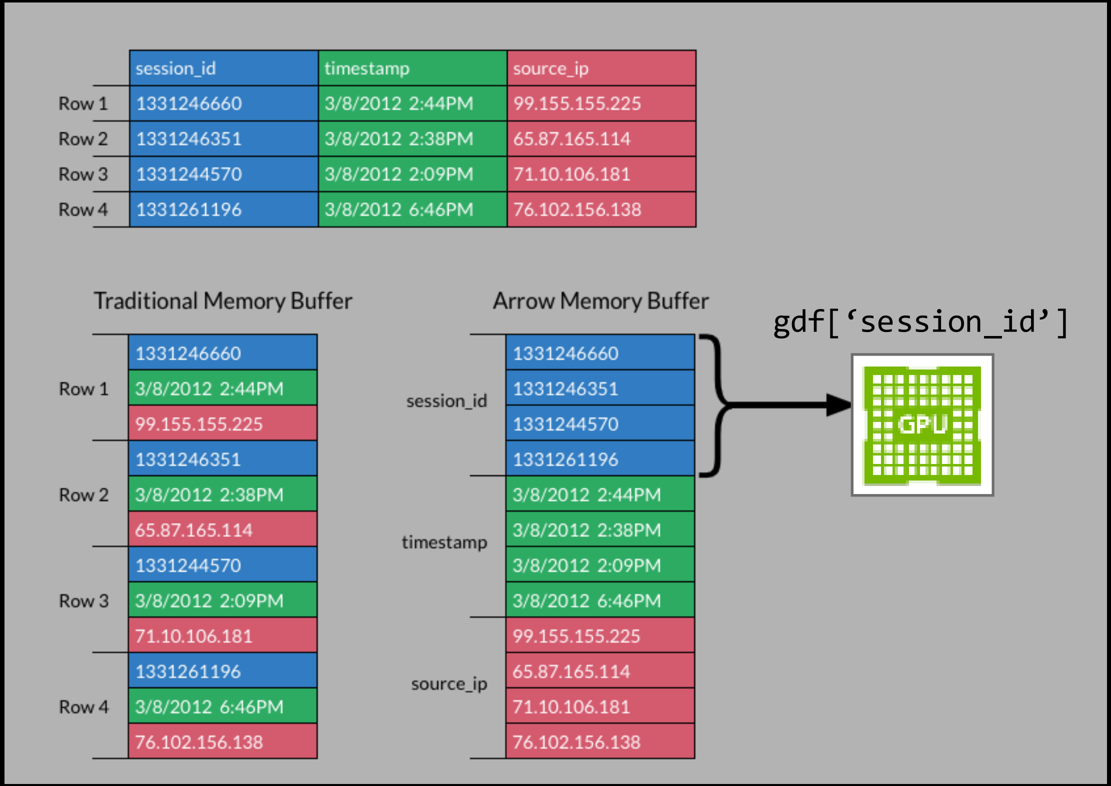
APACHE ARROW

Columnar layout leverages GPU strengths

Emphasis on zero-copy and shallow-copy operations minimizes a key bottleneck

Consistency with CPU version simplifies development and conversion



	session_id	timestamp	source_ip
Row 1	1331246660	3/8/2012 2:44PM	99.155.155.225
Row 2	1331246351	3/8/2012 2:38PM	65.87.165.114
Row 3	1331244570	3/8/2012 2:09PM	71.10.106.181
Row 4	1331261196	3/8/2012 6:46PM	76.102.156.138

Traditional Memory Buffer

Row 1	1331246660
	3/8/2012 2:44PM
	99.155.155.225
Row 2	1331246351
	3/8/2012 2:38PM
	65.87.165.114
Row 3	1331244570
	3/8/2012 2:09PM
	71.10.106.181
Row 4	1331261196
	3/8/2012 6:46PM
	76.102.156.138

