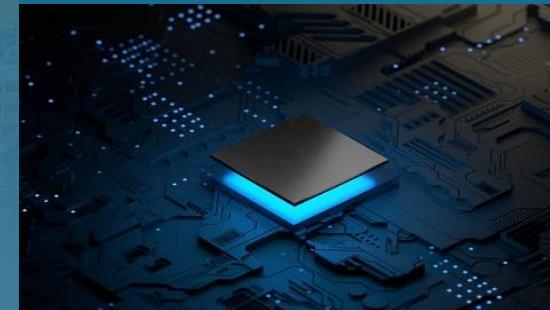




Sandia
National
Laboratories

Sandia Insights – A Data Sciences Architecture and Framework



National Laboratories Information Technology (NLIT) 2022

October 17, 2022



Dr. Patrick Carlson - Sandia National Lab

Dr. Ian Brooks - Cloudera Government



Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

Presenters



Dr. Patrick Carlson

- PhD graduate in Human-Computer Interaction (HCI) from Iowa State University
- Worked at Sandia National Labs as a Data Scientist since 2017
- Leads the Sandia Data Sciences Community of Practice (CoP)
- Interested in the technical aspects of Data Science such as data engineering, programming, analysis, modeling, machine learning, productionization, ml-ops, data-ops, and more



Dr. Ian Brooks

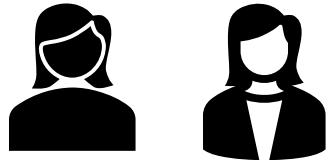
- PhD graduate in Computer Science from the University of North Texas
- Focused on Big Data solutions since 2015
- Previous industry roles include Software Engineer, Data Architect, and Data Scientist
- At Cloudera, he is a Principal Solutions Engineer on the Public Sector team and a Machine Learning SME



Why Sandia Insights



Data Scientists and
Data Engineers



- Rapid access to data
- Robust tooling
- Common environment with libraries preinstalled
- HPC and model training

- Reduce duplication and rework
- Faster turnaround time

Data Governance



- Data security
- Centralized access controls
- Central data catalog management

Leadership



- Data-driven decision making

Vision for Sandia Insights

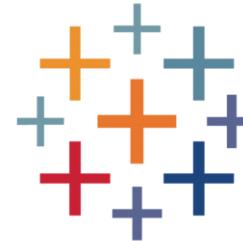


- Empower Data Scientists and Analysts through easy access to vetted enterprise datasets
- Secure and document data through Data Governance and a data catalog
- Productionize and operationalize models, use data-ops and ml-ops practices
- Build out a pipeline and best practices for the entire data-lifecycle
- Focus on people and methods, not specific tools

History of Sandia Insights



- 2015 – Tableau Server
- 2016 – Analytics for Sandia Knowledge (ASK)
 - Custom developed catalog
 - Tableau visualizations and reports
 - Vetted enterprise datasets via Data Central
 - Expertise finder and co-author network
- 2018 – CKAN data catalog
- 2018 – RStudio Connect (previously called Shiny Server)
- 2019 – Cloudera installation
- 2020 – Collibra data catalog



