Efficiently Reproducing Distributed Workflows in Notebook-based Systems

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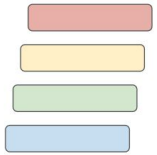


floability

Overview

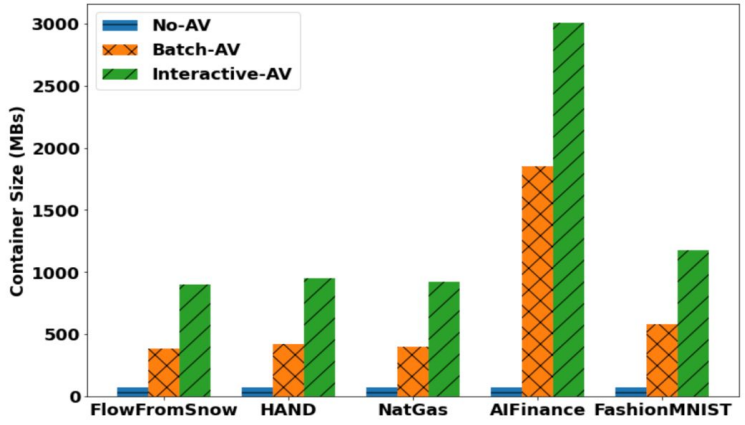
- Primary objective: Improve reproducibility of distributed workflows in notebooks
- Notebooks have become widespread in scientific computing
  - Interactive and iterative development, cell-level execution, easy dissemination
  - Distributed workflows for large-scale data analytics
- Repeating and reproducing distributed workflows is challenging
  - Most techniques like manual savepoints work well for single-node workflows
- We present NBReplay – a tool for efficient, reproducible execution of distributed workflows
  - Checkpoint and restore intermediate workflow state at each cell
  - Avoid redundant execution through selective task caching and replay
  - Shows average performance gains between 2.08x–18.4x for notebook re-execution

Structure of a Notebook

[9]:
```
plt.subplots(figsize =(12, 8))
x = np.arange(len(df2.index))
plt.bar(x, df2['Size 2'], width=bar_width, hatch='-')
plt.bar(x+(1*bar_width), df2['Size 1'], width=bar_width, hatch='x')
plt.bar(x+(2*bar_width), df2['Size 3'], width=bar_width, hatch='/')
```

[9]:
```
plt.ylabel('Container Size (MBs)', fontsize=18, fontweight='bold')
plt.xticks([r + bar_width for r in range(len(x))], df2.index)
plt.legend(labels=labels)
plt.savefig('export_size_containers_all.png', dpi=500)
df2['Size 2'].head(3)
```

[9]:
```
Use Case
FlowFromSnow    72.7
HAND            72.7
NatGas          72.7
Name: Size 2, dtype: float64
```