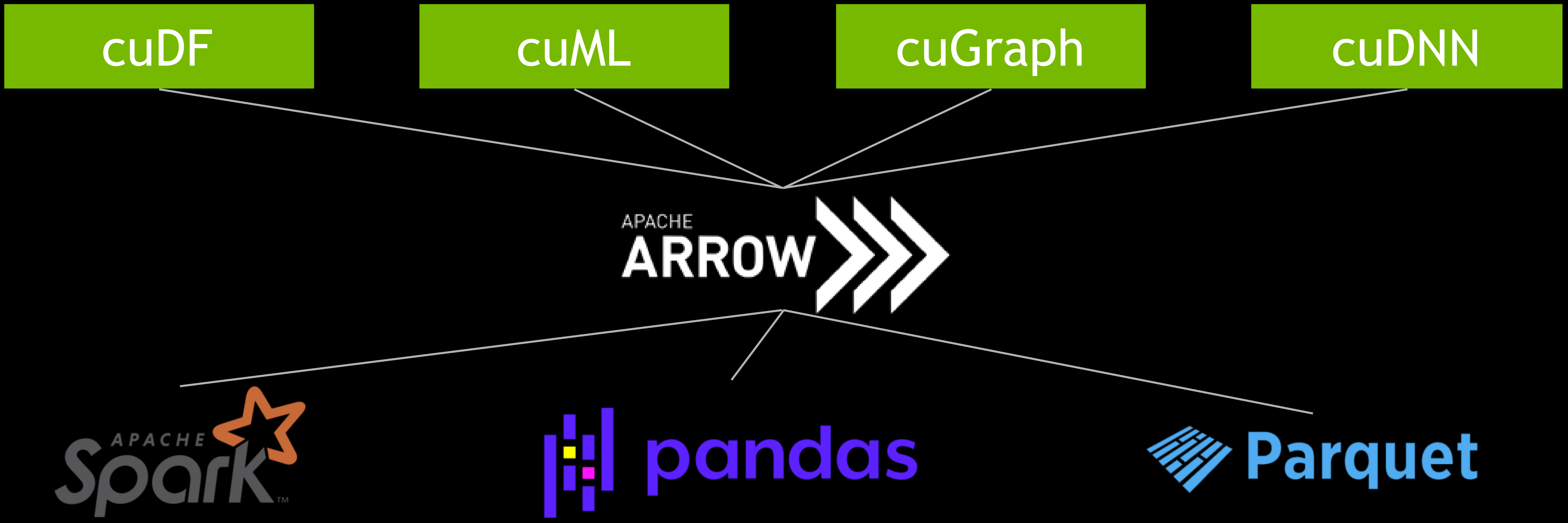
Arrow Memory Buffer

session_id	1331246660
	1331246351
	1331244570
	1331261196
timestamp	3/8/2012 2:44PM
	3/8/2012 2:38PM
	3/8/2012 2:09PM
	3/8/2012 6:46PM
source_ip	99.155.155.225
	65.87.165.114
	71.10.106.181
	76.102.156.138

gdf[‘session_id’]

