On-Demand Column-Joining for End-User Analysis

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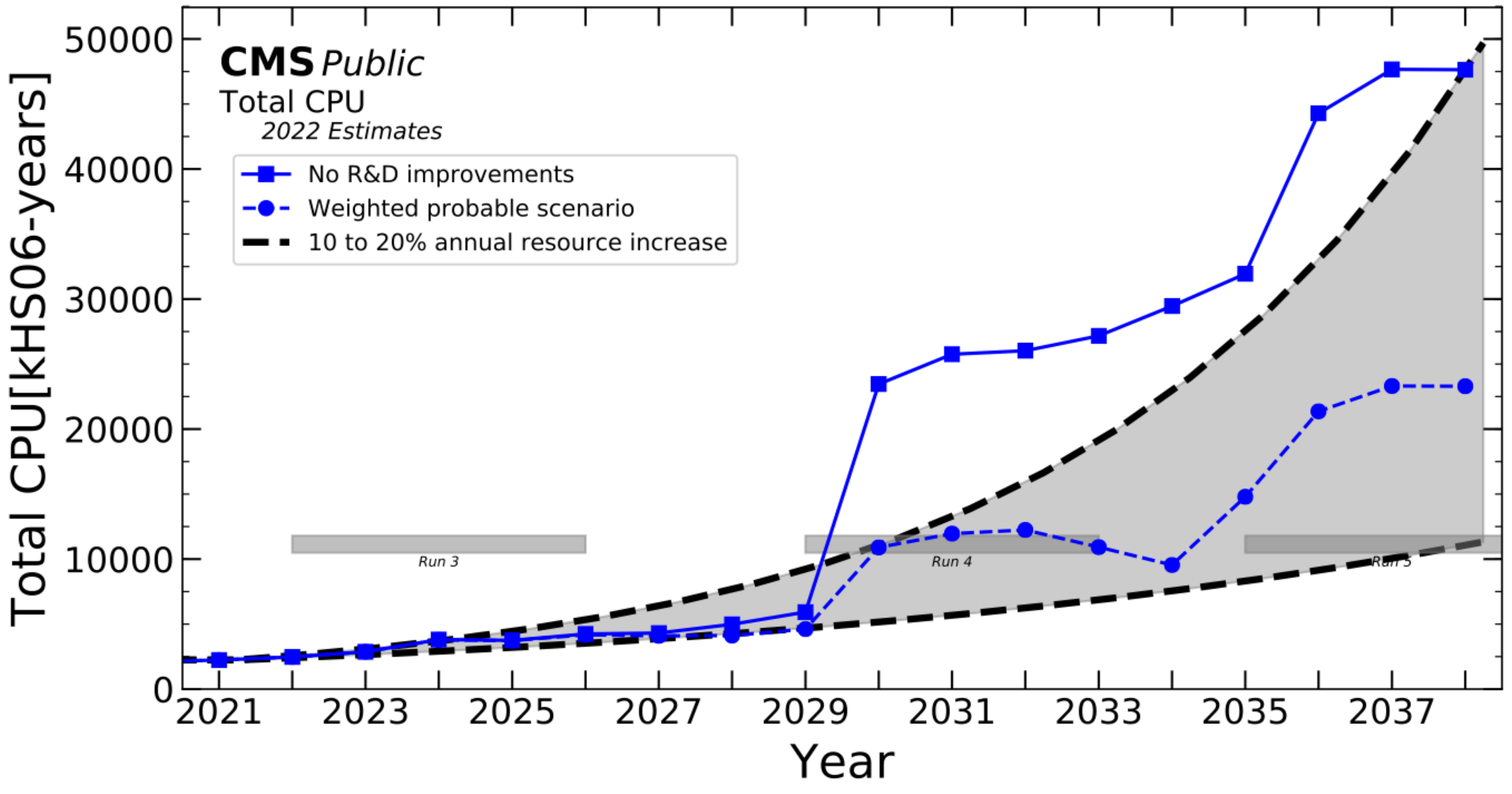
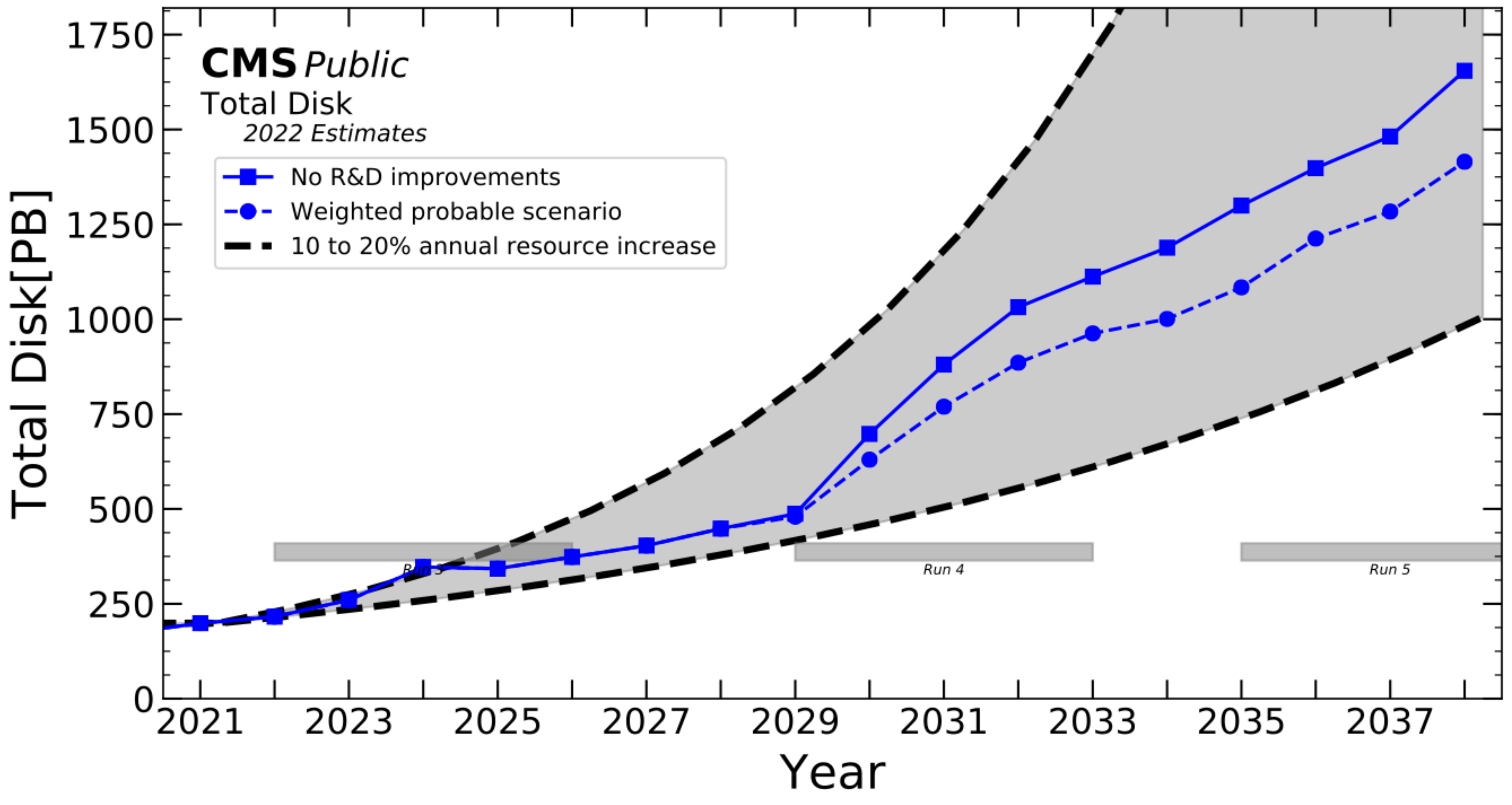
Motivation


CMS Public
Total CPU
2022 Estimates
No R&D improvements
Weighted probable scenario
10 to 20% annual resource increase
Total CPU[kHS06-years]
Year
Run 3
Run 4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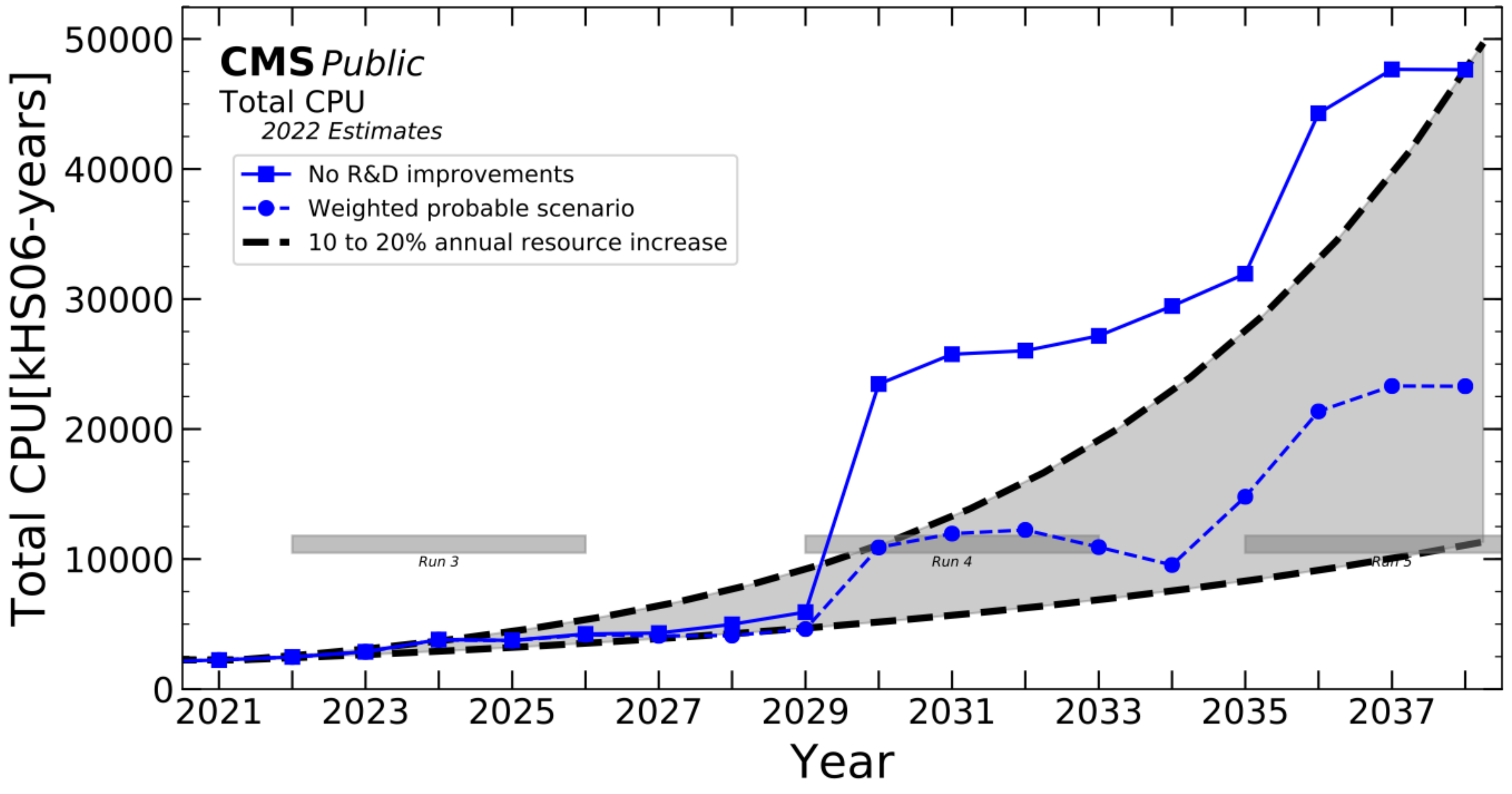

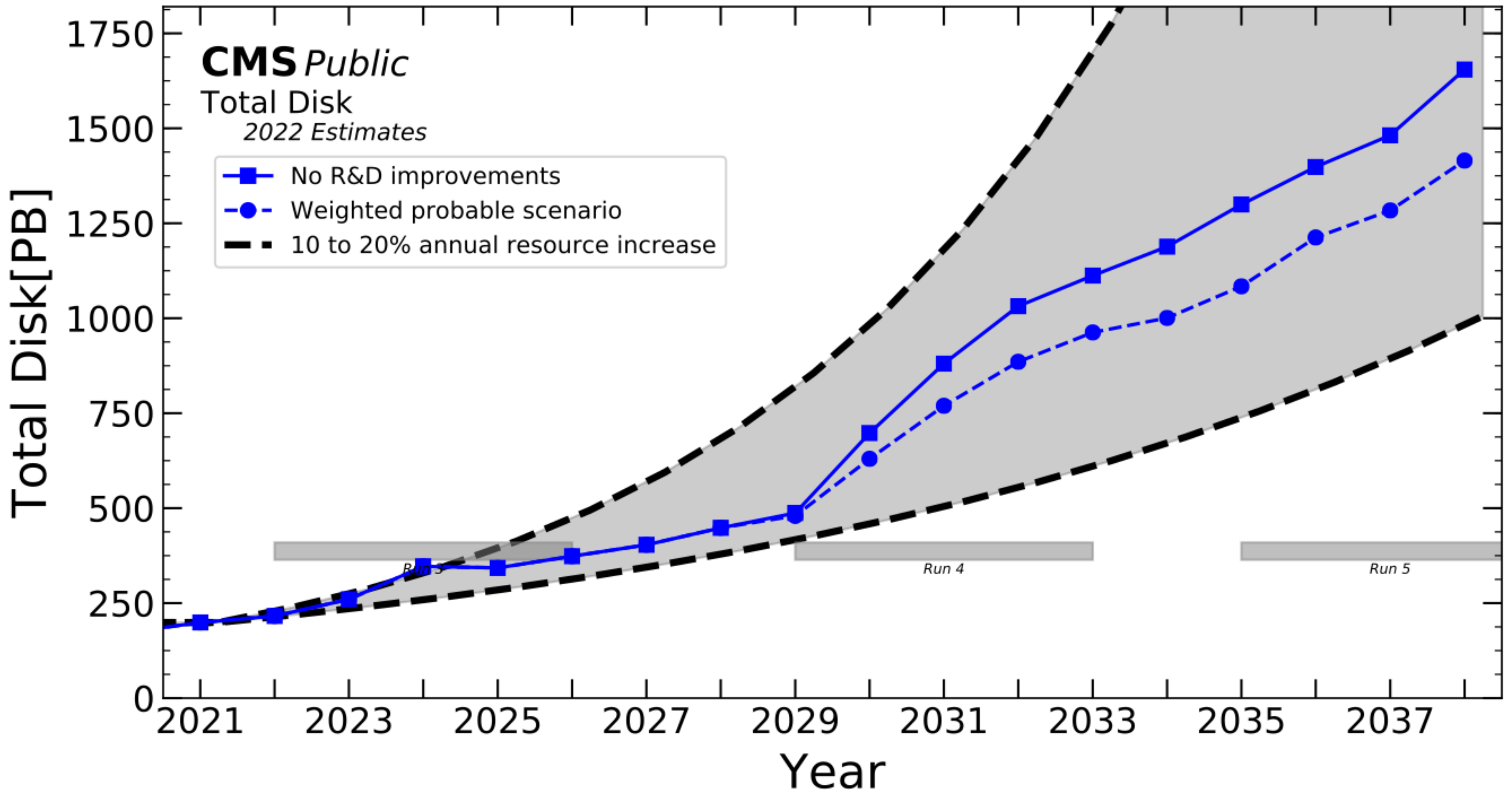

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  - CMS AOD (450kB/event) - Limited Availability, high processing costs, data: C++ classes
  - MiniAOD (45kB/event) - Suitable for nearly all analyses, still large, still significant processing, data: C++ classes
  - NanoAOD(4kB/event) - Suitable for half of analyses, **analysis-ready**, **data: primitives**