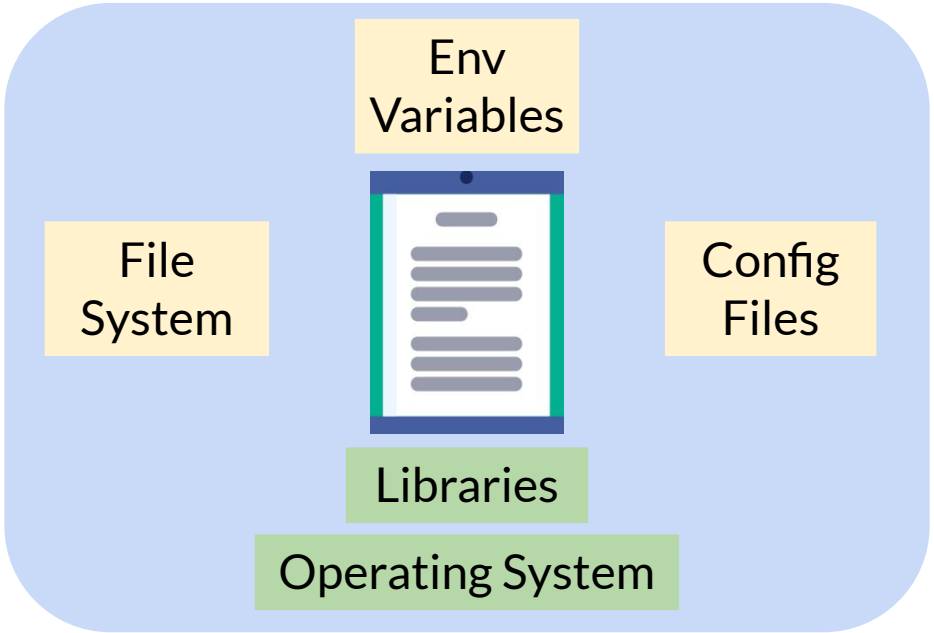


Code Cells

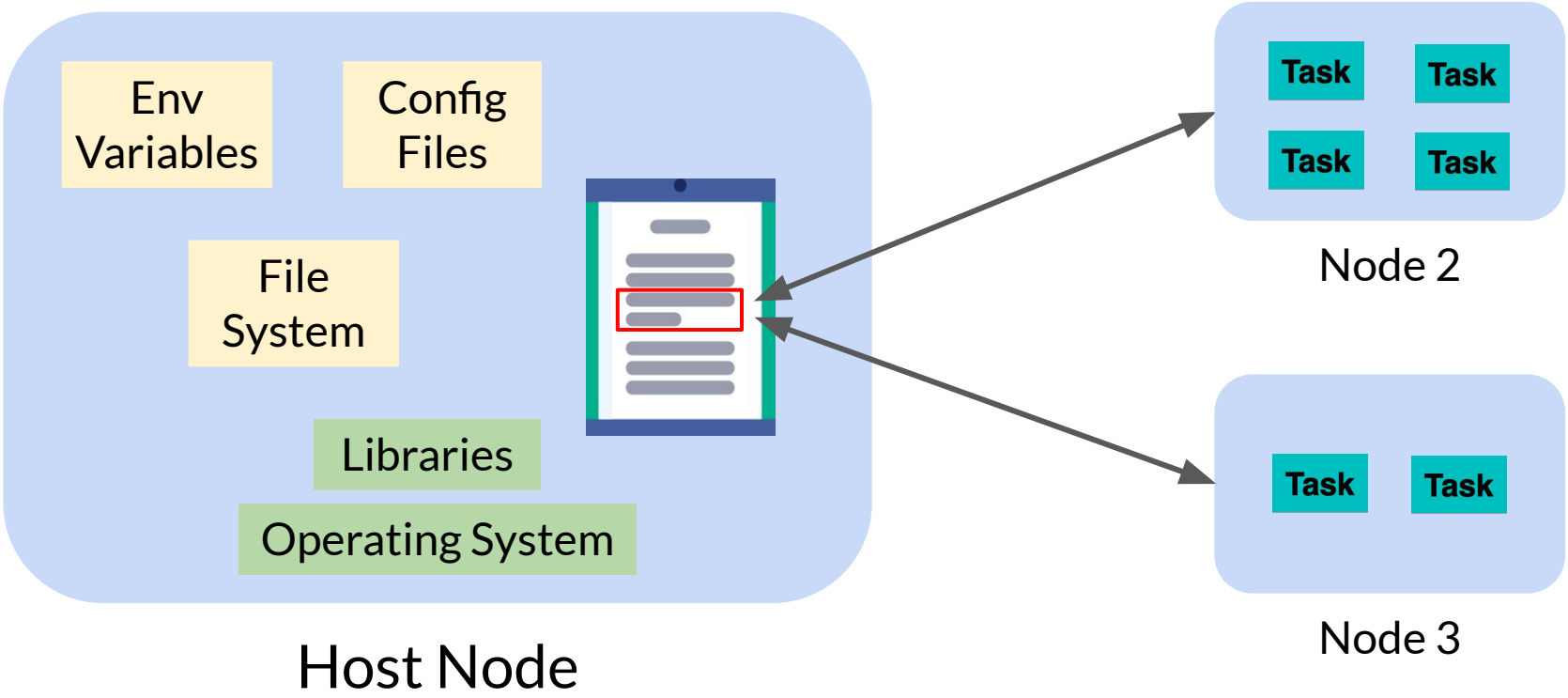
Data & Results

Visualizations

Execution in a Notebook



Distributed Execution in a Notebook



Notebooks for Exploration

Exploratory Analysis

Update the formula

→ risk_score > 10.0

→ risk_score > 5.0

[c1]
```
from dask.distributed import Client
import dask.dataframe as ddf
# Connect to an existing Dask cluster
client = Client("tcp://scheduler:8786")
# Lazy load dataset from shared filesystem
df = ddf.read_parquet("run_24-06.parquet")
# Lazy preprocessing
df = df[df["temperature"].notnull()]
df = df.assign(anomaly = df["temperature"]-
     df["temperature_baseline"])
raw_df = df
```