APACHE ARROW

One format for interoperability and efficiency



cuDF

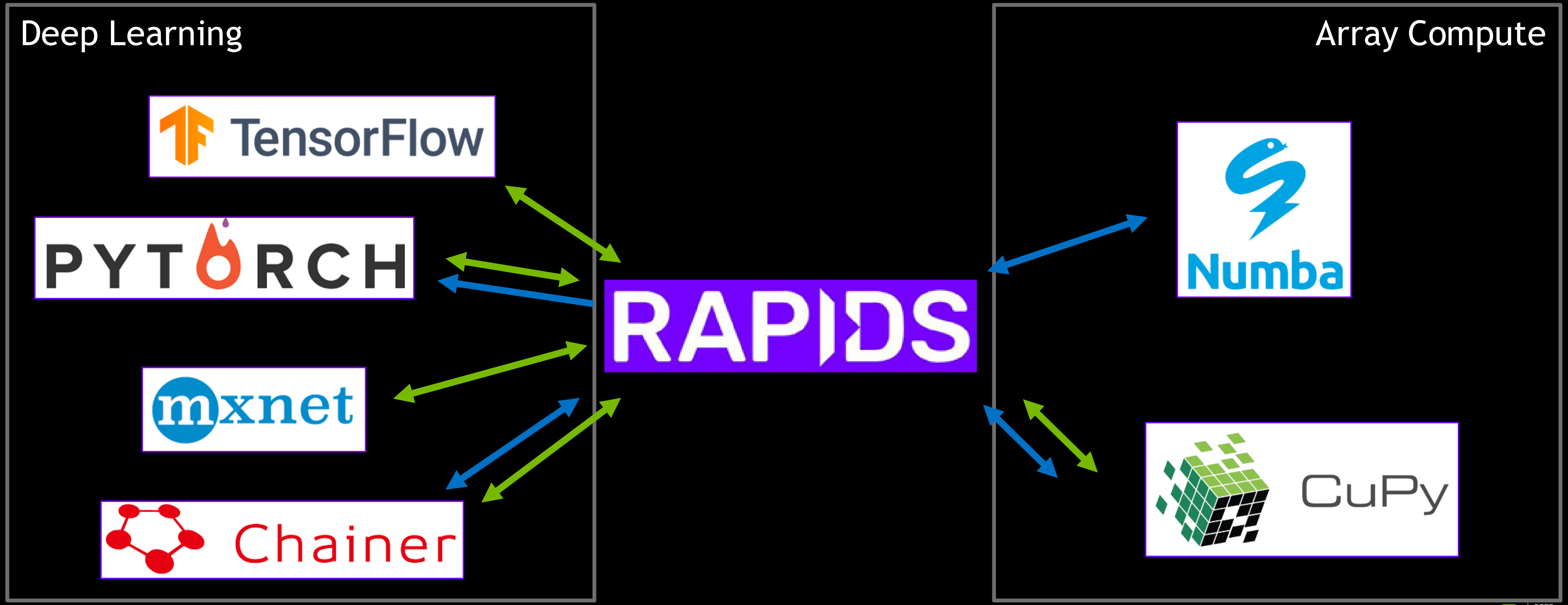
cuML

cuGraph

cuDNN

INTEROPERABILITY

DLPack and __cuda_array_interface__



TRY NOTEBOOKS 01 - 04 NOW

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SECTION 1

05

INTEROPERATING WITH CUPY

CuPy:cuDF :: numpy:pandas

Not as fast as an optimized CUDA kernel, but very efficient for coding

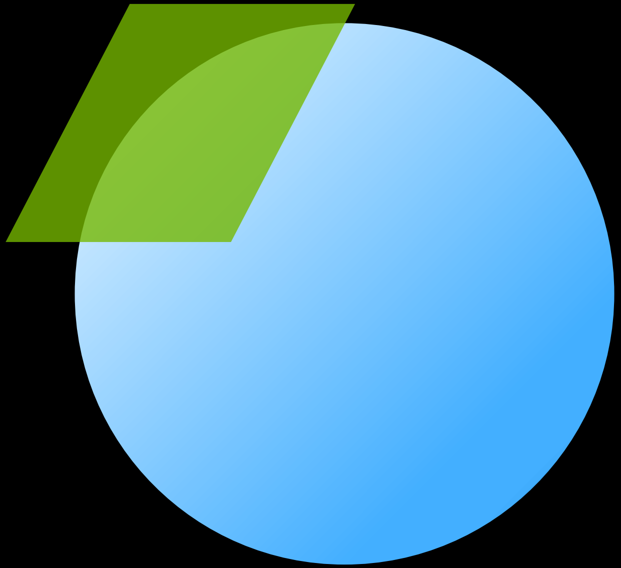
Important to keep track of data type requirements (e.g. contiguity)

COORDINATE SYSTEMS

We will be using data that was provided in both ellipsoidal and grid coordinate formats

Grid coordinates make distance calculations more convenient within a specific area

Fusing geospatial datasets like this requires complex coordinate conversions—a perfect job for GPU acceleration!



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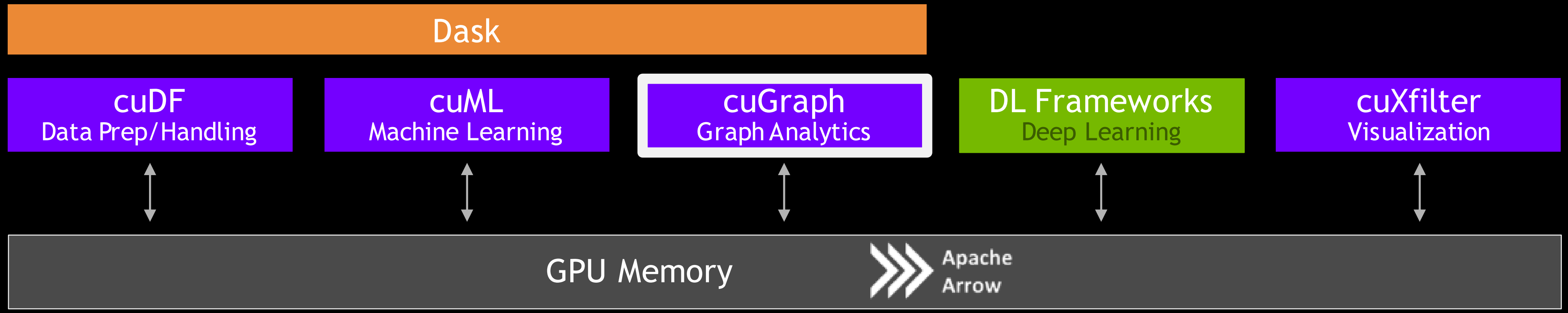
SECTION 1
06