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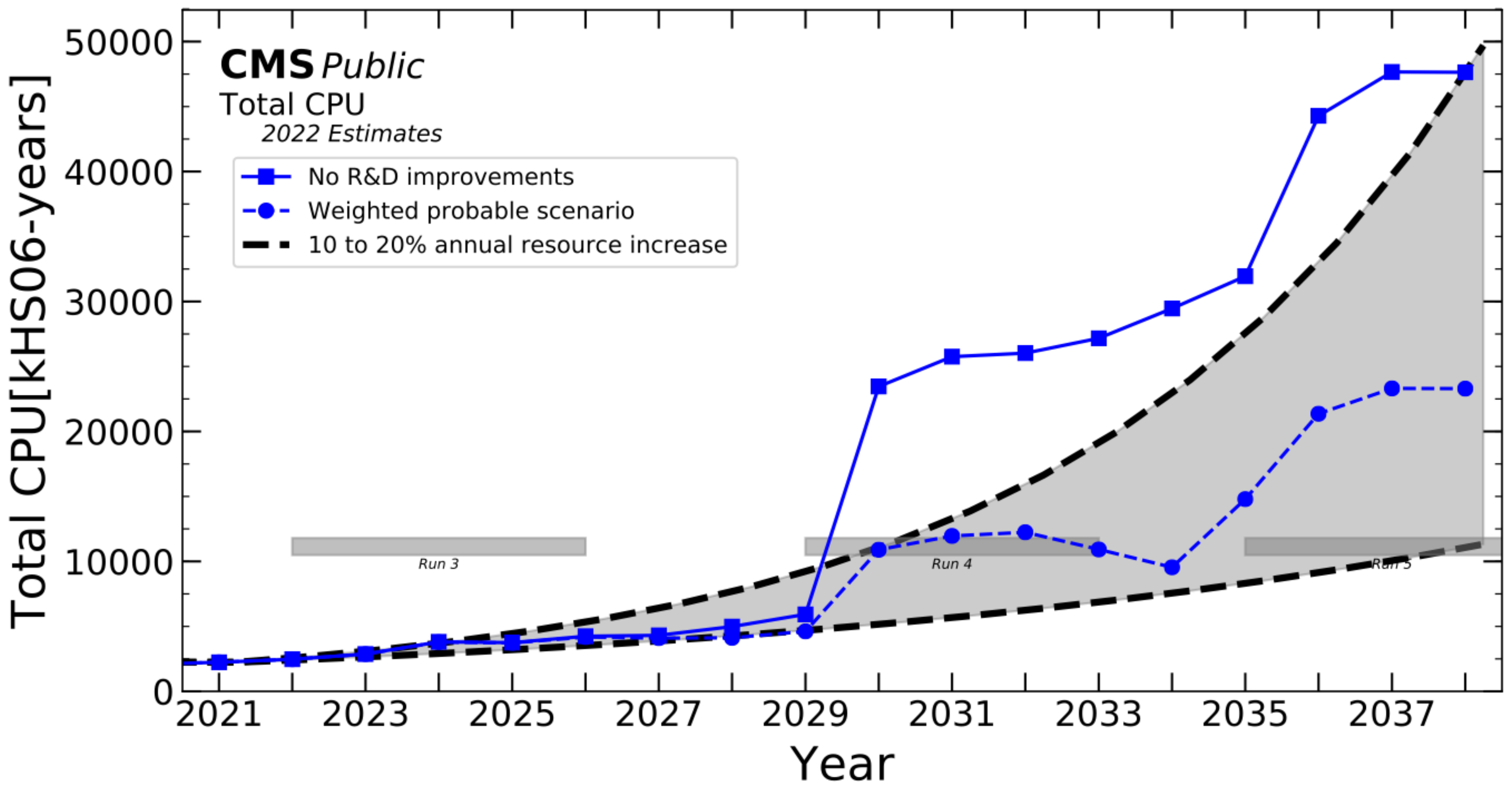

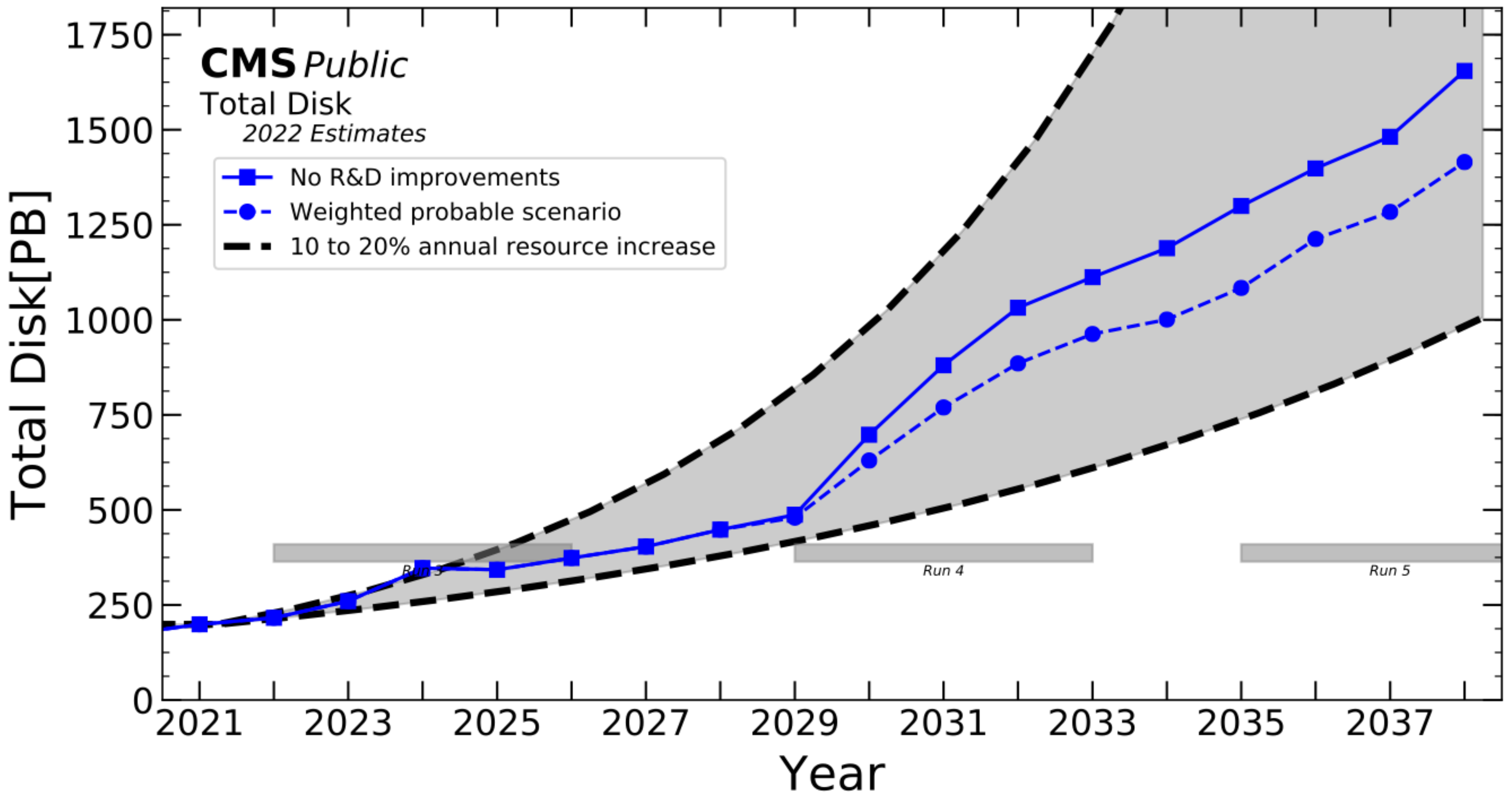

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- Several competing needs create an impedance mismatch
  - Disk space comes at a premium
  - High throughput requires high availability and duplication across sites around the world
  - Traditional analysis workflows tend to **duplicate information** from large data-tiers (Mini/AOD) via custom “Ntuples”, in order to create more streamlined but self-contained input data - for the half of analyses able to use NanoAOD (a “generalized” ntuple), it’s nearly optimal and can obviate the need for intermediate Ntuples
  - Fast turnaround (for analyzers) is paramount to getting the science **done**!

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- An analysis may have 90% of data needs met by NanoAOD, but the additional requirements drive it to use MiniAOD or AOD
  - Custom NanoAOD variant (superset of central variation) or custom NTuple format created from larger datatier (labor and compute-intensive), **duplicating** a significant amount of centrally-stored events in Nano and Mini formats (inefficient disk utilization)

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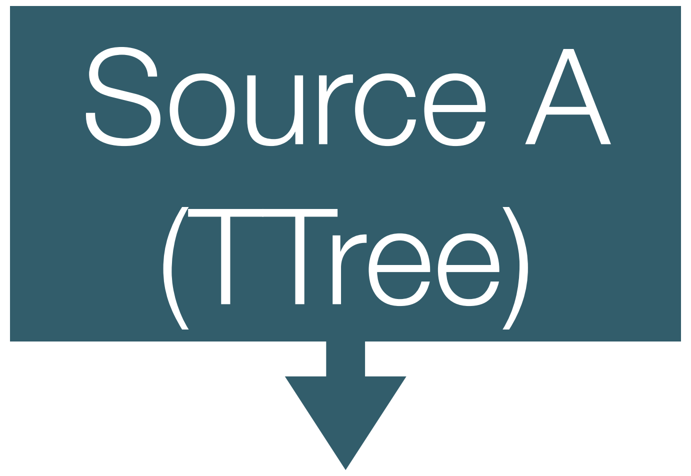

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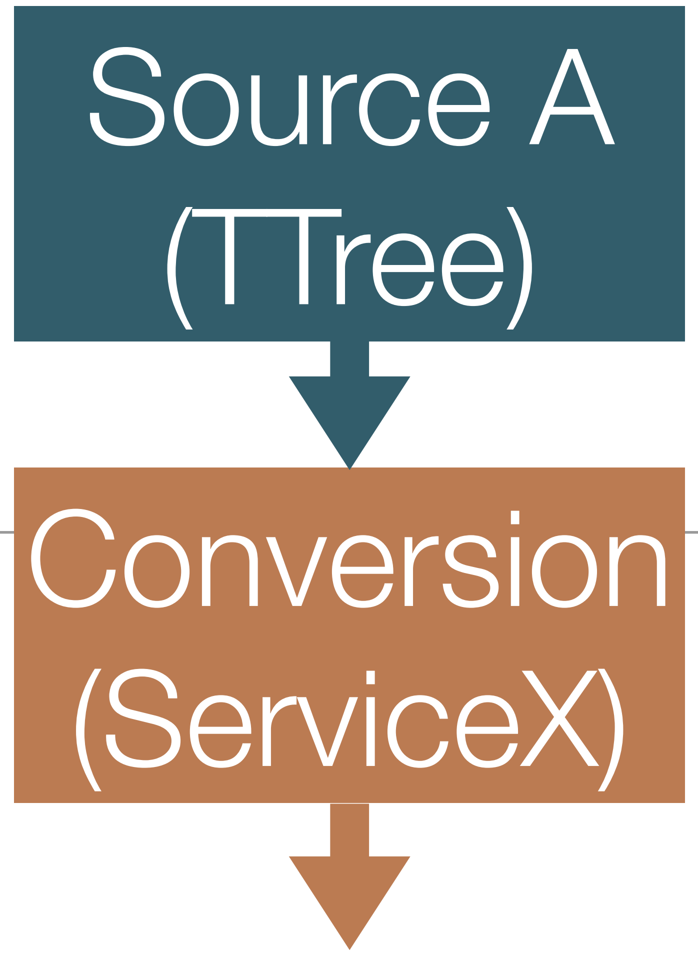

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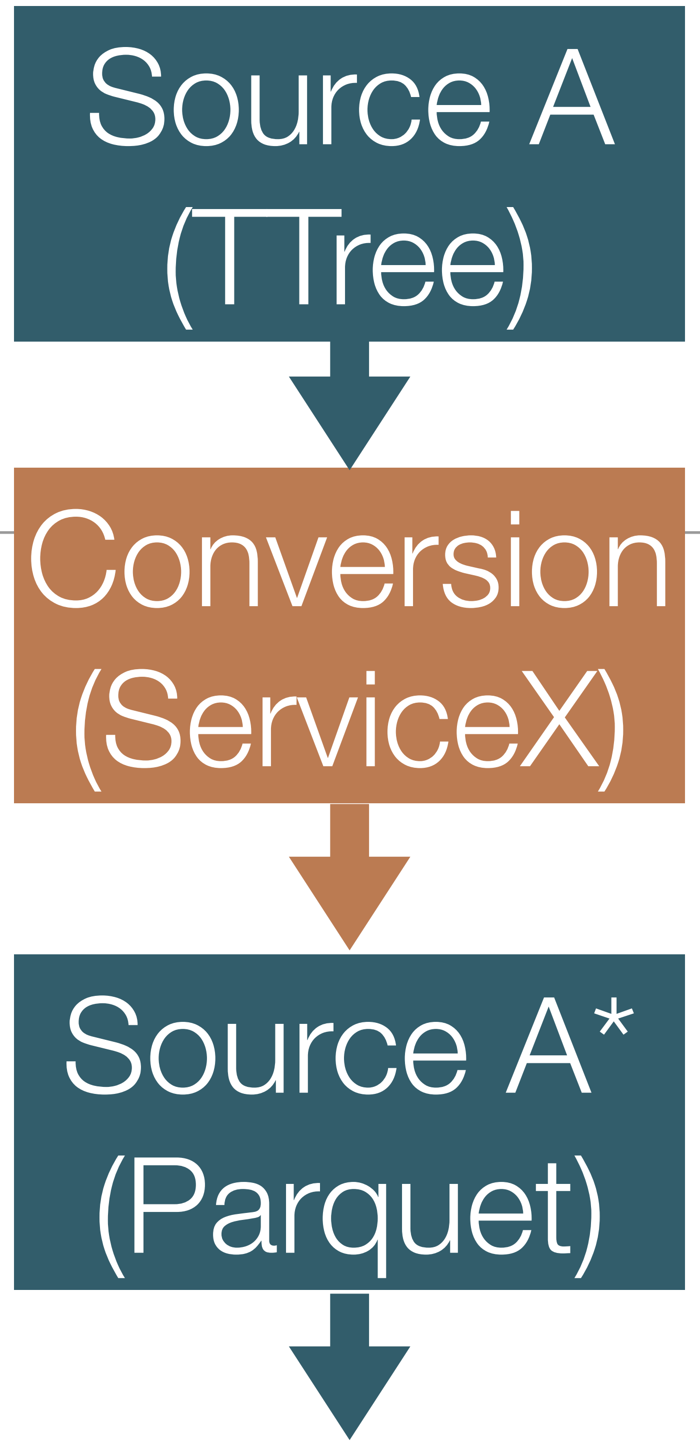

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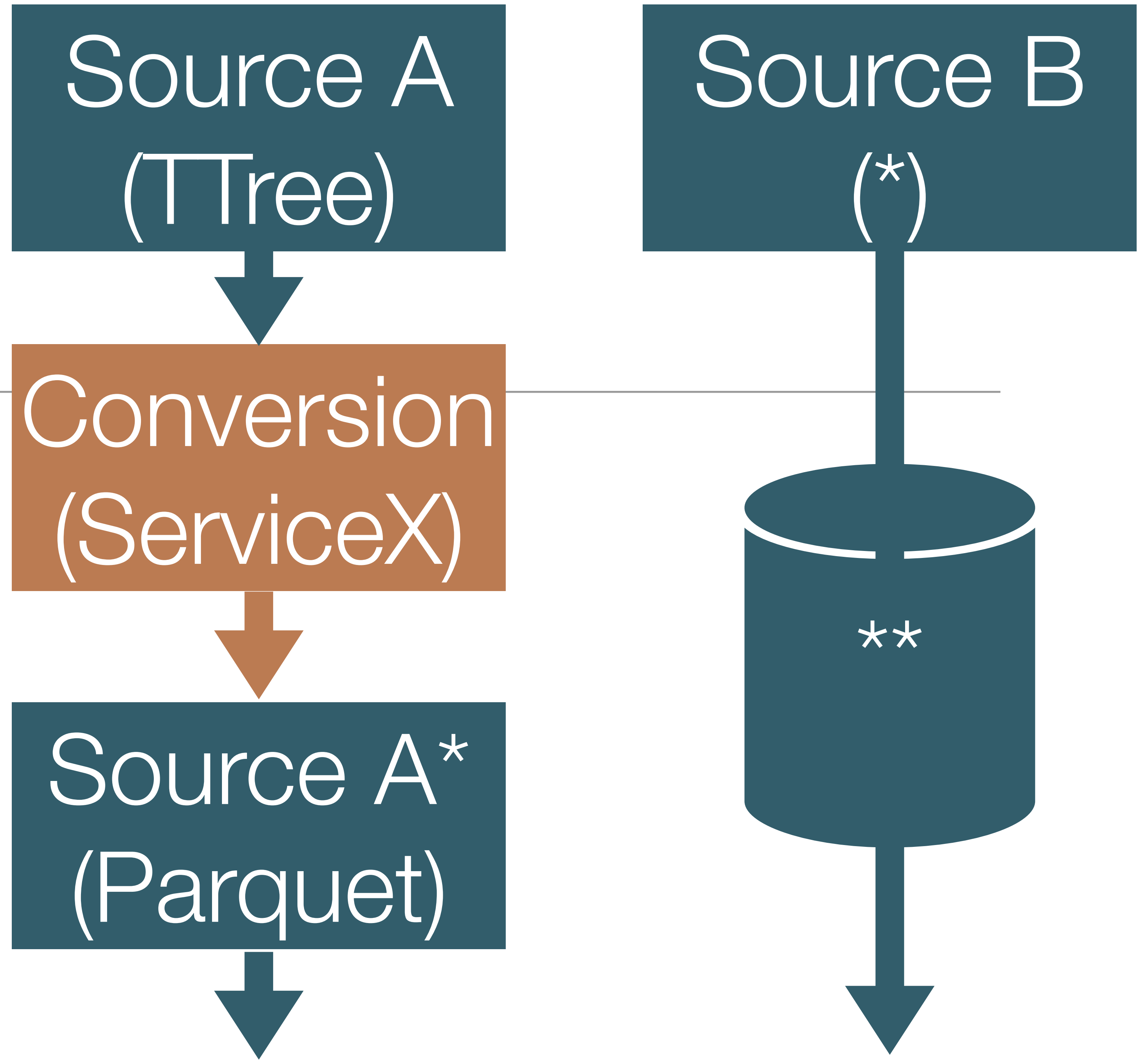