CLOUDERA



Current State

Data Lifecycle



Advanced Analytics Data Lifecycle



Business Analyst



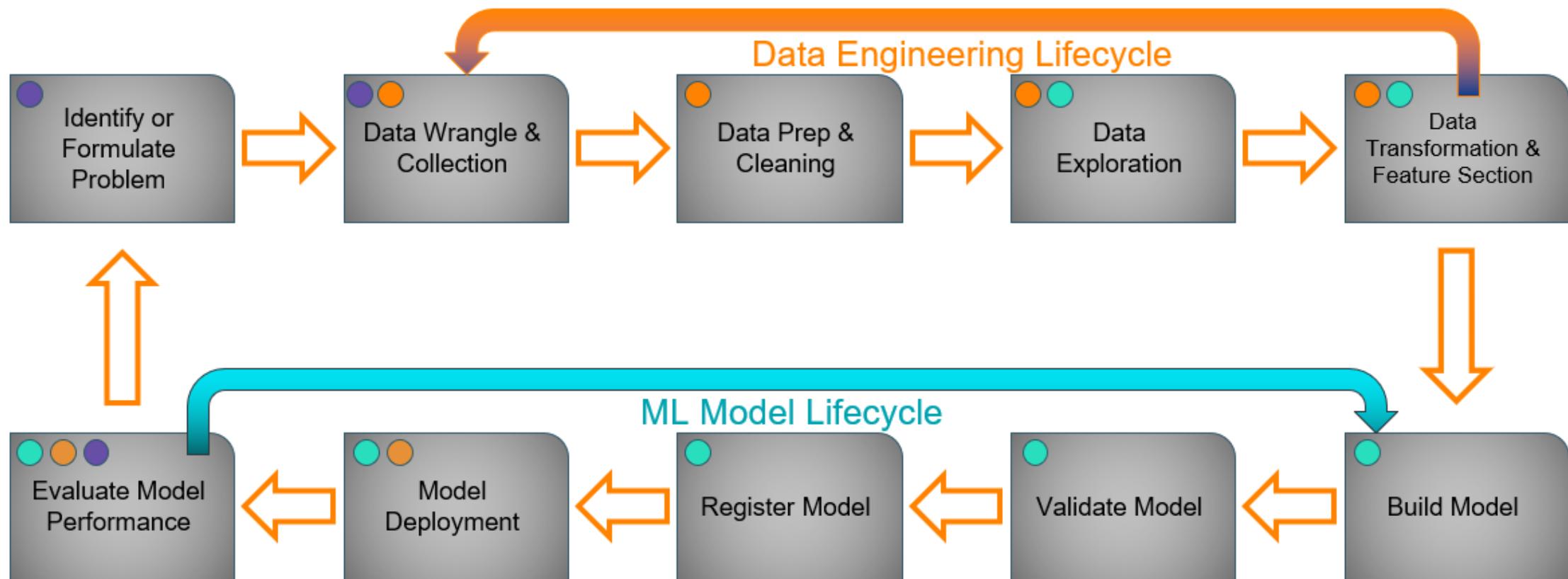
Data Engineer



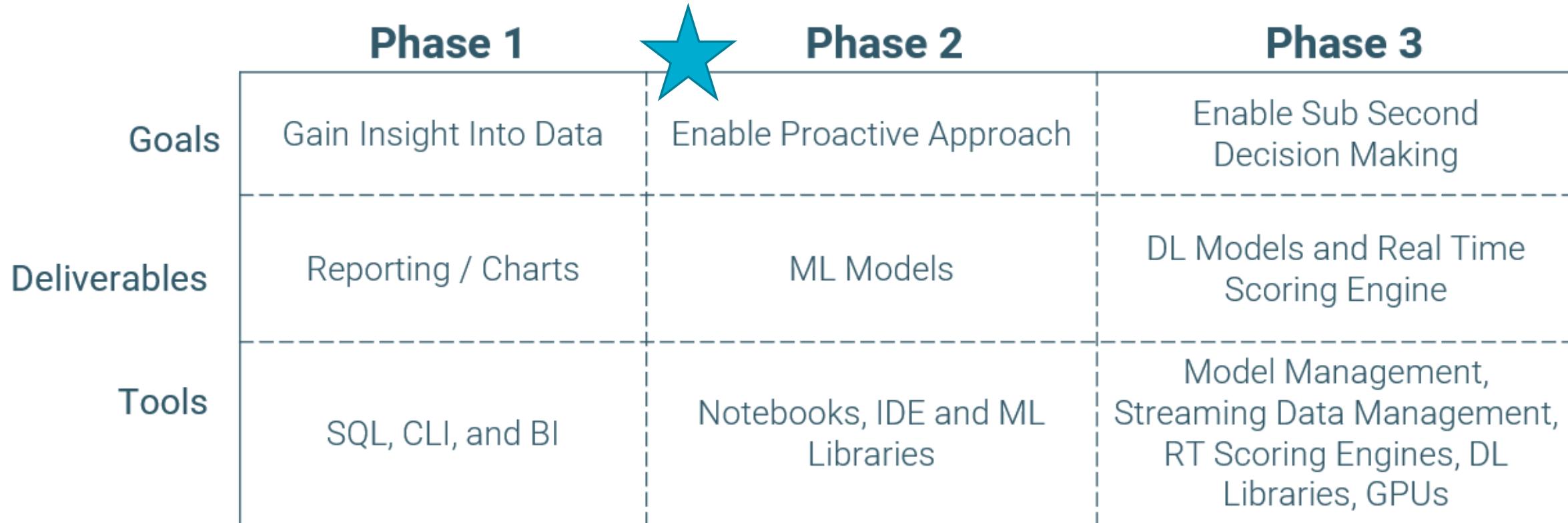
Data Scientist



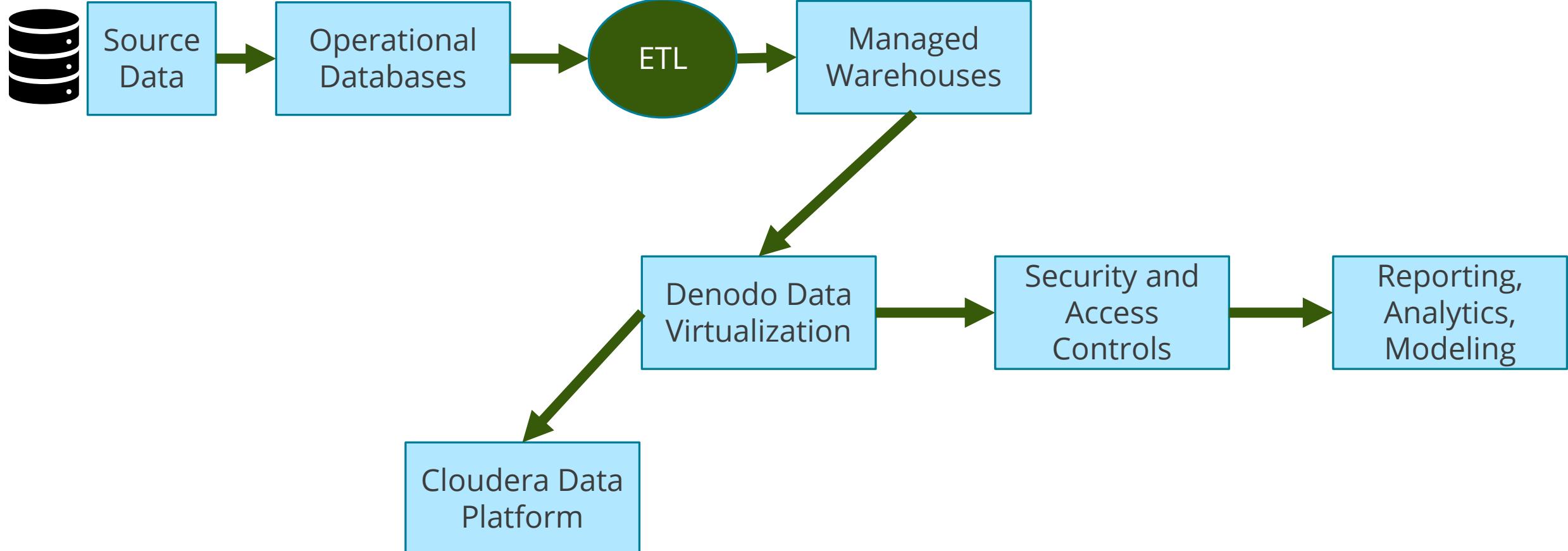
ML Engineer



Progression of Enterprise Data Science Practices



Current Data Pipeline



Challenges



- Existing legacy ETL process
- Batch ETL process is well suited for slowly changing datasets or tables (once a week updates)
- Batch ETL process ties up system for many hours, prevents usage of data for reporting and analytics
- Existing process is rigid and prevents agile development

Future State

Productionization of Data Science and Collaboration

- ml-ops – productionizing machine learning applications
- Cloudera Data Science Workbench (CDSW) – containerized environment for Data Scientists, collaborative development
- Future MLFlow support for experiment tracking and hyper-parameter tuning