RAPIDS PLATFORM



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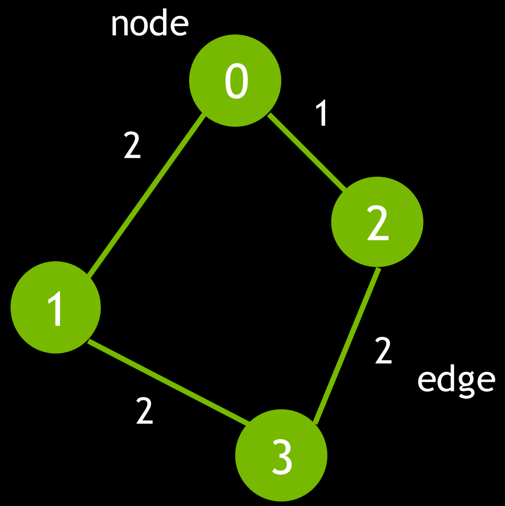
CUGRAPH

Follows NetworkX convention for graph object

Key differences to take advantage of GPU power

Exercises

- Now: steps to build a graph with `from_cudf_edgelist`
- Later: traversing the graph with single-source shortest path



Not shown today: analyzing a graph for centralities, communities, link prediction…

BUILDING A GRAPH

With `from_cudf_edgelist`

Undirected (Graph) vs directed (DiGraph)

Single vs Multi graphs

One source column, one destination column, one edge weight column

TRY NOTEBOOK 06 NOW

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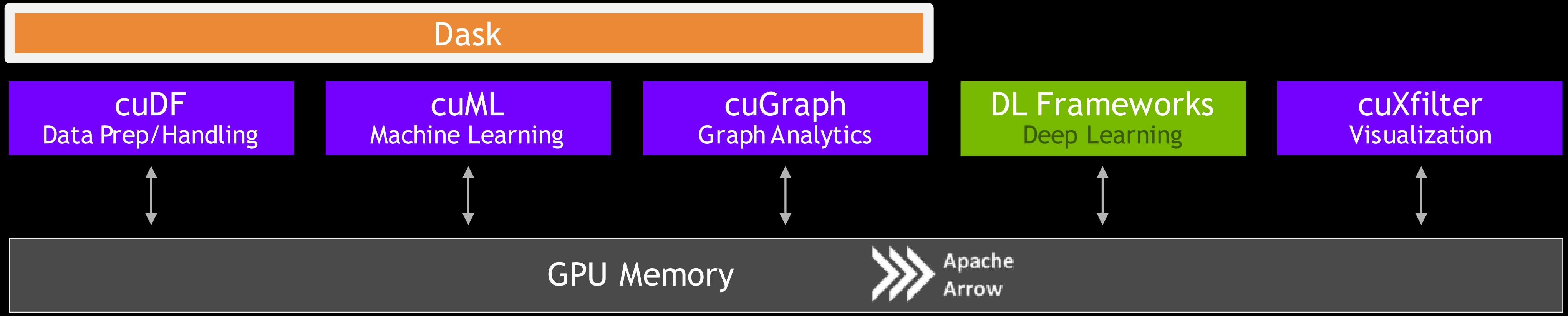
SECTION 1
07 - 08