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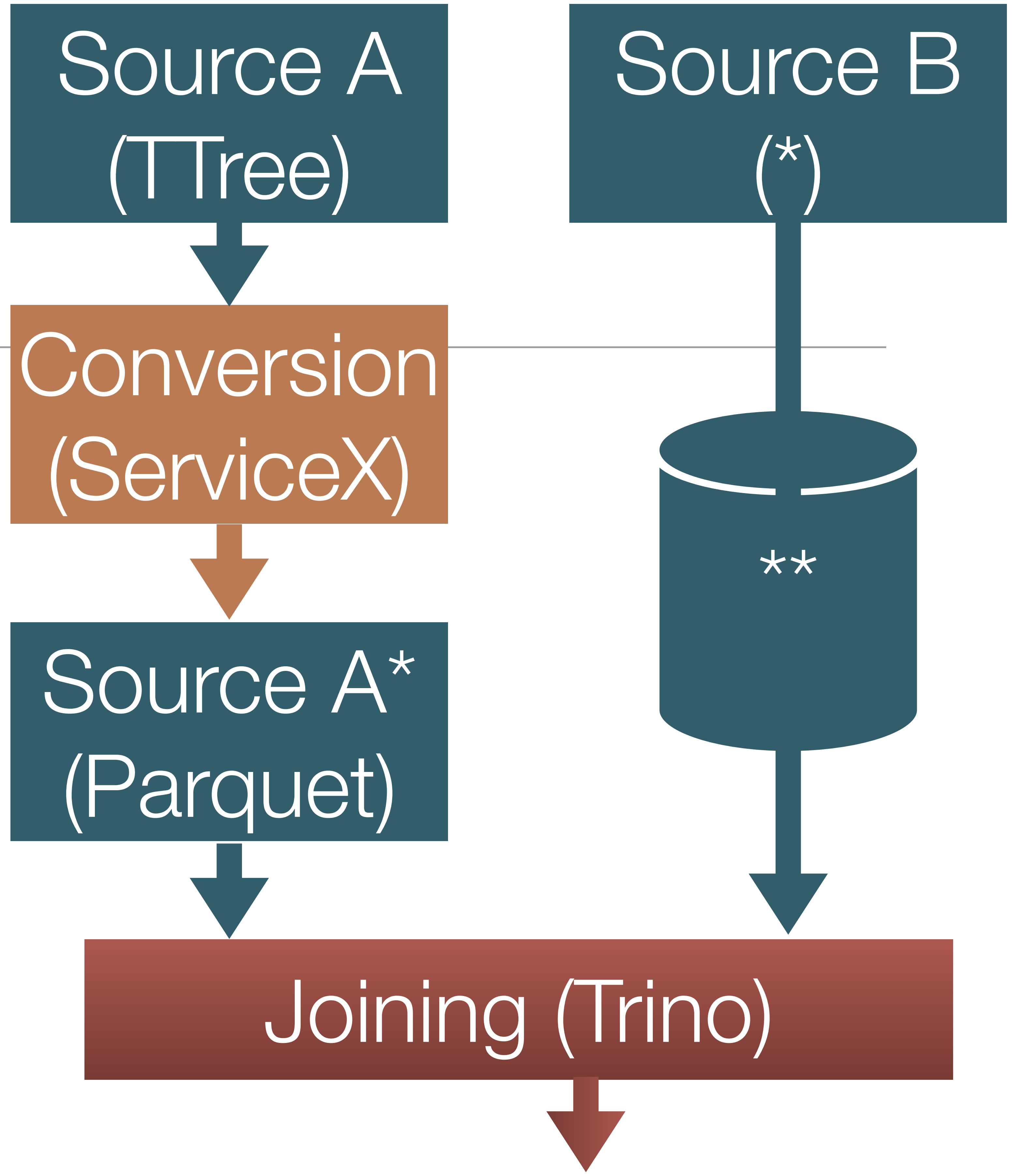

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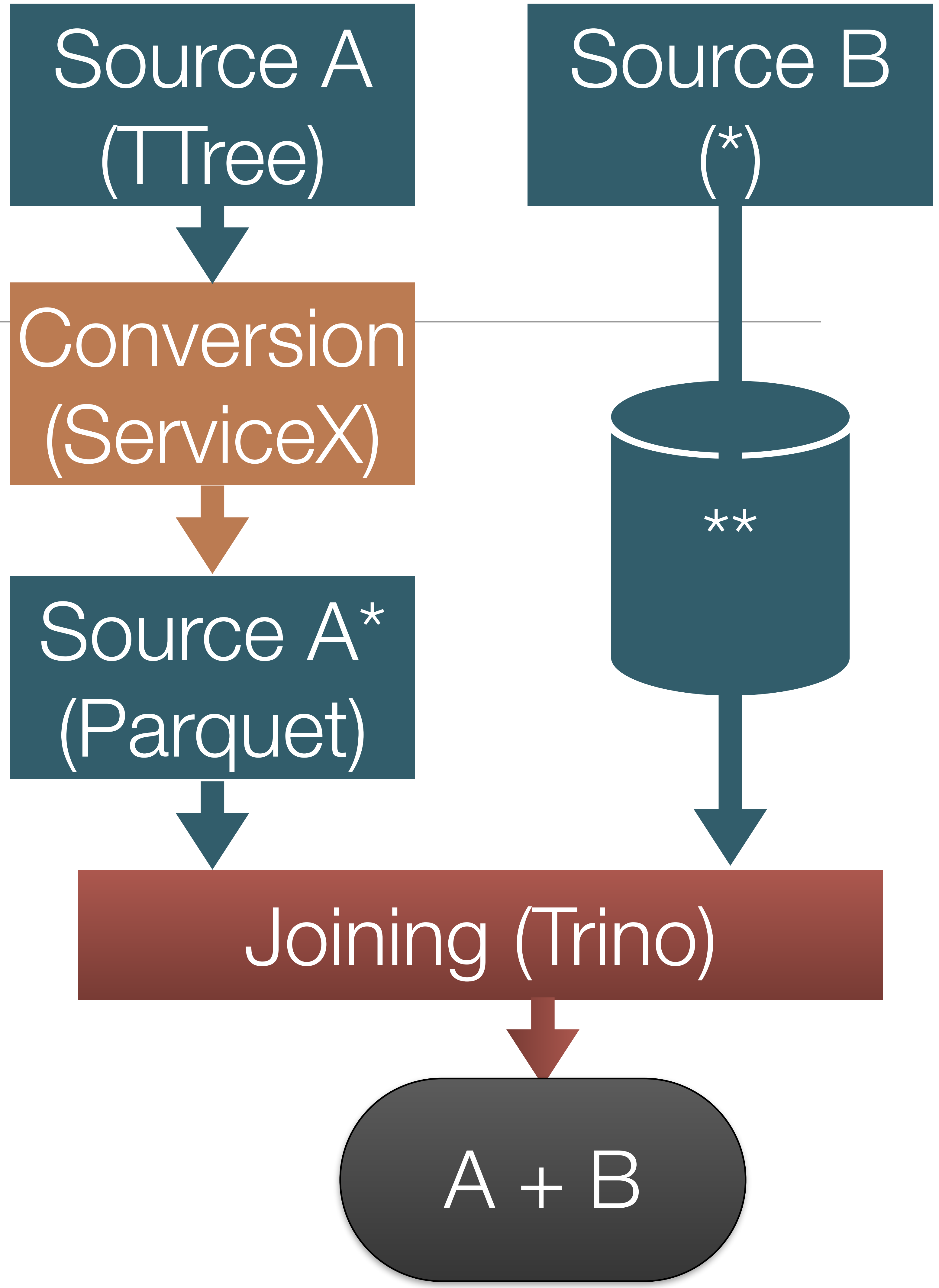

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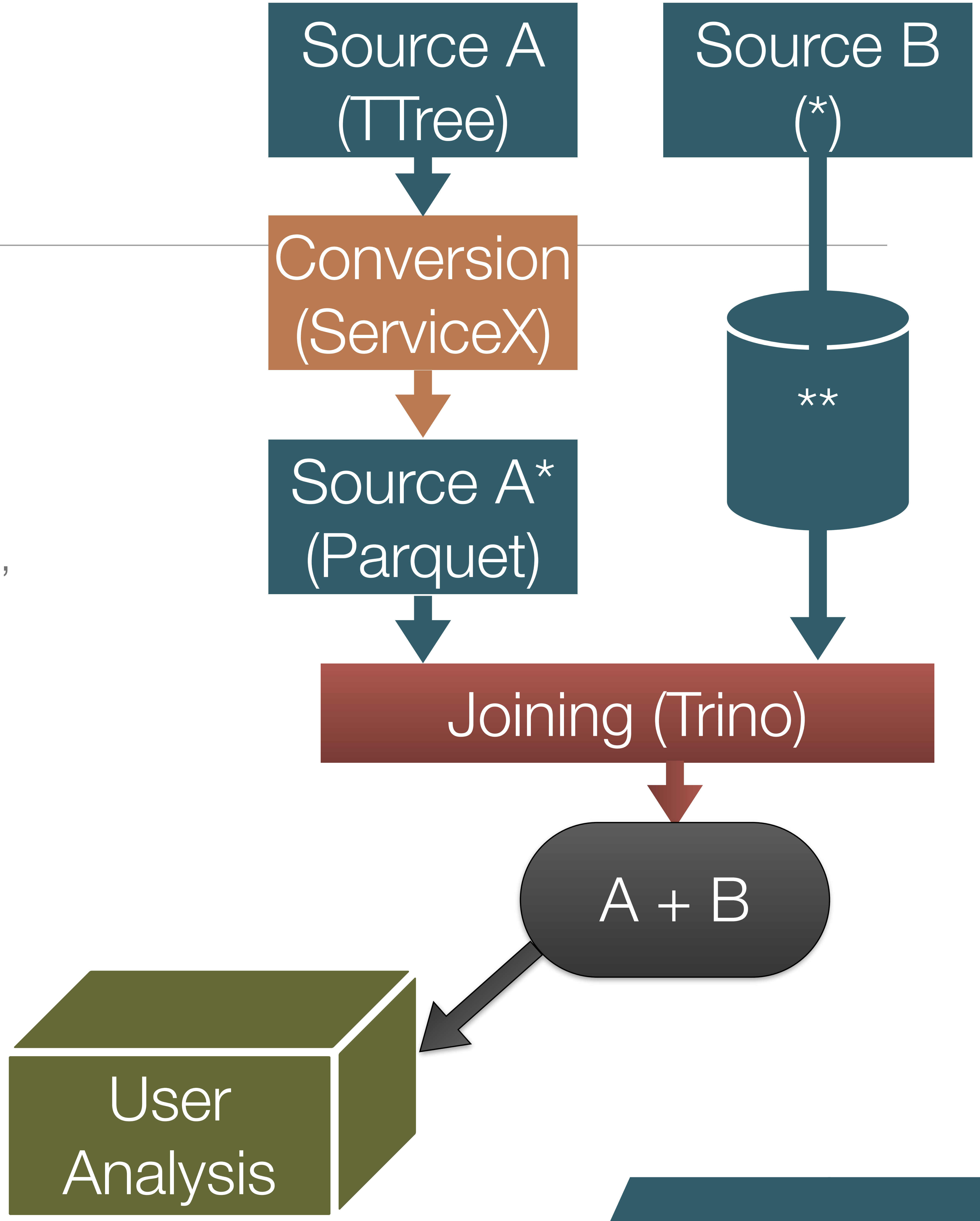
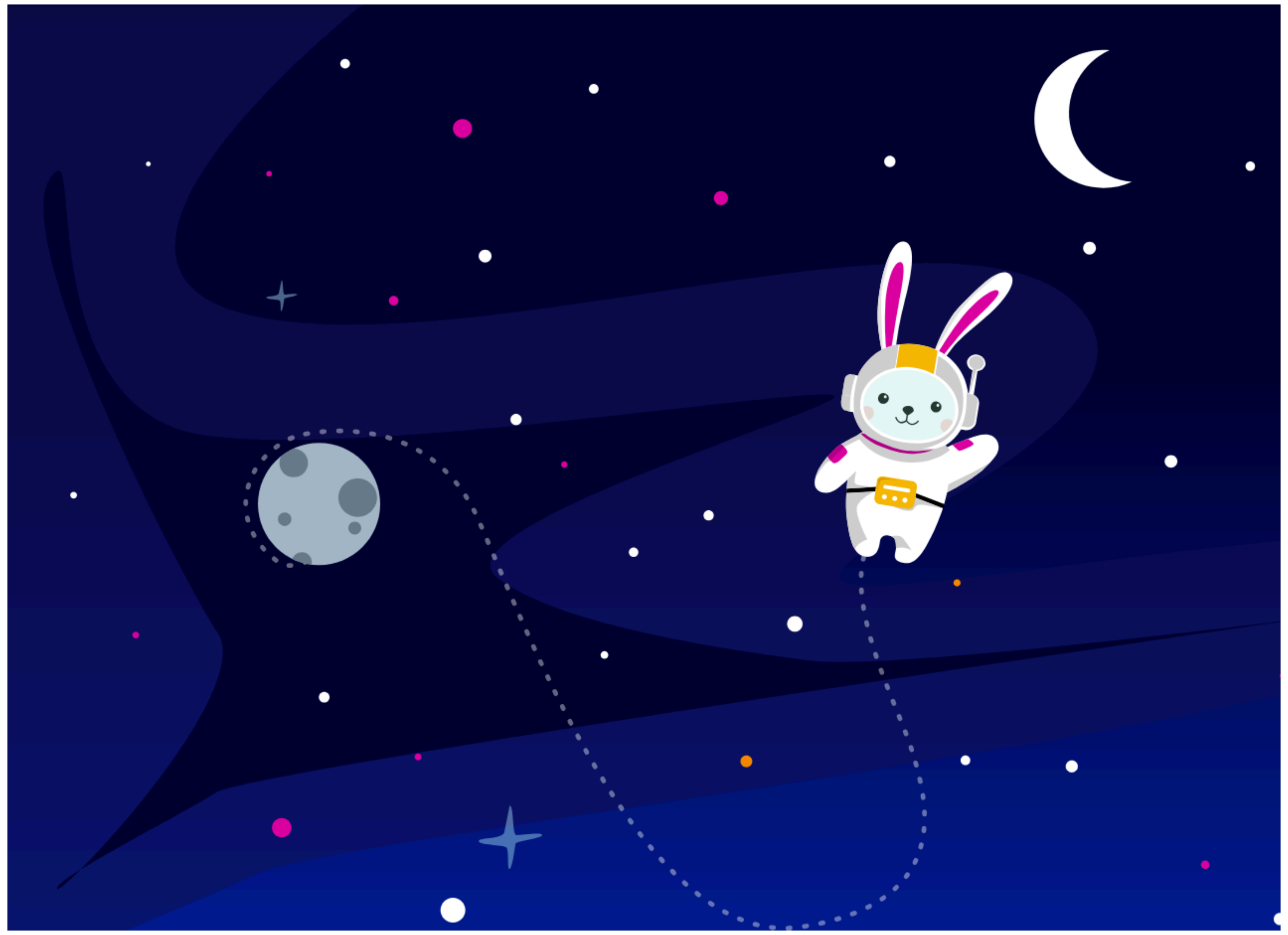


Trino (as described by o1-mini)

Trino is a high-performance, distributed SQL query engine designed for running interactive analytic queries against various data sources of all sizes. Originally developed by Facebook under the name **Presto**, Trino was forked in 2020 by the original creators to foster a more open and community-driven development model. Trino has since evolved into a robust, open-source project maintained by the **Trino Software Foundation**.