File Edit View Navigate Run

quake.r

```

10 # Setting Up Spark Context
11 sc <- spark_connect(master = "yarn",
12   spark.shuffle.service.enabled = "True",
13   spark.dynamicAllocation.enabled="True",
14   spark.sql.broadcastTimeout = "1200",
15   app_name = "Quakes!")
16 sc
17
18 #Load Training and Test Data Frames
19 train <- spark_read_csv(sc, name="train", path = "hdfs://tmp/quake/train/train.csv", header
20 train <- spark_read_csv(sc, name="train", path = "hdfs://tmp/quake/train/train_sample.csv",
21
22 test <- spark_read_csv(sc, name="test", path = "hdfs://tmp/quake/test/*.csv", infer_schemas
23 test <- spark_read_csv(sc, name="test", path = "hdfs://tmp/quake/test/sed_000307.csv", infer
24
25 summary(train)
26 summary(test)
27
28 #Show Tables
29 src_tbls(sc)
30 dfd_schema(test)
31 dfd_schema(train)
32
33 #Display Dataframe Values
34 summarise(train, acoustic_data, time_to_failure)
35
36 featureList <- list("acoustic_data")
37
38 # Linear Regression Model
39 LinearReg_pipeline <- ml_pipeline(sc) %>
40 ft_vectorAssembler(
41   input_cols = featureList,
42   output_col = "feature_vector"
43 ) %>
44 ft_standard_scaler(
45   input_col = "feature_vector",
46   output_col = "scaled_features"
47 ) %>
48 ft_r_formula(formula = "time_to_failure ~ acoustic_data",
49   prediction_col = "predicted_failure_time",
50   label_col = "time_to_failure"
51 ) %>
52 ml_linear_regression( features_col = "scaled_features",
53   label_col = "time_to_failure",
54   standardization = TRUE)
55
56 LinearReg_pipeline
57
58 #fitted_pipeline <- ml_fit(LinearReg_pipeline, train)

```

Line 20, Column 25

File Edit View Navigate Run

quake.r

```

10 # Setting Up Spark Context
11 sc <- spark_connect(master = "yarn",
12   spark.shuffle.service.enabled = "True",
13   spark.dynamicAllocation.enabled="True",
14   spark.sql.broadcastTimeout = "1200",
15   app_name = "Quakes!")
16 sc
17
18 #Load Training and Test Data Frames
19 train <- spark_read_csv(sc, name="train", path = "hdfs://tmp/quake/train/train.csv", header
20 train <- spark_read_csv(sc, name="train", path = "hdfs://tmp/quake/train/train_sample.csv",
21
22 test <- spark_read_csv(sc, name="test", path = "hdfs://tmp/quake/test/*.csv", infer_schemas
23 test <- spark_read_csv(sc, name="test", path = "hdfs://tmp/quake/test/sed_000307.csv", infer
24
25 summary(train)
26 summary(test)
27
28 #Show Tables
29 src_tbls(sc)
30 dfd_schema(test)
31 dfd_schema(train)
32
33 #Display Dataframe Values
34 summarise(train, acoustic_data, time_to_failure)
35
36 featureList <- list("acoustic_data")
37
38 # Linear Regression Model
39 LinearReg_pipeline <- ml_pipeline(sc) %>
40 ft_vectorAssembler(
41   input_cols = featureList,
42   output_col = "feature_vector"
43 ) %>
44 ft_standard_scaler(
45   input_col = "feature_vector",
46   output_col = "scaled_features"
47 ) %>
48 ft_r_formula(formula = "time_to_failure ~ acoustic_data",
49   prediction_col = "predicted_failure_time",
50   label_col = "time_to_failure"
51 ) %>
52 ml_linear_regression( features_col = "scaled_features",
53   label_col = "time_to_failure",
54   standardization = TRUE)
55
56 LinearReg_pipeline
57
58 #fitted_pipeline <- ml_fit(LinearReg_pipeline, train)