RAPIDS PLATFORM



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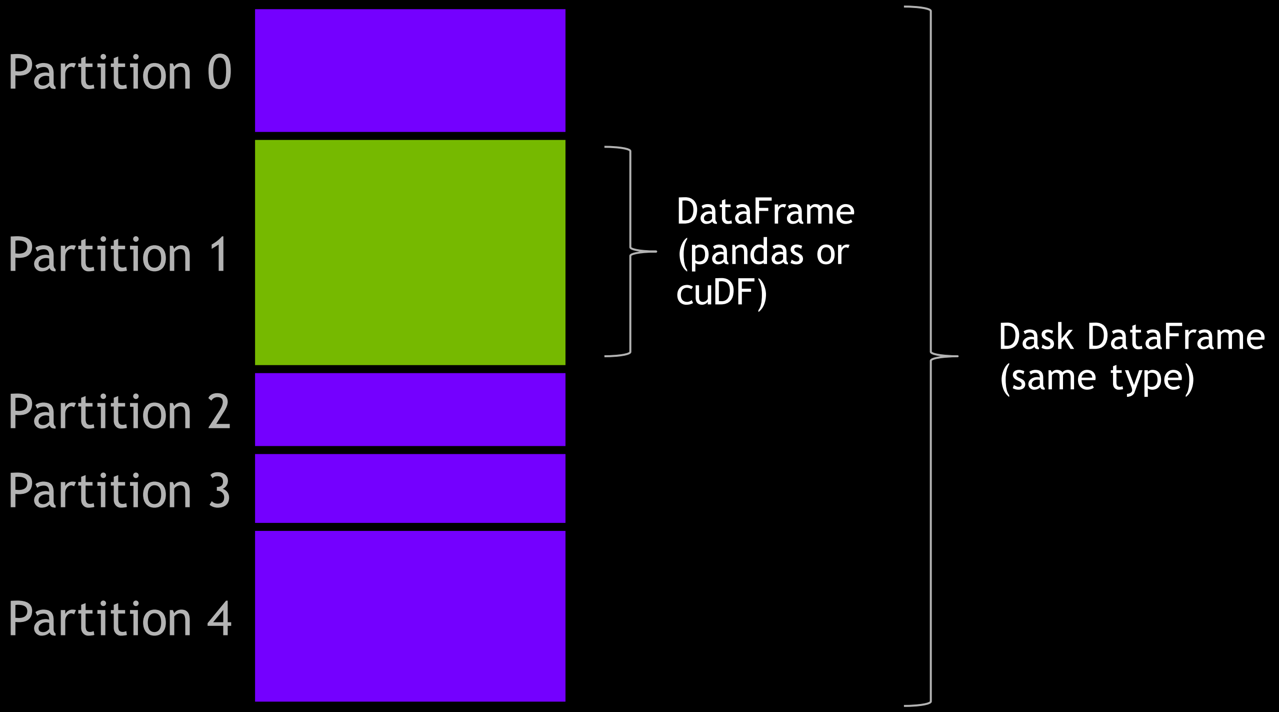
DISTRIBUTED DATAFRAMES

Scaling seamlessly



WORKING WITH PARTITIONS

No intrinsic row ordering, so no `.iloc` row selection, and index is essential

Key methods operate on whole dataframe partitions

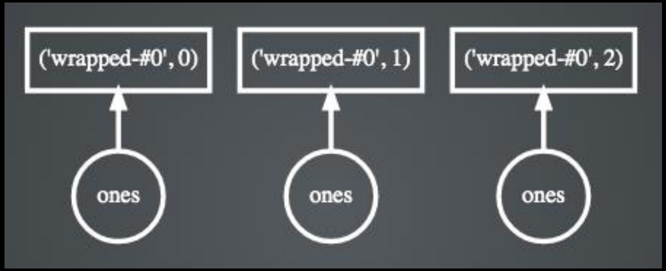
Remember distinction between multi-GPU and multi-node/multi-GPU algorithms

Rebalance across workers when necessary

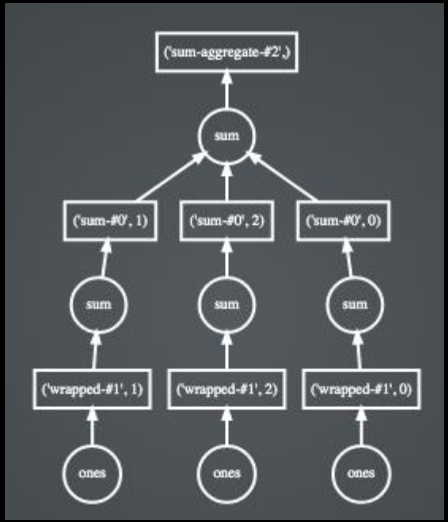
TASK SCHEDULER

Enabling efficient compute

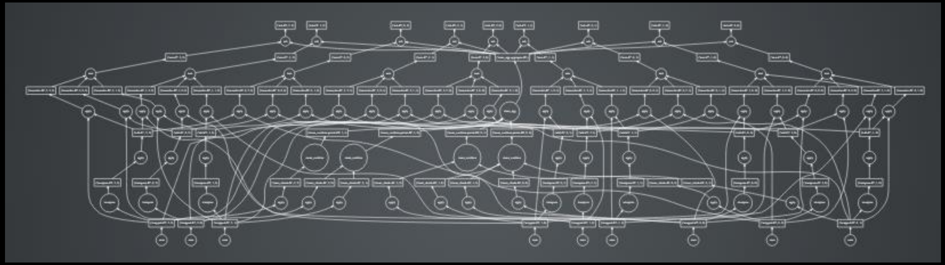
Simple operations



Compound operations



Complex DAG task chains



WORKING WITH THE SCHEDULER

Let Dask help you overcome your storage I/O barriers

Limit `.compute` (stay in Dask) until necessary

For exploratory and experimental data science, don’t be afraid to `.persist`

Remember that everything in a graph will be rerun without `.persist`/`.compute`—including random number generation

TRY NOTEBOOKS 07 - 08 NOW

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