- **Key Features of Trino:**
  - Distributed Architecture
  - SQL Compatibility
  - Federated Querying
  - Performance Optimization
  - Extensibility and Customization:
    - Plugin Architecture: Users can develop **custom connectors** and functions to extend Trino's capabilities.
    - Community-Driven: Being open-source, it benefits from contributions and innovations from a broad community of developers and organizations.
  - Security and Access Control:
    - Authentication and Authorization: Supports various security protocols and integrates with enterprise security systems.
    - Data Encryption: Ensures data privacy through encryption in transit and at rest.



Benchmarking Trino

Source File 1

1:1
1:2
…
1:N

Source File A

A:1
A:2
…
A:M

- We've prepared several benchmark datasets using CMS OpenData
  - Source datasets ranging from ~2GB to ~500GB (converted to parquet, ZSTD:5, full NanoAOD)
  - GNN Inference (parquet, 8 scalar-float columns / event)
    - fully-aligned, intra-file-reversed, intra-file-shuffled, globally-shuffled variants
  - Testing various combinations (from a few scalar columns from source + inference, to dozens of ragged fields in source + all 8 inference columns)

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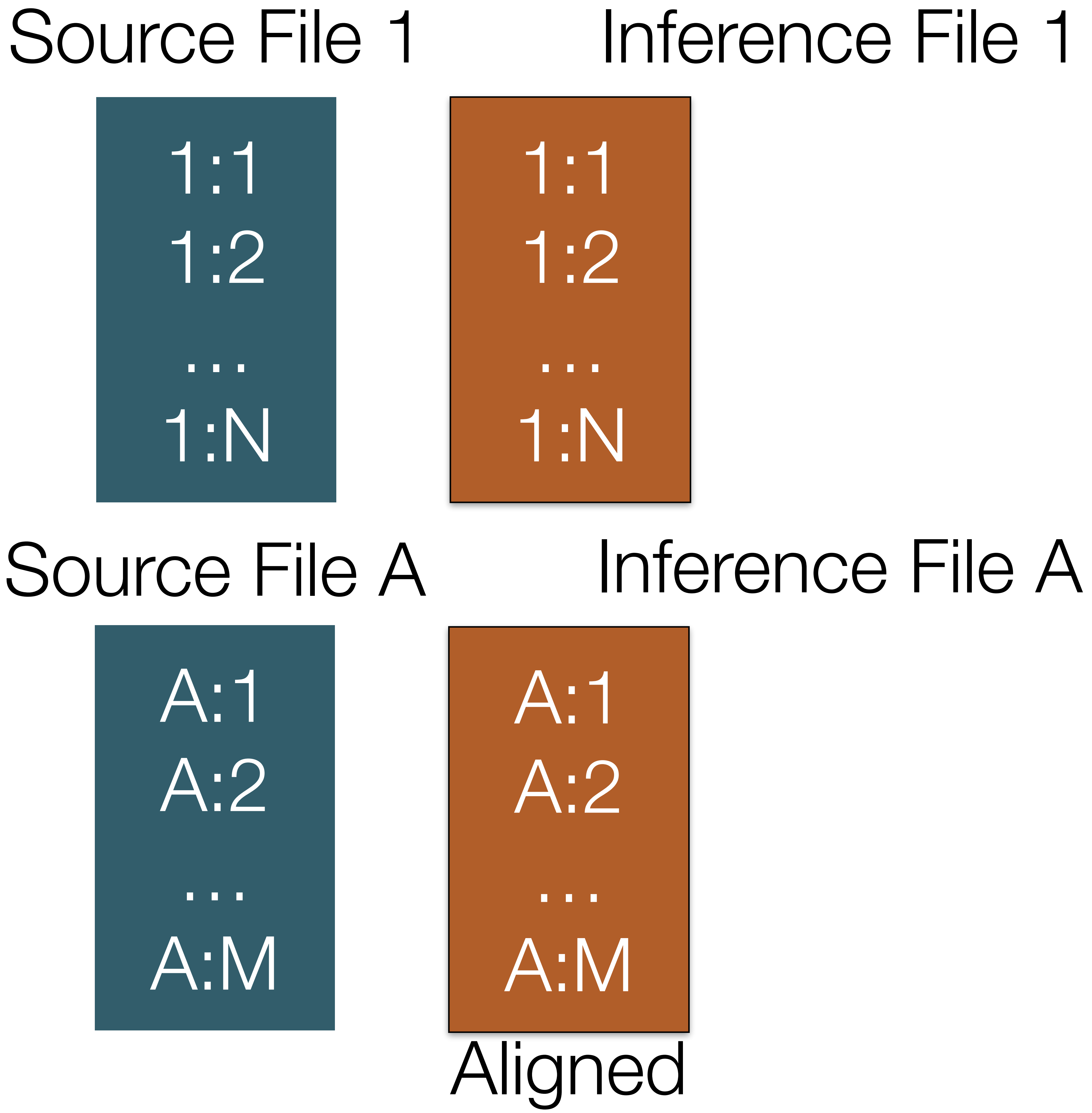

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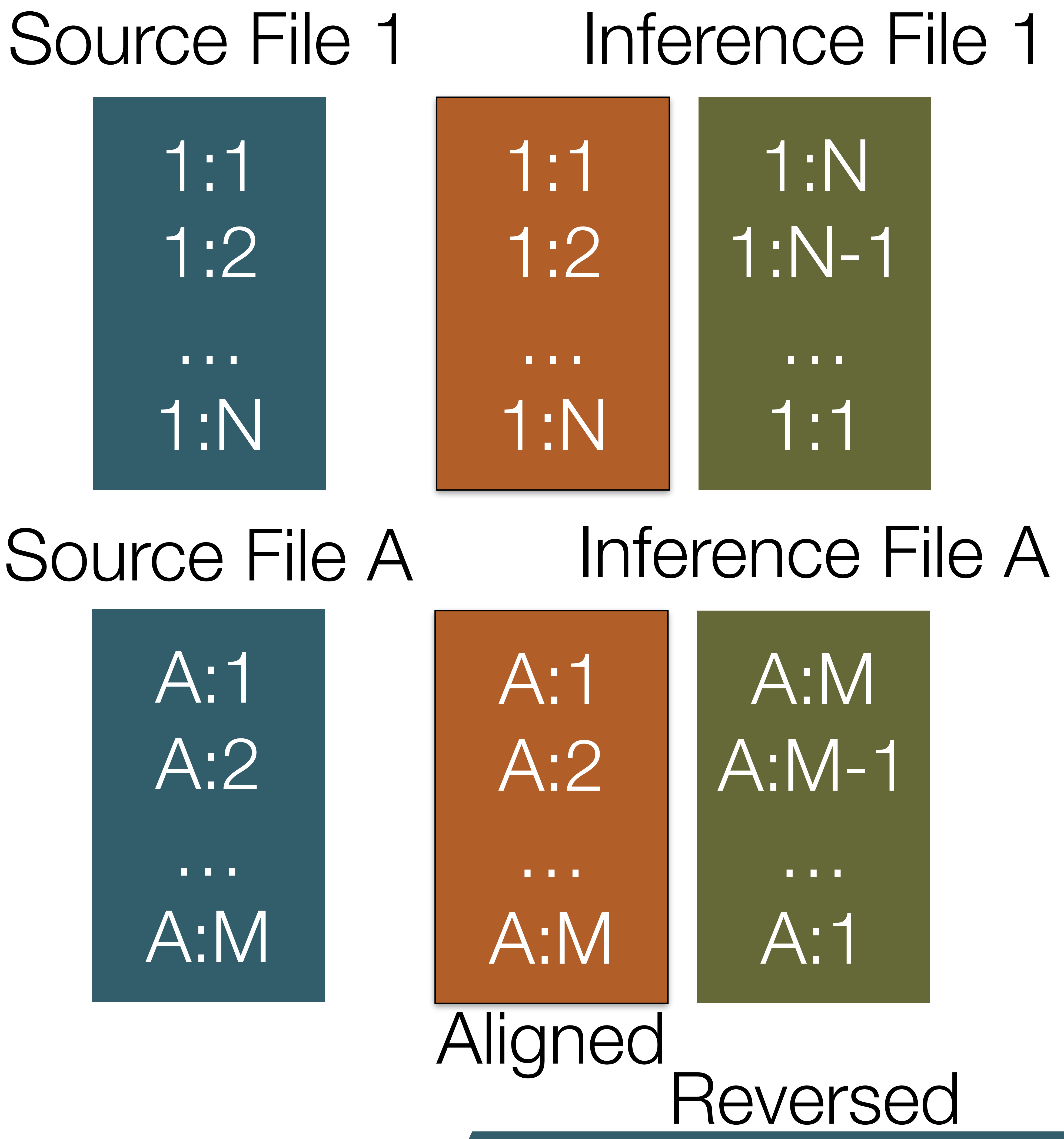

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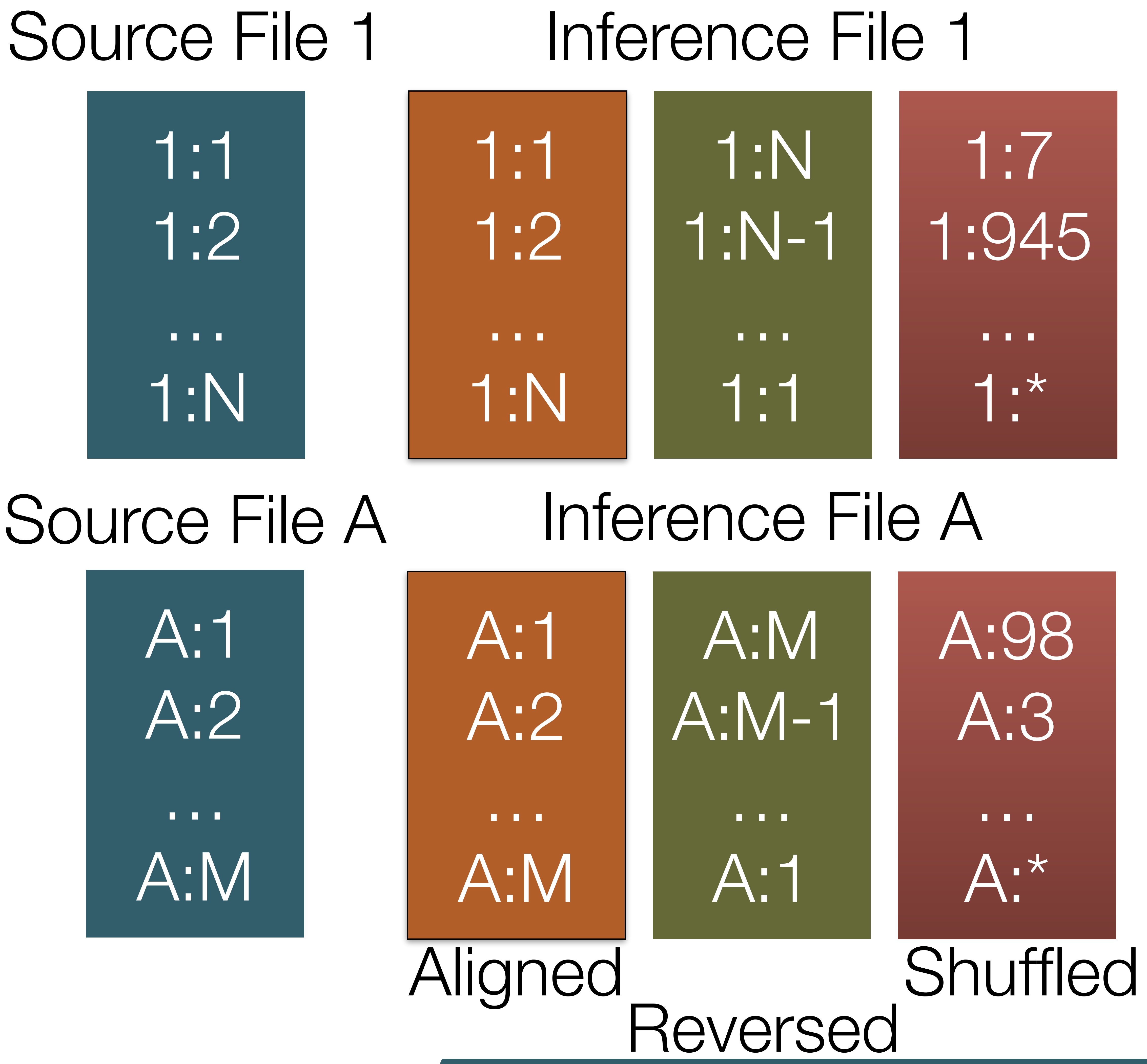

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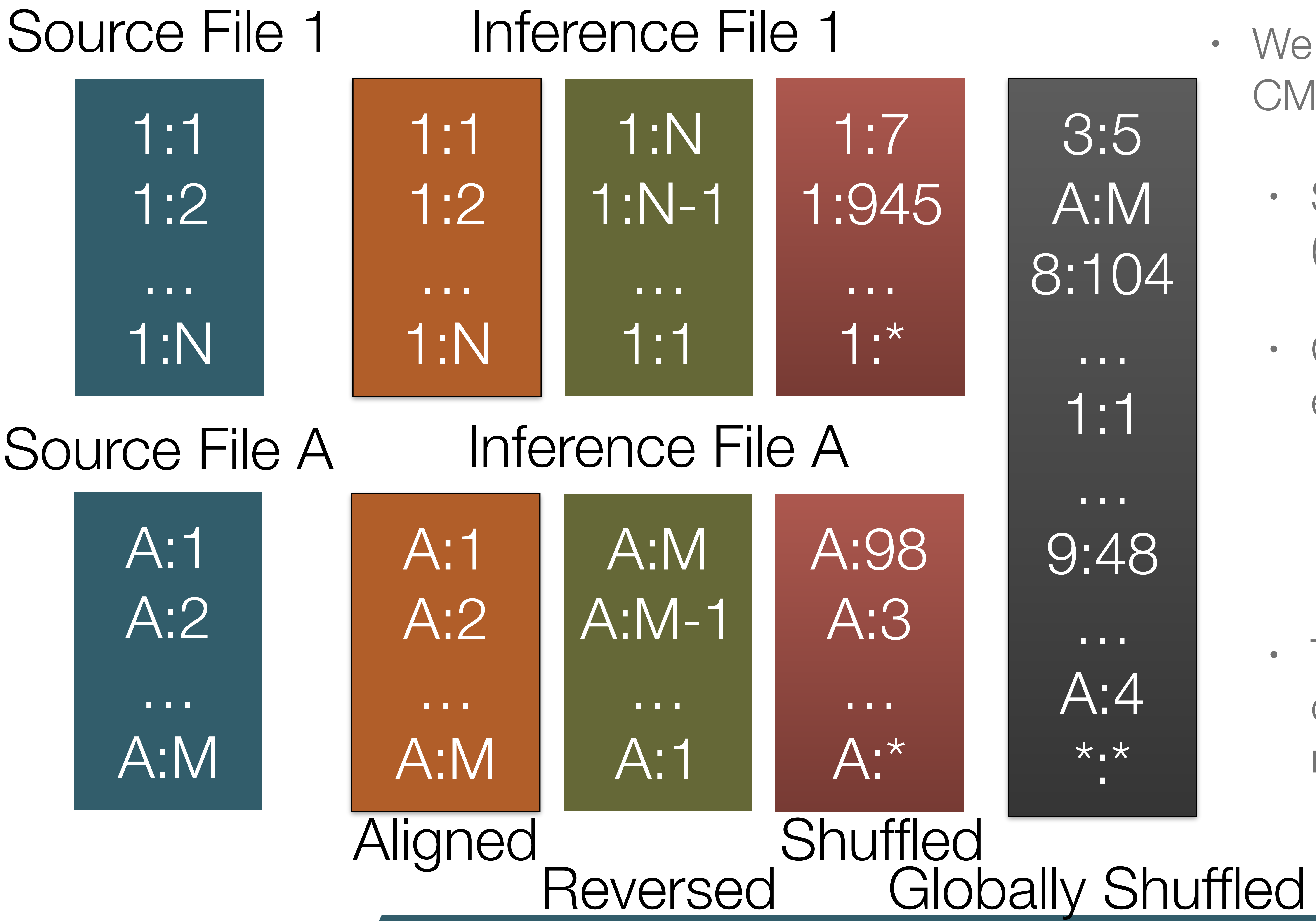