```

Line 20, Column 25



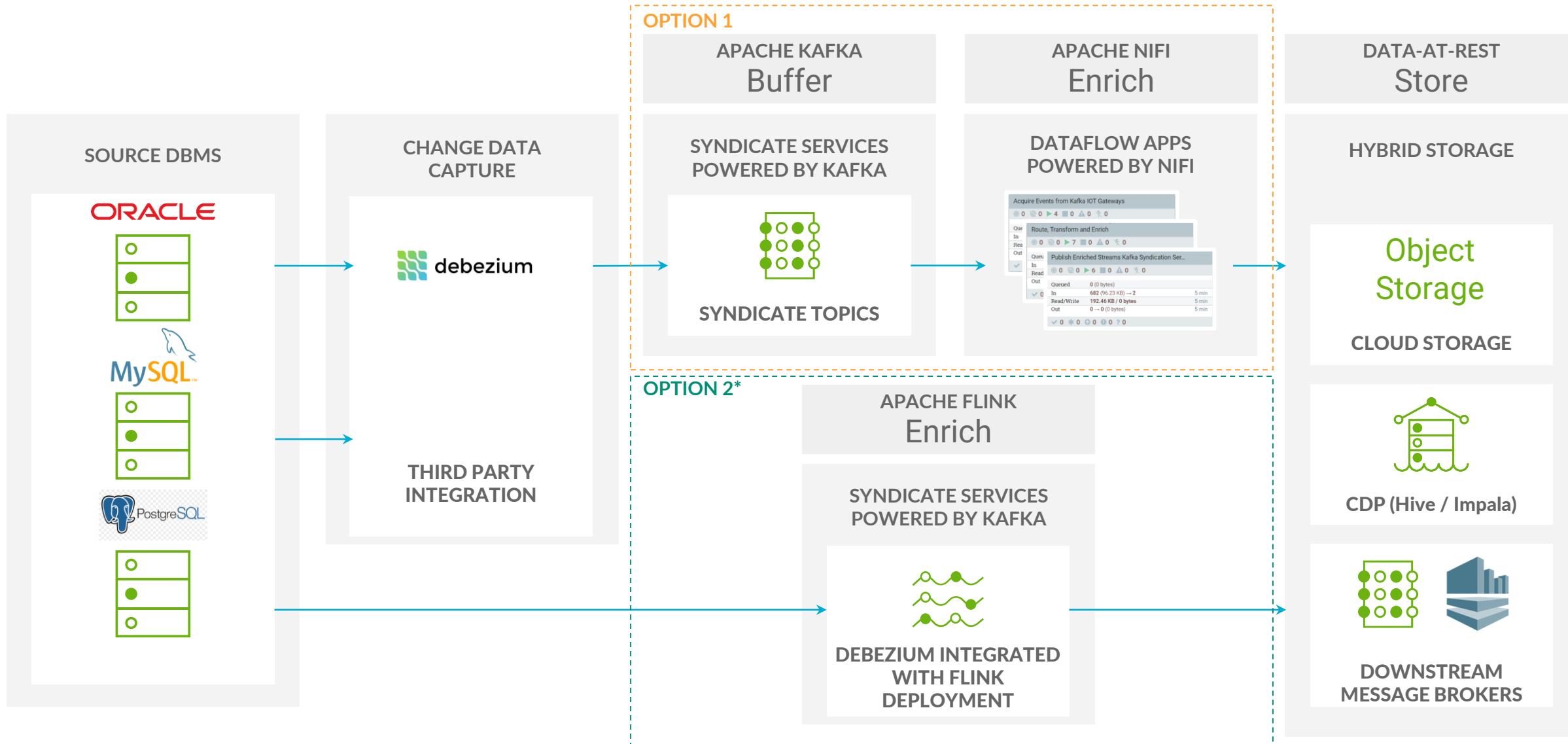
Data Governance and Cataloging



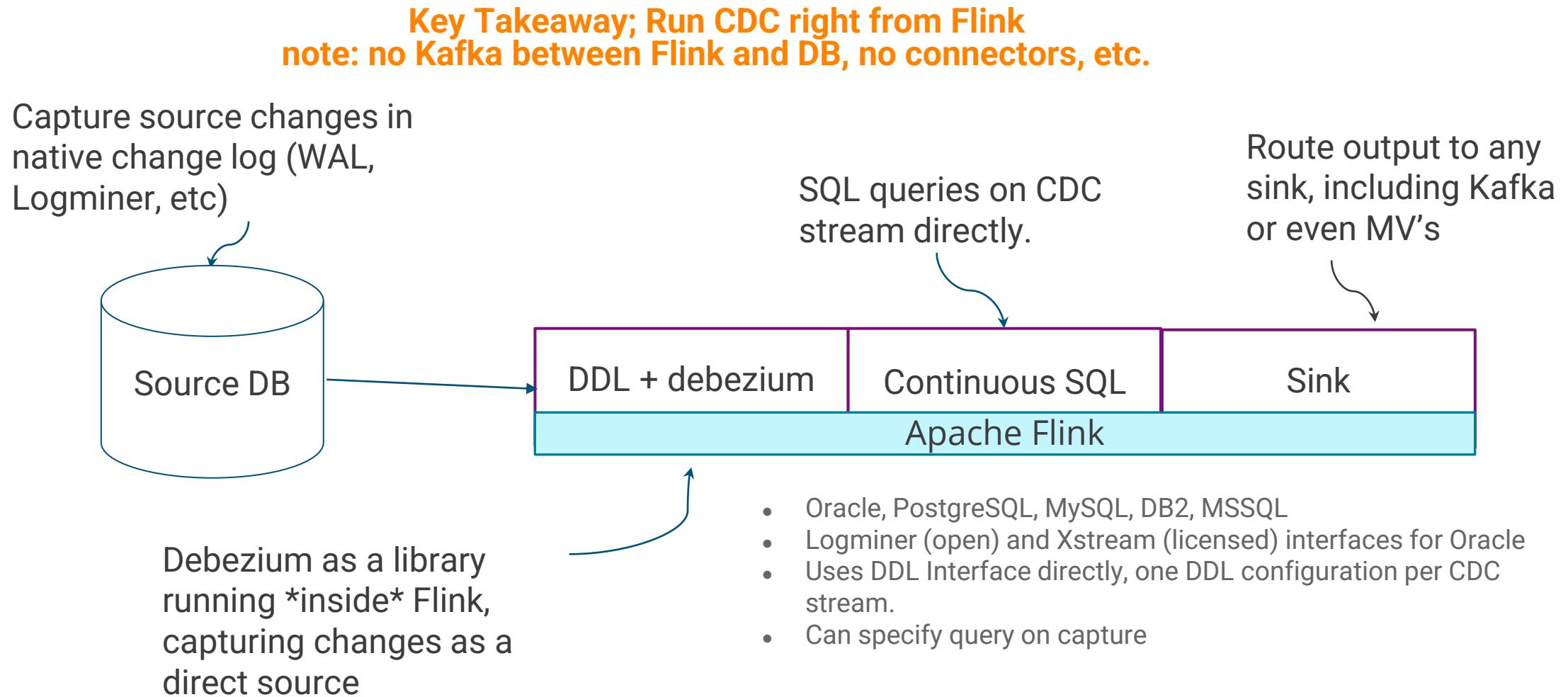
- Document more datasets with descriptions and metadata
- Leverage Denodo as singular integration point for structured data and access controls
- Tagging data in Denodo and Cloudera (Apache Atlas)
- Test attribute-based access controls in Denodo and Cloudera (Apache Ranger)
- Working on labels and sensitivity categories to address Controlled Unclassified Information (CUI) requirements