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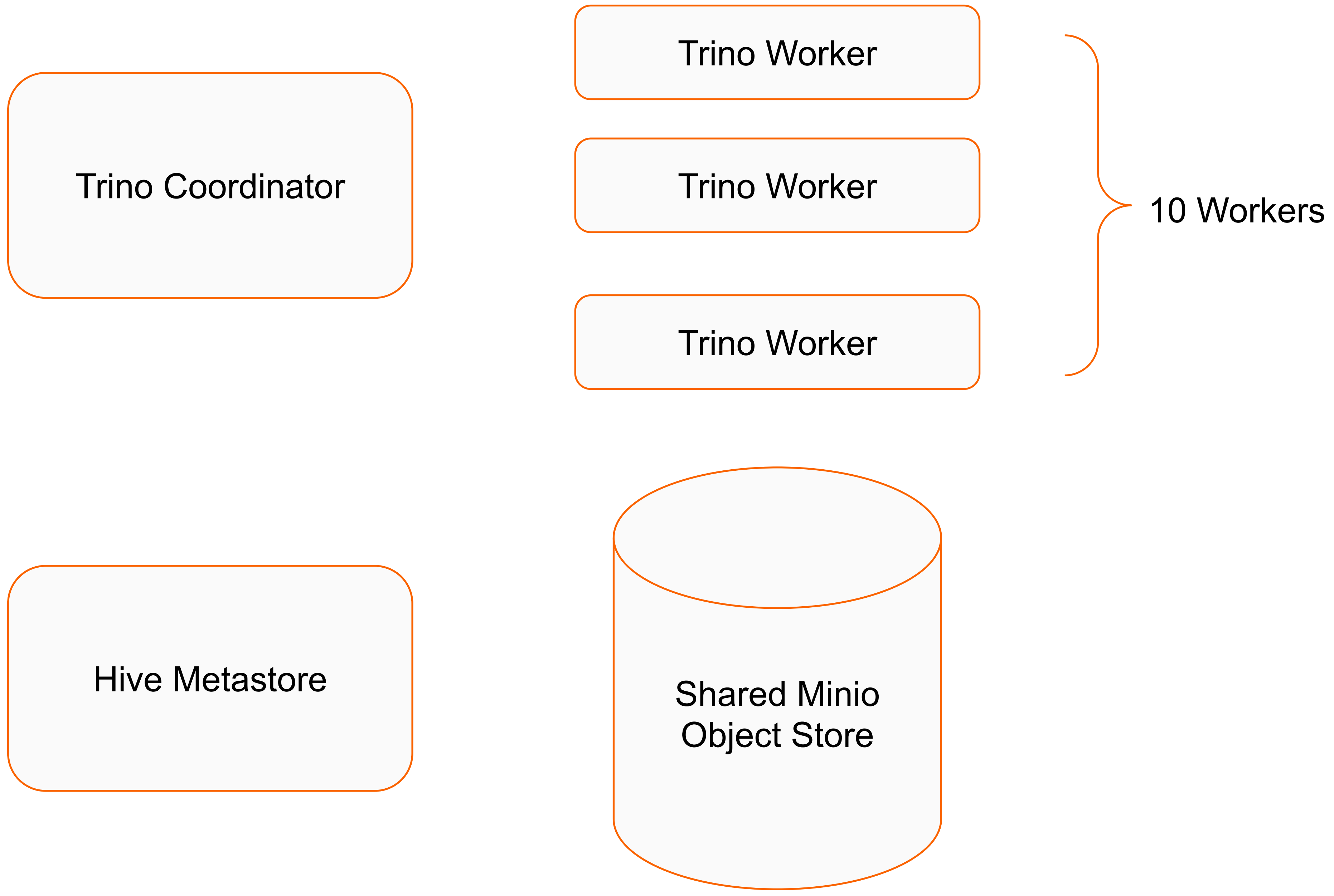
Cluster Configuration

See more in Ben's slides:
https://indico.cern.ch/event/1369601/contributions/5883602/

- Heterogeneous Cluster
    - 3 Nodes: Intel Xeon Silver 4212 @ 2.20GHz (22 cores) - 88GB RAM - Ceph on NVME storage
    - 1 Node: Intel Xeon Silver 4210 @ 2.20GHz (39 cores) - 100GB RAM - Ceph on NVME storage
- Shared resource
    - 10 Workers for Trino on Cluster

Exploratory Environment at FNAL

- Deployed in FNAL OpenShift cluster
- Shared Mino Object Store



Small Dataset Join Benchmark

```
CREATE TABLE single_top_s_chan_join
WITH (
  format = 'PARQUET',
  external_location = 's3a://servicex/nanotest/parquet/AGC/single_top_s_chan/join_out/'
)
AS
  SELECT single_top_s_chan.run, single_top_s_chan.event, single_top_s_chan.luminosityBlock,
    Electron_pt,
    Electron_eta,
    Electron_phi,
    Electron_cutBased,
    Electron_ip3d,
    Electron_sip3d,
    Electron_mass,
    Electron_pfRelIso03_all,
    Electron_pfRelIso03_chg,
    Muon_pt,
    Muon_eta,
    Muon_phi,
    Muon_mass,
    Muon_tightId,
    Muon_ip3d,
    Muon_sip3d,
    Muon_pfRelIso04_all,
    Jet_mass,
    Jet_pt,
    Jet_eta,
    Jet_phi,
    Jet_jetId,
    Jet_btagCSVV2,
    Jet_btagDeepFlavB,
    Jet_btagDeepFlavCvB,
    Jet_btagDeepFlavCvL,
    Jet_btagDeepFlavQG,
    Jet_chEmEF,
    Jet_chHEF,
    Jet_muEF,
    Jet_neEmEF,
    Jet_neHEF
    Jet_puIdDisc,
    Jet_qgl,
    Jet_rawFactor,
    Jet_bRegCorr,
    Jet_bRegRes,
    Jet_electronIdx1,
    Jet_electronIdx2,
    Jet_muonIdx1,
    Jet_muonIdx2,
    GNN_p1, GNN_p2, GNN_p3, GNN_p4
  FROM single_top_s_chan
  JOIN single_top_s_chan_infer ON
    single_top_s_chan.run = single_top_s_chan_infer.run AND
    single_top_s_chan.luminosityBlock = single_top_s_chan_infer.luminosityBlock AND
    single_top_s_chan.event = single_top_s_chan_infer.event;
```

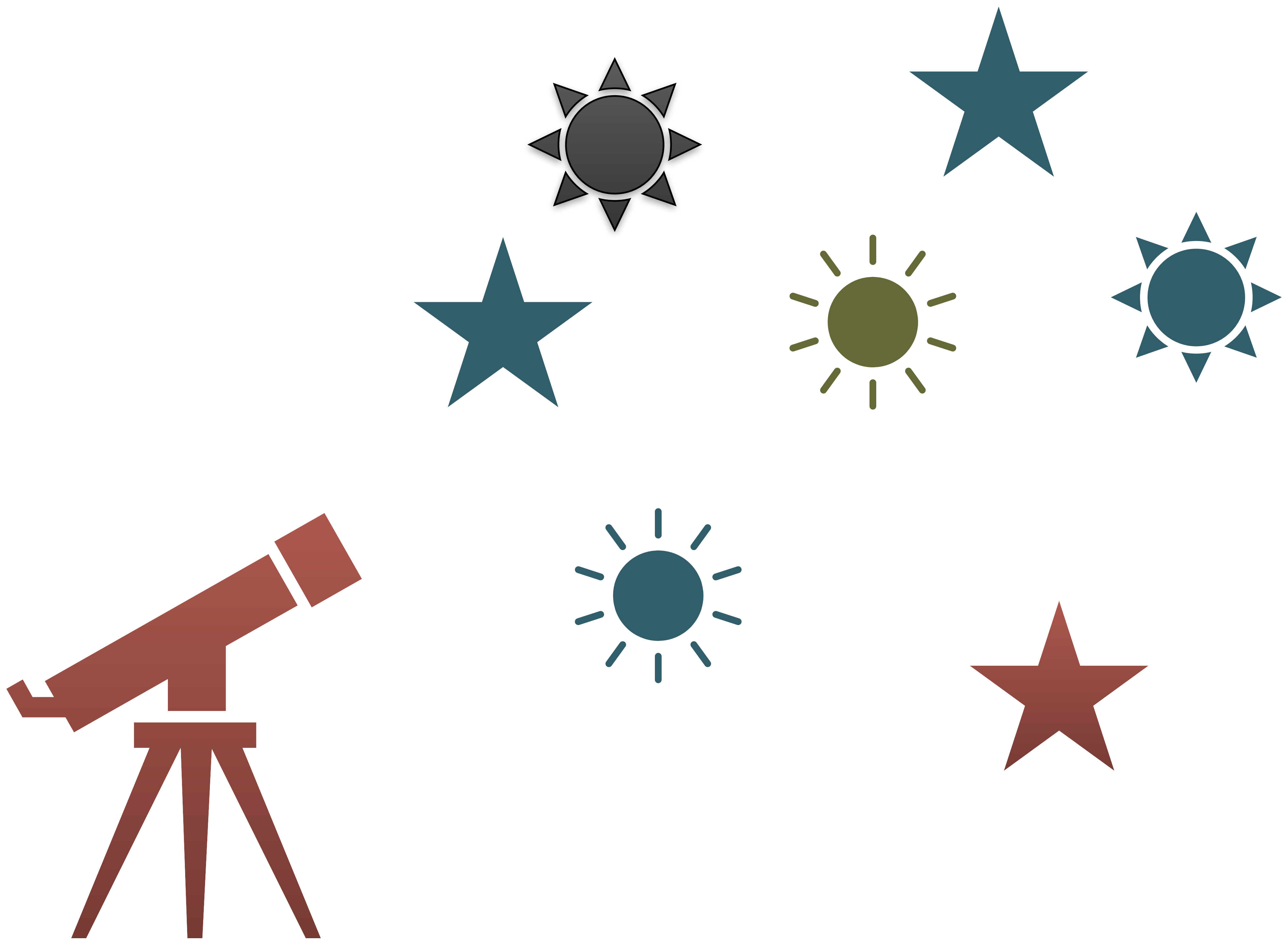
- Dataset with 2.8M events (rows), ragged primitive data for most columns (3.7GB source + 93MB inference)
- Encouraging result: seemingly **invariant* to permutations** being joined

2.2M events/s

```
single_top_s_chan_infer
    Query 20240927_183428_00028_au69m, FINISHED, 11 nodes
    Splits: 862 total, 862 done (100.00%)
    16.64 [34.4M rows, 1.48GB] [2.07M rows/s, 91.3MB/s]

    trino:servicex> select count(*) from single_top_s_chan_join;
      _col0
    ---------
     2867199
    (1 row)

single_top_s_chan_infer_reversed
    Query 20240927_184139_00033_au69m, FINISHED, 11 nodes
    Splits: 862 total, 862 done (100.00%)
    14.54 [34.4M rows, 1.48GB] [2.37M rows/s, 104MB/s]

    trino:servicex> select count(*) from single_top_s_chan_join;
      _col0
    ---------
     2867199
    (1 row)

single_top_s_chan_infer_intrafileshuffle
    Query 20240927_184318_00036_au69m, FINISHED, 11 nodes
    Splits: 862 total, 862 done (100.00%)
    15.49 [34.4M rows, 1.5GB] [2.22M rows/s, 98.9MB/s]

    select count(*) from single_top_s_chan_join;
      _col0
    ---------
     2867199
    (1 row)

single_top_s_chan_infer_globalshuffle
    Query 20240927_184518_00039_au69m, FINISHED, 11 nodes
    Splits: 859 total, 859 done (100.00%)
    15.00 [34.4M rows, 1.5GB] [2.29M rows/s, 102MB/s]

    select count(*) from single_top_s_chan_join;
      _col0
    ---------
     2867199
```

* stat fluctuations, warm-caching to be eliminated as sources of differences in high-stat testing

“All that glitters is not gold”



Large Dataset Join Benchmark

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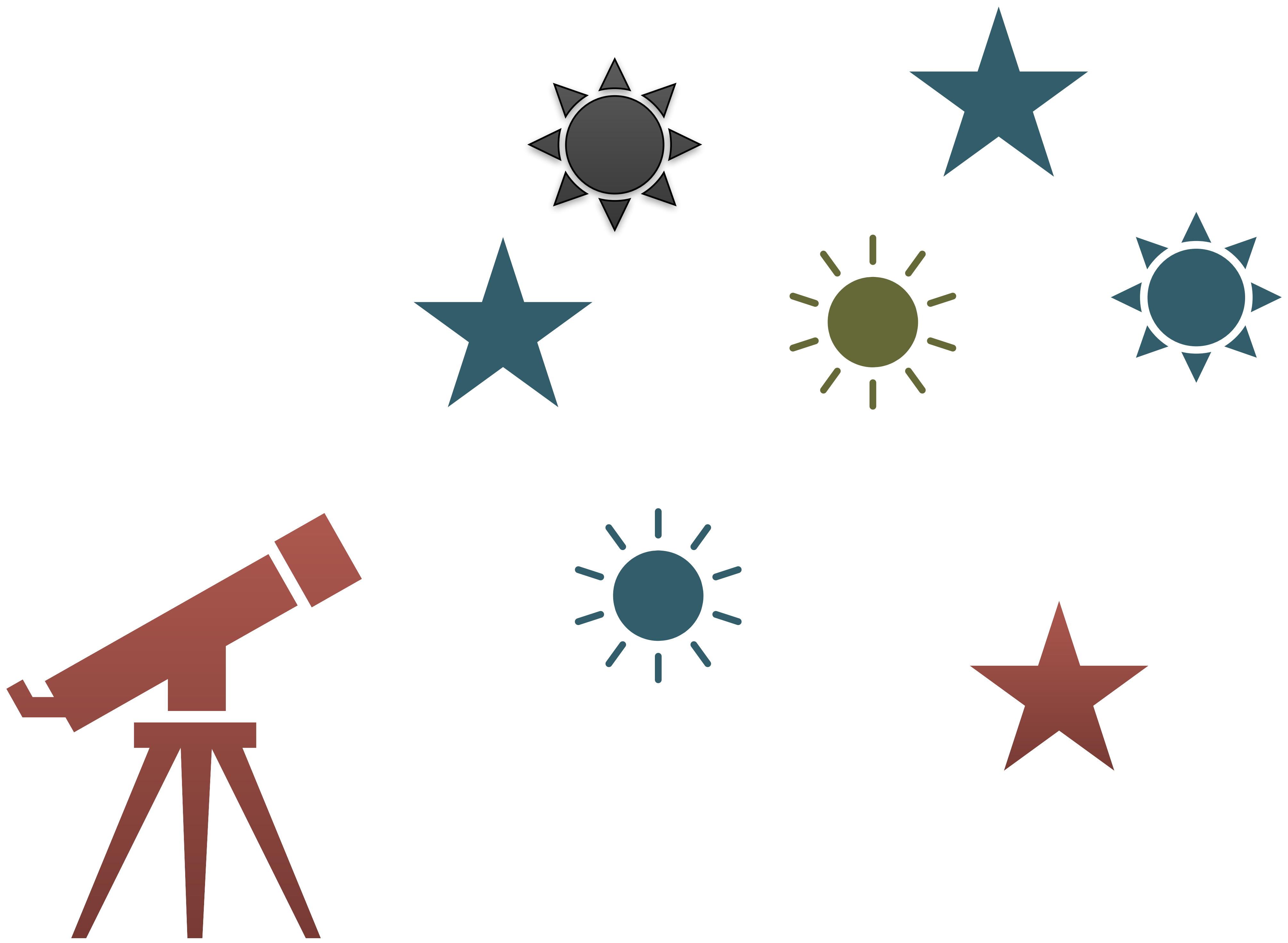

Large Dataset Join Benchmark

- Largest dataset of 500GB (ttbar) crashed trino deployment*

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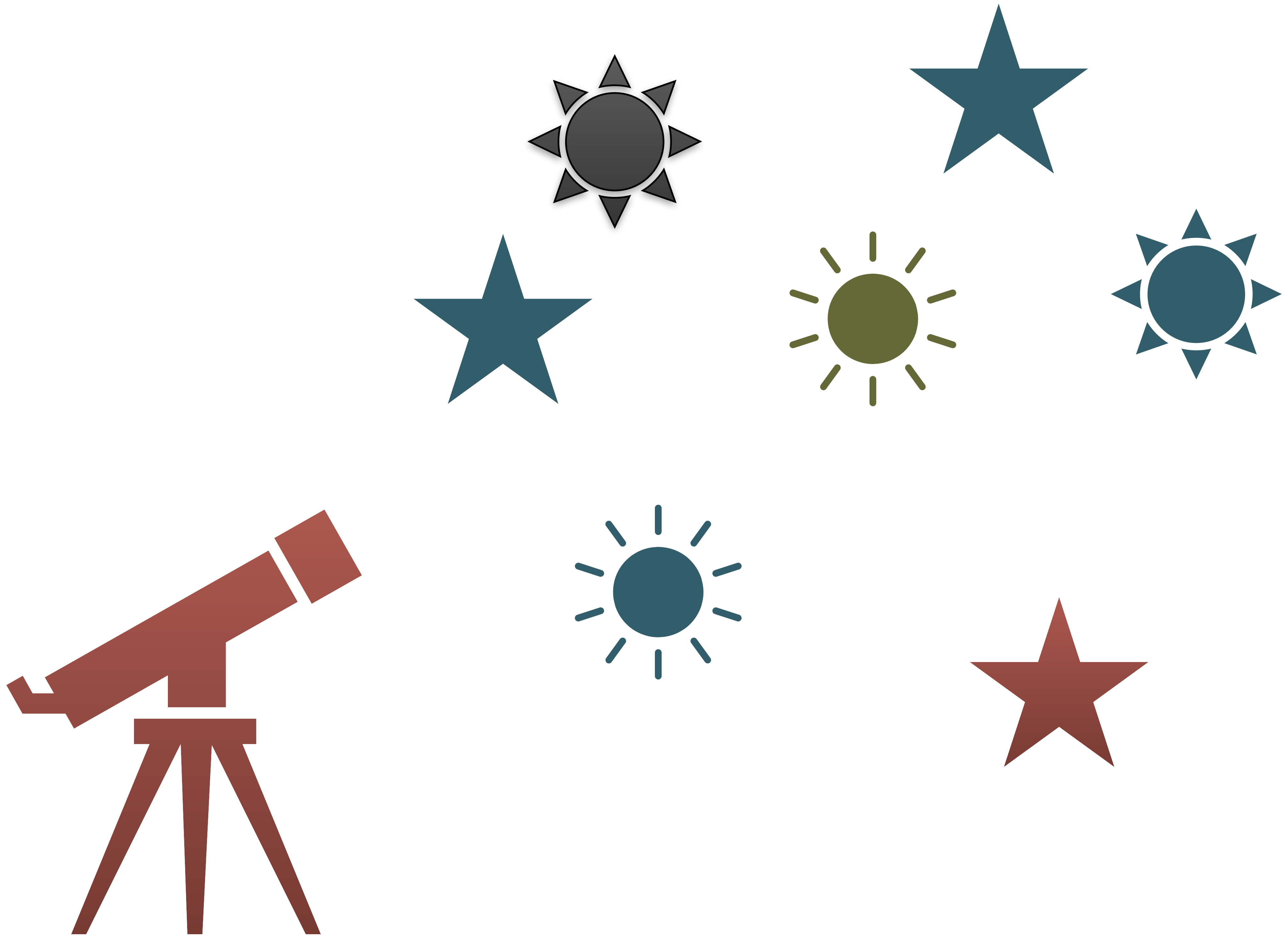

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* Incorrect resource limits set for trino in OKD

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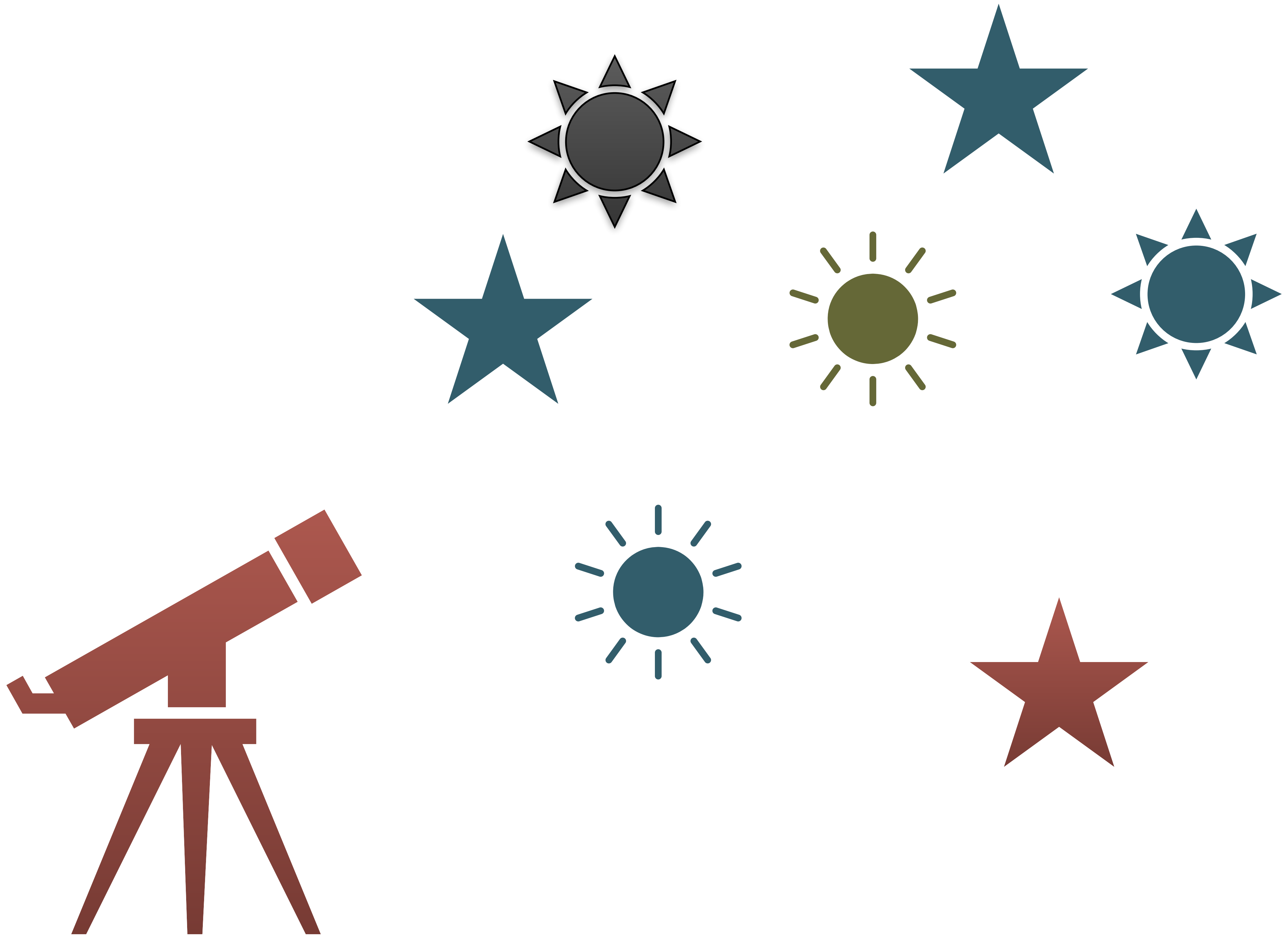

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- Largest dataset of 500GB (ttbar) crashed trino deployment*

- May indicate that partitioning the joins into dask-task sized elements will be a necessity to use trino as our distributed SQL engine (already a desirable element, as described later)

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Benchmark of “analysis” read-speed

Stats computed over 7 runs, 5 loops (timeit)

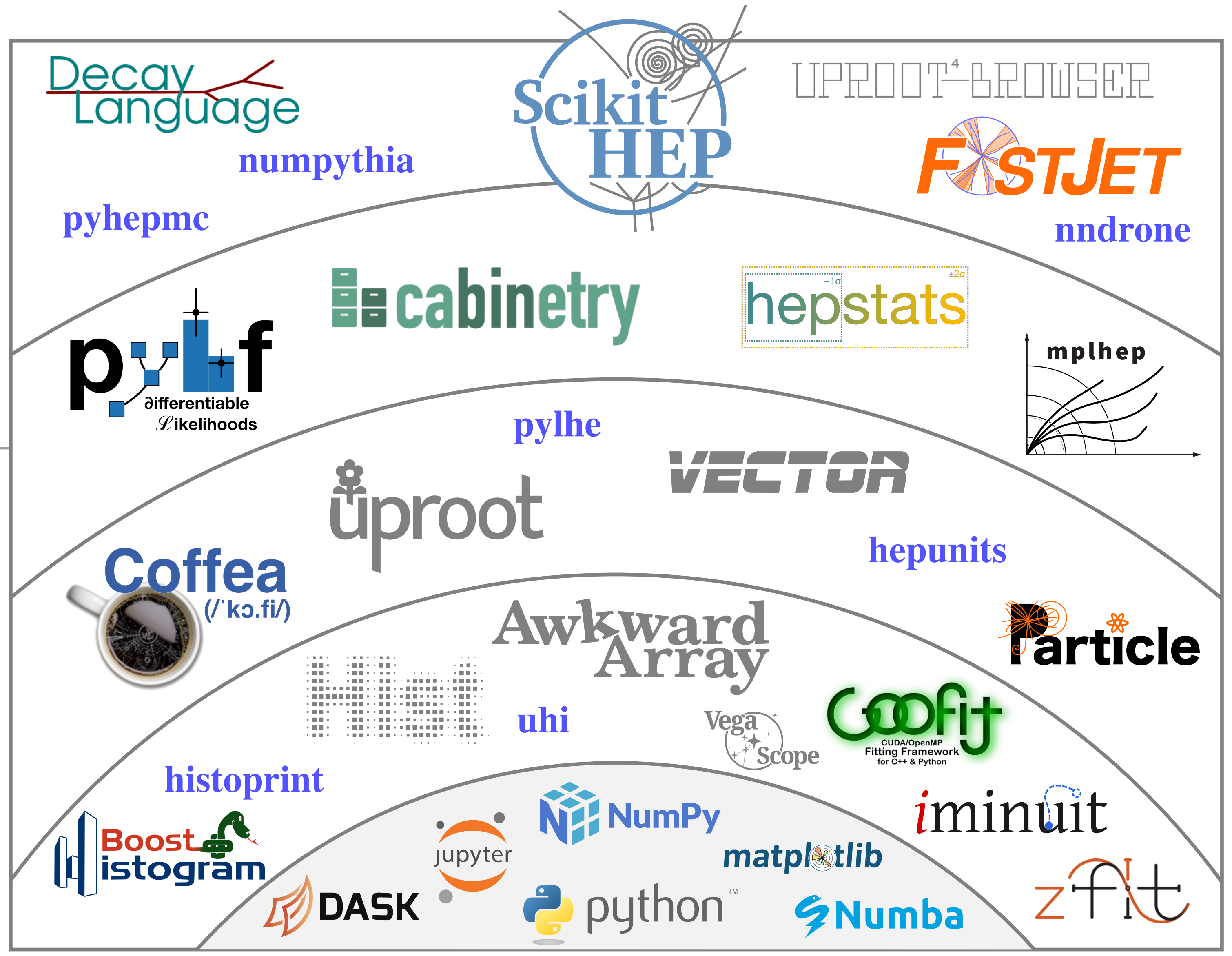
1,334,428 events processed

Benchmark Output Analysis Formats

Test of a simple pseudo-analysis running on various root TTree and parquet files, in various compression schemes

Format	Source	How Made	Compression	Time
ROOT	AGC	N/A	ZLIB:1	11.7 s ± 389 ms
ROOT	converted	root hadd	LZMA:9	11.9 s ± 551 ms
ROOT	converted	root hadd	ZSTD:5	10.9 s ± 477 ms
Parquet	converted	hepconvert	ZSTD:5	4.73 s ± 61 ms
Parquet	joined	trino	GZIP	3.99 s ± 129 ms

Coffea analysis



- coffea brings together individual scikit-hep elements needed for a full analysis, and provides **schema-application, corrections, scaleout**(-patterns)
  - and often the first place something is prototyped and tested before being spun out into it's own package
- Tightly integrated with dask:
  - User's analysis code is broadcast over datasets to create **task graphs**
  - Typetracer setup per dataset records operations (lazy, no data executed on)
  - Task graphs are distributed to compute resources to execute
  - Results returned to user's client (histograms, small arrays, locations of output root/parquet files, …)
- Task graphs are key: allow programmatic optimization of analysis, understanding **necessary inputs** as mapped to **requested outputs**

Joins R&D (End-to-End Processing with dask)

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Source A
(Format A)

Source B
(Format B)

Source C?
(Format C)

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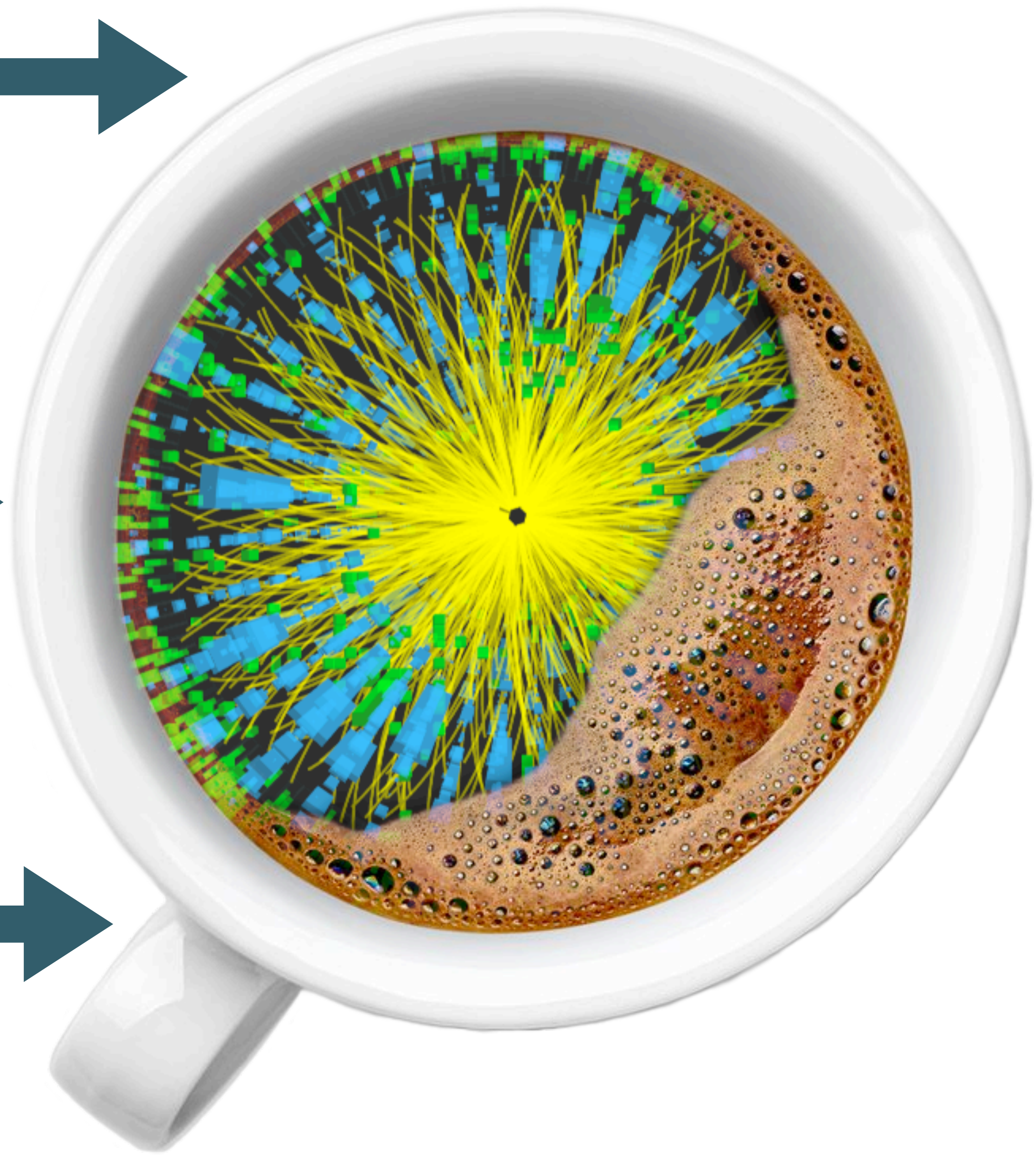