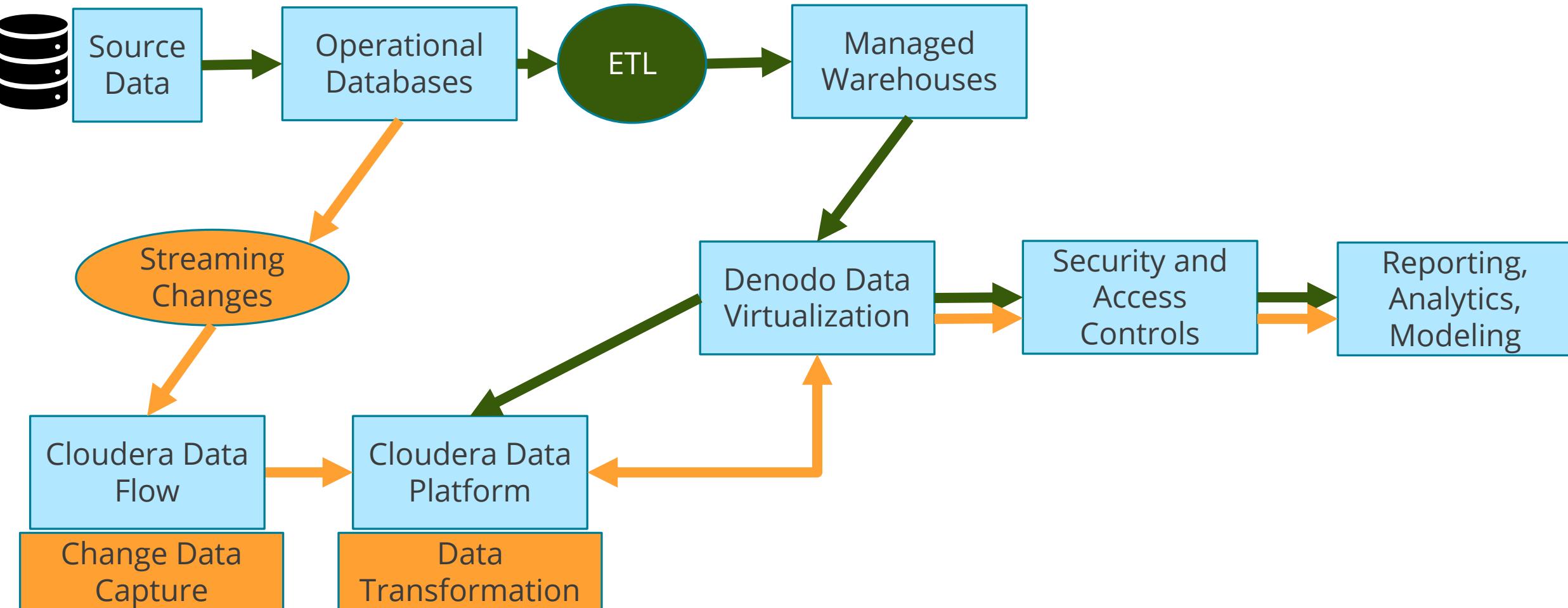
Change Data Capture (CDC)



Integrated Change Data Capture



Sandia Automated Data Pipeline



Demo or Video of CDC



Impact of Automated Data Pipelines



- Rapid access to current data enables reporting and analytics access to quickly changing datasets or tables
- Providing robust tooling to augment and not interfere with existing data pipelines such as ETL
- More agile development of future data pipelines
- Ensure end-to-end security and governance throughout entire pipeline
- Provide leadership with real-time dashboards and decision-making opportunities



Lessons Learned and Best Practices

Challenges	Actions
Culture of “ownership” of data	Implement Data Governance
Pockets of Data Scientists around the lab	Data Sciences Community of Practice (CoP)
Lack of leadership support and direction	Get a Chief Data Office (CDO) or Deputy Chief Data Officer
Lack of documentation around data	Implement a data catalog
Data architecture is old	Understand architectural paradigms: ETL, ELT, data warehouse, data lake, lambda and kappa architectures, etc.

PRIORITIZE:
 People
 Processes
 Architectures
 Culture
 Results



Tools
 Software
 One-Off Projects



Comments or Questions?

pcarlso@sandia.gov



<https://carlsonp.github.io>
<https://www.linkedin.com/in/patrick-carlson-13753628>



ibrooks@cloudera.com



<https://github.com/Brookslan>
<https://www.linkedin.com/in/ianrbrooksphd/>