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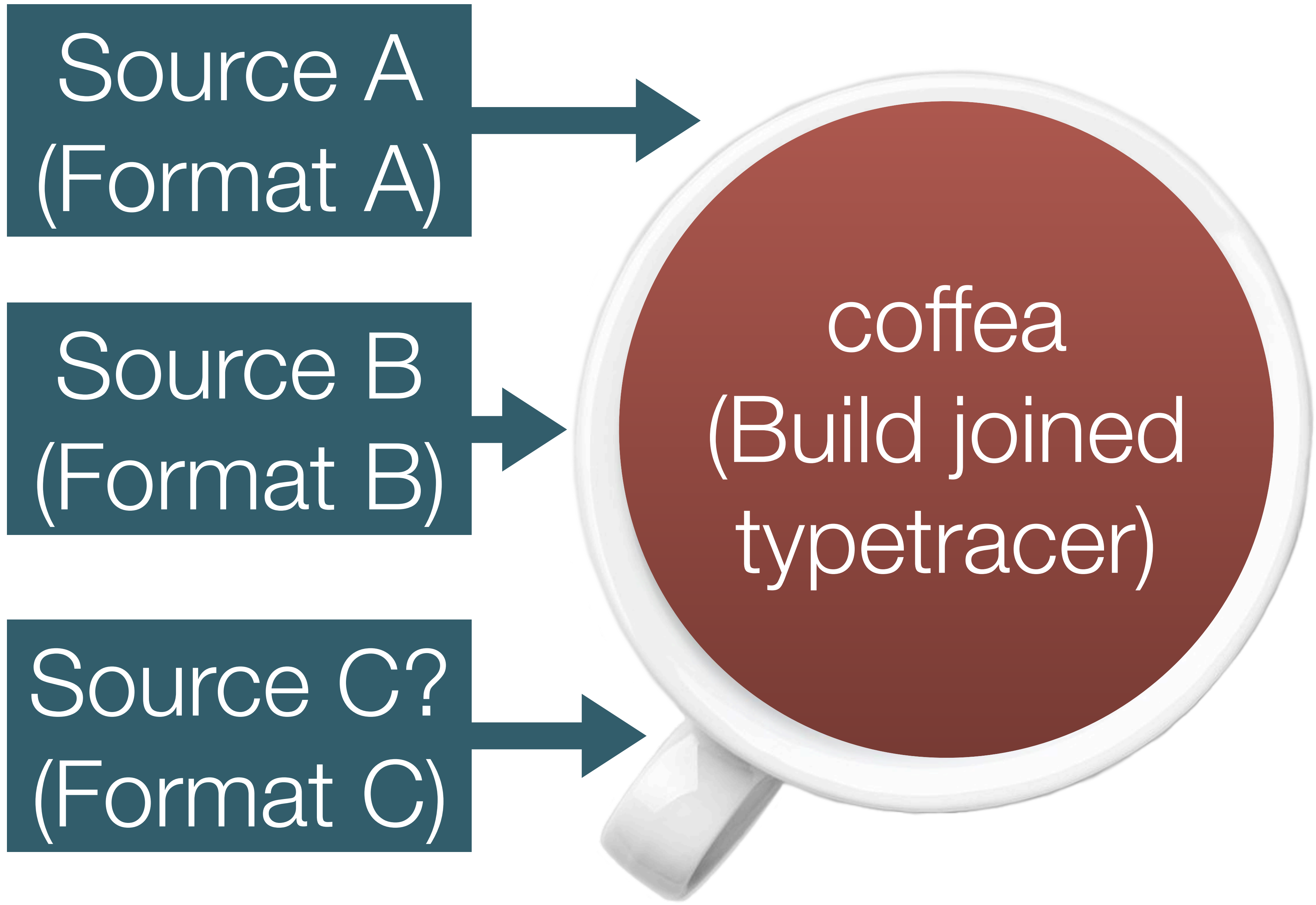

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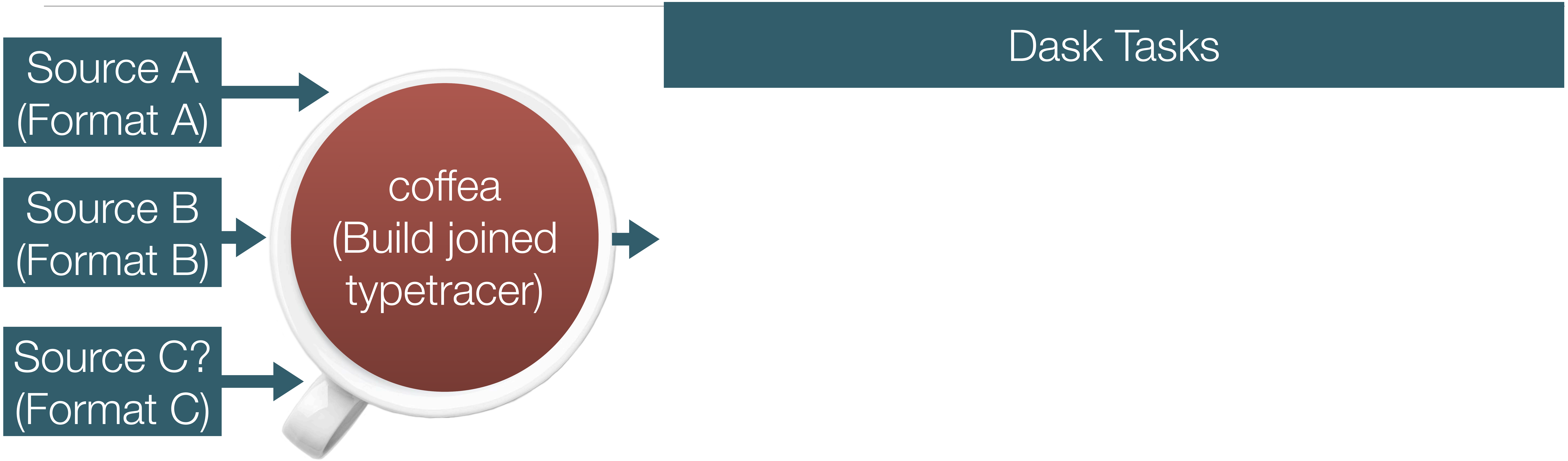

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Dask Tasks

Dataset 1, Chunk 1 (N events)

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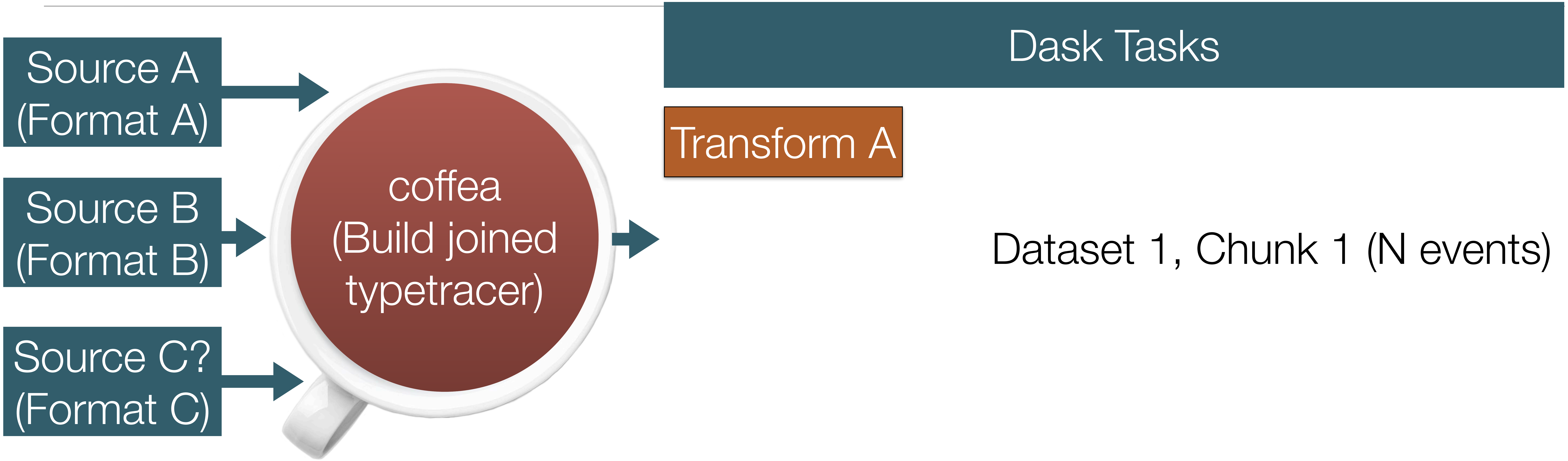

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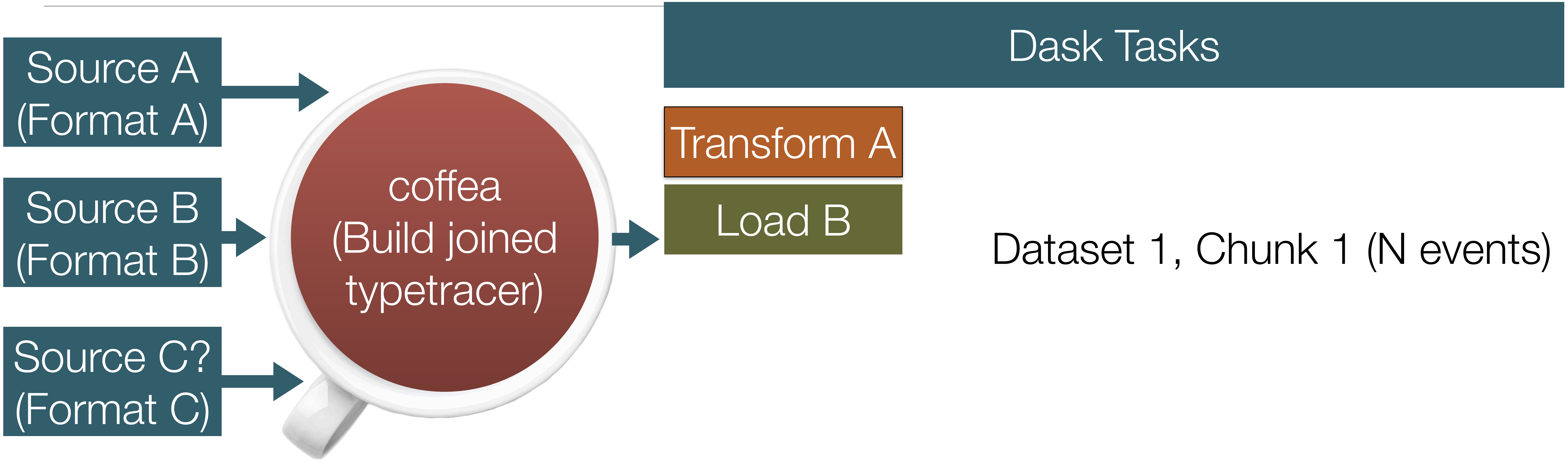

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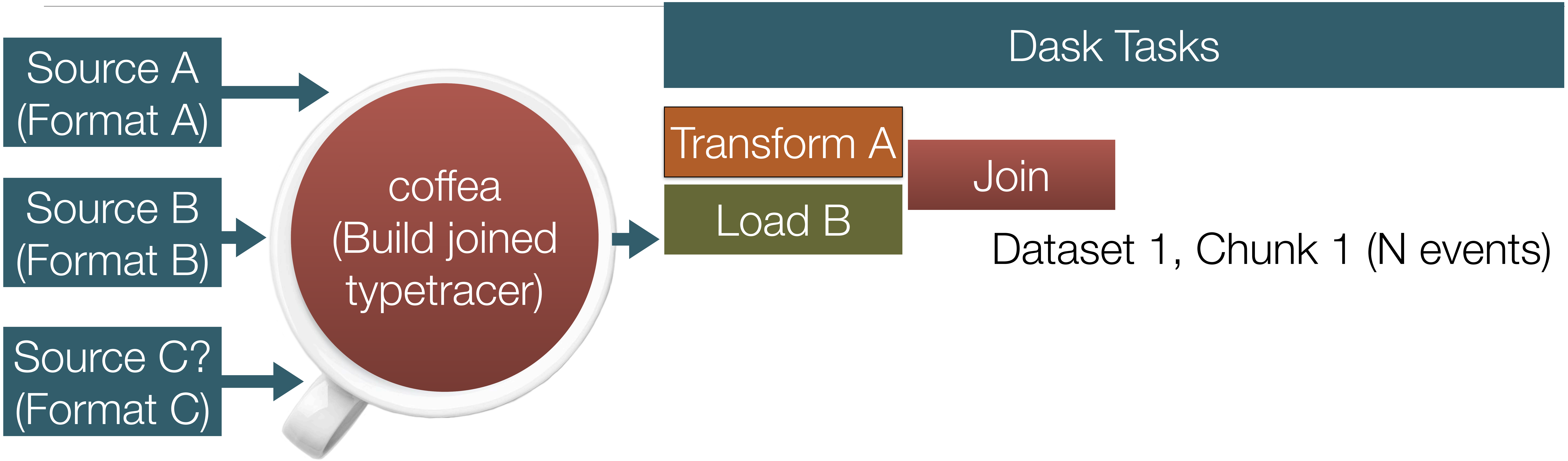

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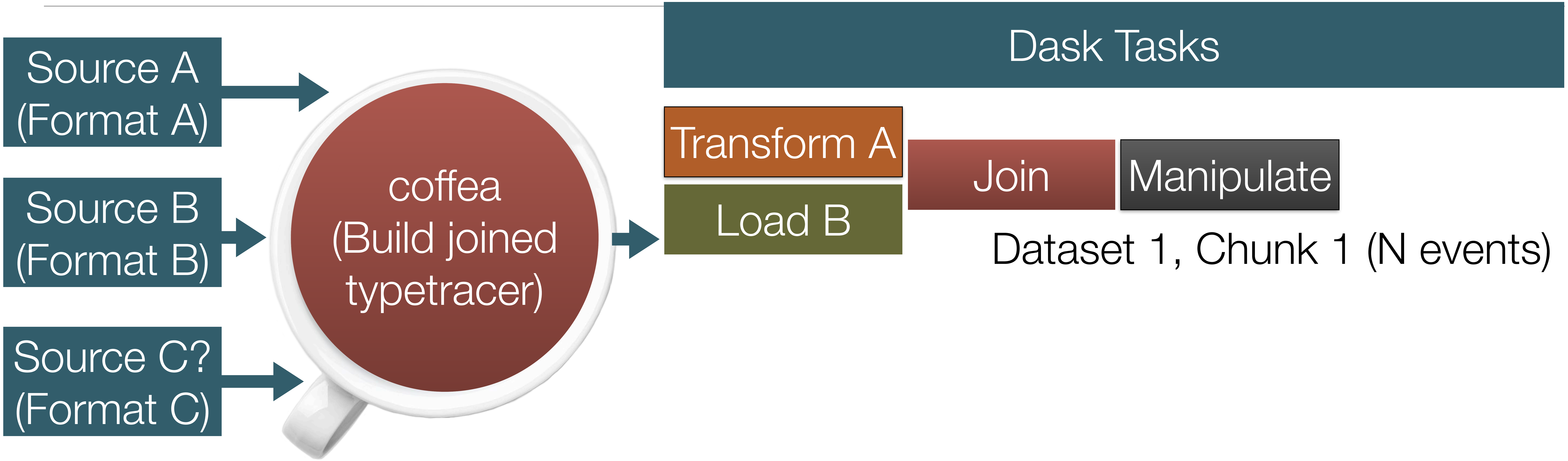

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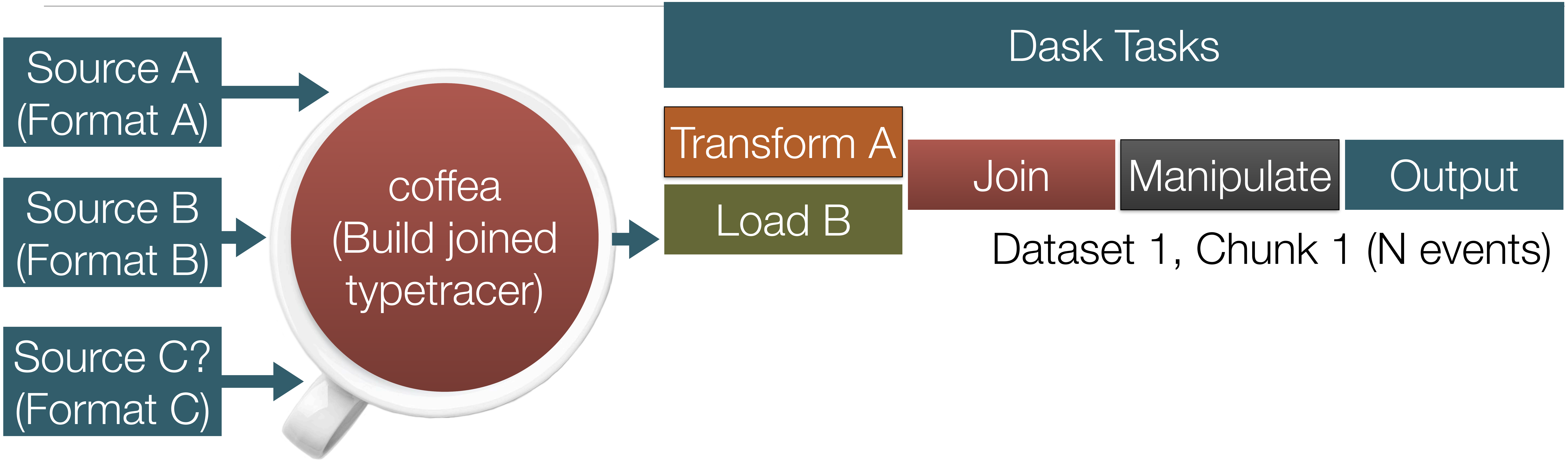

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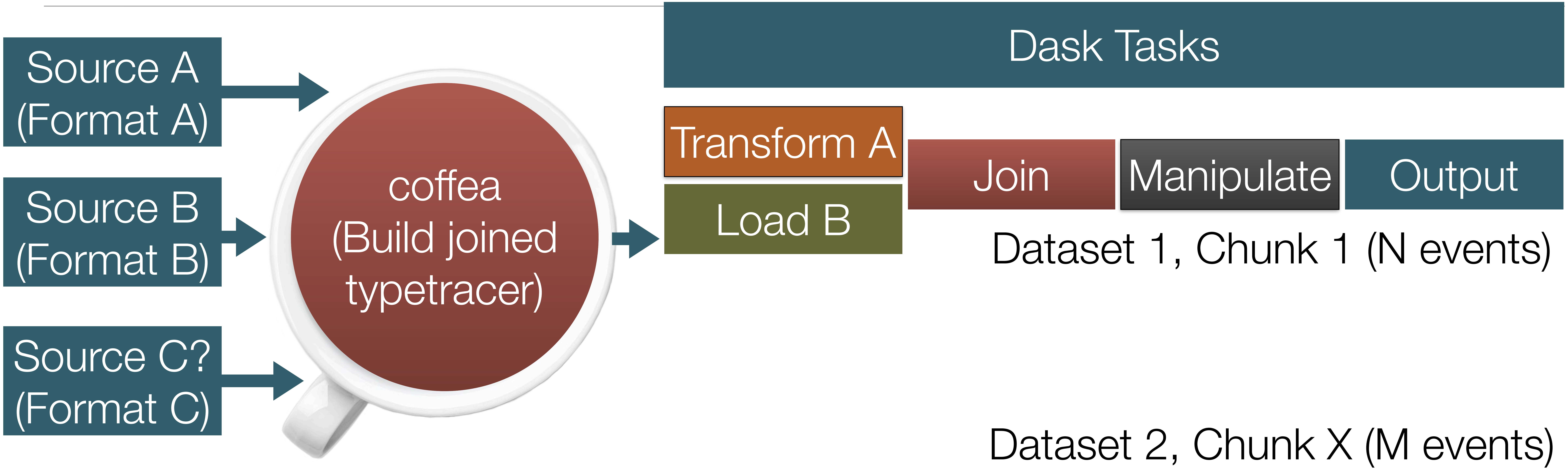

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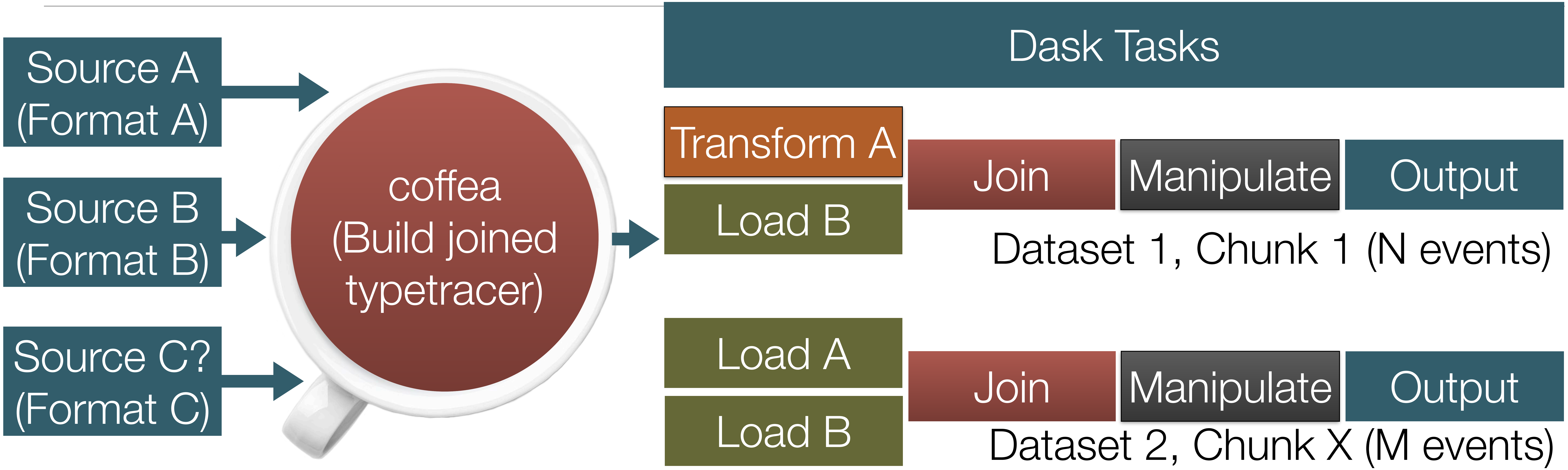

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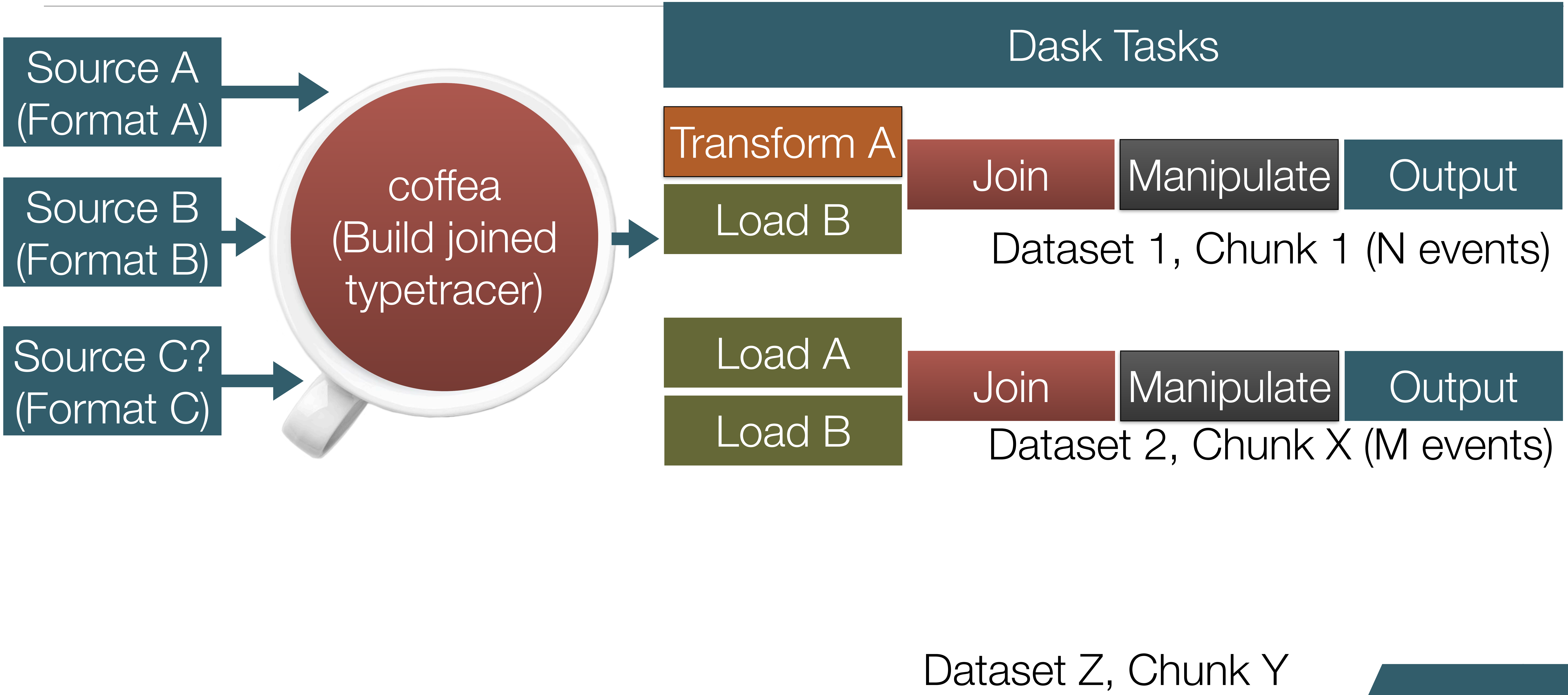

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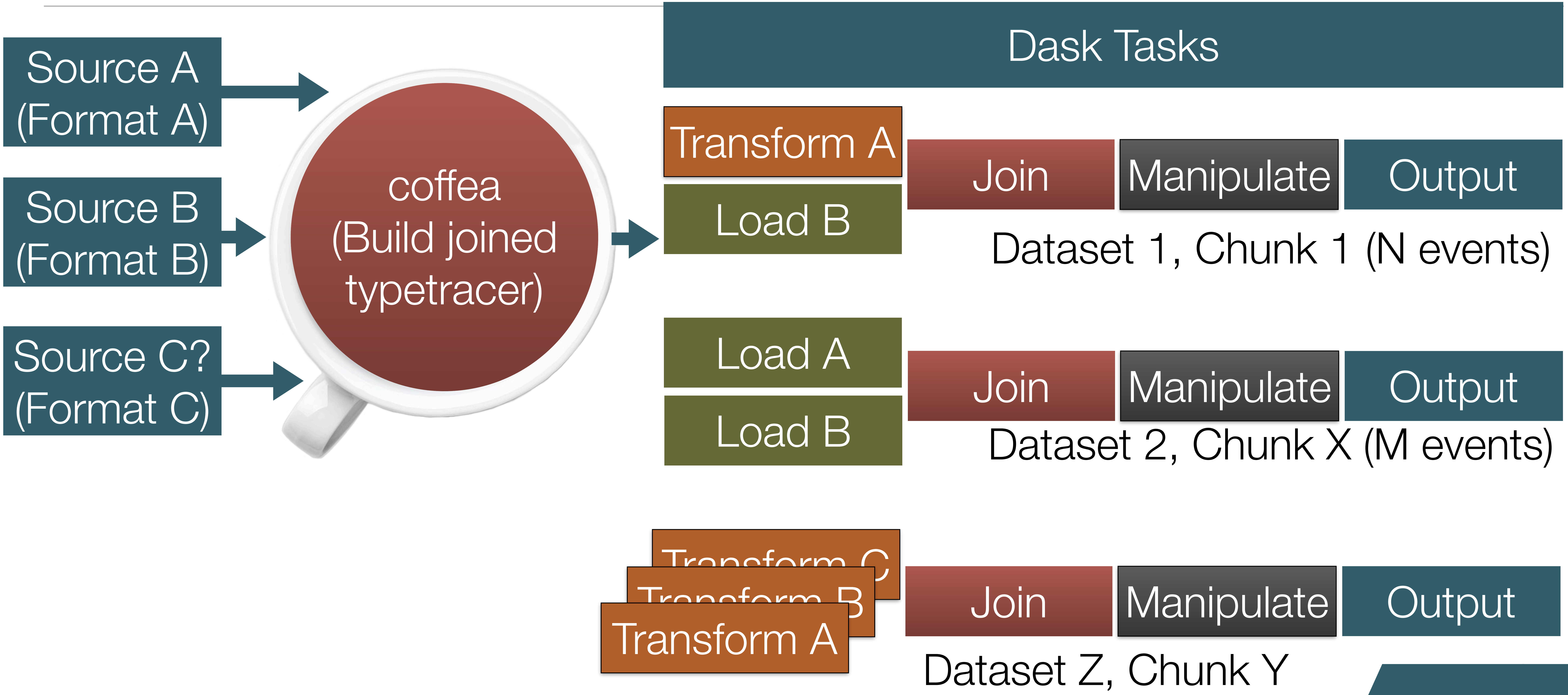

Ongoing and Future Developments

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- Baseline and Optional Targets of US CMS HL-LHC R&D Program (2024) in collaboration with IRIS-HEP
  - Building Typetracer for pseudo-joined data
  - Generation of ServiceX conversion tasks
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    - Native Ceph Object Store usage (Currently object -> file -> object)
- Future developments within US CMS and IRIS-HEP
    - Kafka integration for streaming output
    - RNTuple support in trino

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  - Adding ParticleFlow candidates for reclustering
  - Full set of ML taggers
- Caching Experiment-wide objects (systematic variations, CMS ParticleTransformer, FlashSim?)
  - Versioning potential
- Caching Analysis-specific non-ML (derived quantities, systematic variations) and ML results (event, object classifiers)

Funding Acknowledgements

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BACKUP

US CMS Software and Computing - HL-LHC R&D (WBS4)

2 Grand Challenges for HL-LHC Computing and Software

In order to effectively focus and structure the U.S. CMS R&D efforts, we organize the innovation, research, and development needs for HL-LHC computing into the four *Grand Challenges* that encompass the advances needed for HL-LHC computing to succeed:

(1) **Modernizing Physics Software and Improving Algorithms**

Exploit novel algorithms, including ML/AI, reduce algorithmic complexity, increase computational intensity, and provide core software infrastructure to enable effective use of modern hardware and accelerators. The work is organized in the following work packages:

- Core Software Framework and Software Portability
- Establish Performance Metric and Performance Baseline for Physics Software
- U.S. Contributions to the Charged Particle Tracking Software
- U.S. Contributions to Software for High Granularity Calorimeter
- U.S. Contributions to CMS Advanced Algorithms Work

(2) **Building Infrastructure for Exabyte-Scale Datasets**

Build infrastructure to archive, store, transfer, and provide access to exabyte-scale datasets. Explore data lakes and custodial storage: establish a technology and cost model for custodial/archival storage facilities which manages operations costs, and optimizes hardware costs. Orchestrate computational services and data access, provide intelligent

FriendTrees

- Traditional ROOT workflows have some functionality that can alleviate the data duplication issues, via the FriendTree mechanism
  - Supports joining entry-by-entry events in two separate (groups of) files
  - Can accommodate some situations with non-aligned (out-of-order) joins with BuildIndex (major + minor keys, i.e. run + event)
    - https://root.cern/doc/master/classTTree.html#a3f6b5bb591ff7a5bd0b06eea6c12b998
    -

O1-mini's description of TTrees, Parquet, RNTuple

2. Technology Descriptions

a. ROOT TTrees

ROOT TTrees are a fundamental data structure within the ROOT framework, widely used in HEP for storing and analyzing large datasets.

- Structure: TTrees store data in a hierarchical, tree-like structure with branches representing different variables (columns).
- Features:
  - Custom Compression: Supports various compression algorithms tailored for HEP data.
  - Provenance Tracking: Maintains metadata and provenance information essential for reproducible research.
  - Integration with ROOT: Seamless integration with ROOT's data analysis tools and C++/Python interfaces.

b. Apache Parquet

Apache Parquet is an open-source, columnar storage format optimized for performance and interoperability across different data processing frameworks.

- Structure: Stores data in column chunks, enabling efficient compression and encoding schemes.
- Features:
  - Language Agnostic: Supports multiple programming languages (e.g., Java, C++, Python).
  - Wide Ecosystem Support: Integrates with big data tools like Apache Spark, Hive, and Pandas.
  - Efficient Compression: Utilizes advanced compression techniques to reduce storage footprint.

c. ROOT RNTuple

ROOT RNTuple is a newer addition to the ROOT framework, designed to address some limitations of TTrees and to provide a modern, efficient, and scalable storage solution.

- Structure: Similar to TTrees but optimized for better performance and scalability.
- Features:
  - Asynchronous I/O: Enhances read/write performance by supporting non-blocking operations.
  - Better Parallelism: Designed to leverage multi-threading and distributed computing environments.
  - Improved Data Model: Offers a more flexible and robust data schema compared to TTrees.

Trino Use Cases (as described by o1-mini)

- **Use Cases of Trino**
  - **Interactive Analytics**:
    - Ideal for business intelligence (BI) tools and dashboards that require **real-time or near-real-time query responses**.
  - **Data Lake Querying**:
    - Facilitates querying large-scale data lakes stored in platforms like Amazon S3, Google Cloud Storage, or HDFS without the need for data movement.
  - **Federated Data Access**:
    - Enables organizations to query and analyze data spread across multiple heterogeneous systems from a single interface.
  - **ETL and Data Transformation**:
    - Can be used in Extract, Transform, Load (ETL) processes to transform and move data between systems efficiently.

Model o1-mini says…

Trino in the Context of Data Storage Technologies

Given your previous interest in **ROOT TTrees**, **Apache Parquet**, and **ROOT RNTuple**, it's valuable to understand how Trino interacts with these and other columnar storage formats:

- **Apache Parquet**:
  - **Integration**: Trino has robust support for querying Parquet files, allowing users to perform SQL queries directly on Parquet-formatted data stored in data lakes or distributed file systems.
  - **Performance**: Leveraging Parquet's columnar storage, Trino can efficiently read only the necessary columns, reducing I/O and speeding up query execution.
- **ROOT TTrees and RNTuple**:
  - **Integration**: While Trino is primarily designed to work with widely-adopted data formats like Parquet, CSV, JSON, and various databases, integrating with specialized formats like ROOT TTrees or RNTuple may require custom connectors or data transformation steps.
  - **Use in HEP**: In High Energy Physics (HEP), where ROOT formats are prevalent, Trino could be used alongside data processing pipelines that convert ROOT data to more Trino-friendly formats for broader analysis and integration with other data sources.