Data Loading & Pre-processing

[c2]
```
# Compute summary stats across worker nodes
daily_stats = (raw_df.groupby
              (["region","day"])
              .agg({"anomaly":["mean","std"],
               "precipitation":"sum"})
               .persist())
# Compute risk score
def risk_score(row):
    return 1.0*row[("anomaly", "mean")] + 0.1
    *row[("precipitation", "sum")]
stats_ref = daily_stats
daily_stats = daily_stats.map_partitions(
              lambda part: part.assign(
              risk_score = part.apply(
              risk_score, axis=1)))
```

Computational Logic

[c3]
```
# Run dist. computation, get subset of result
high_risk = daily_stats[daily_stats
            ["risk_score"] > 10.0]
# large-scale distributed execution
result = high_risk.compute()
# Save summary for analysis and visualization
result.to_parquet("high_risk_24-06.parquet")
```

Execution, Result & Analysis

Scenario 1: Share and Repeat

[c1]
```
from dask.distributed import Client
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```

Share the notebook with a collaborator to repeat on another machine

[c3]
```
# Run dist. computation, get subset of result
high_risk = daily_stats[daily_stats
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# large-scale distributed execution
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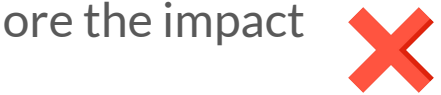
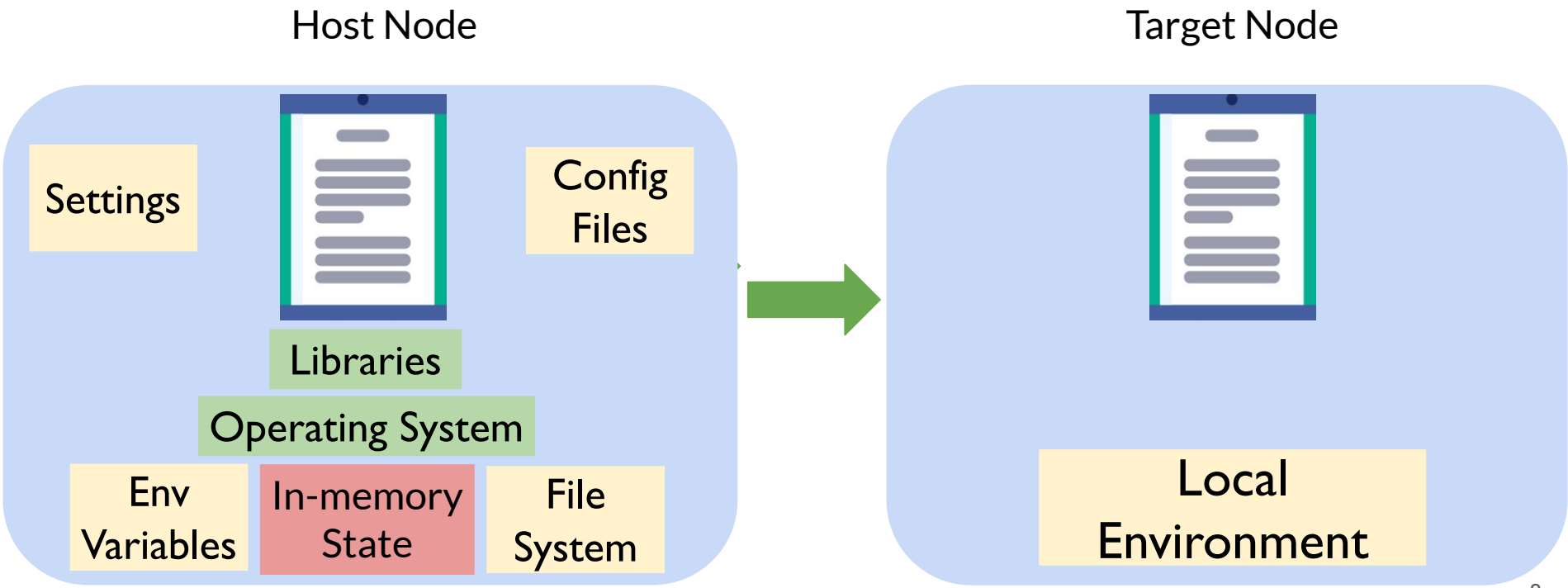
```

Only run cell 3 to explore the impact of **risk_score**



Problem: Sharing the Notebook ONLY



Scenario 2: Repeat Part of a Cell

Update **risk_score** function definition in cell 2

[c_2]
```
# Compute summary stats across worker nodes
daily_stats = (raw_df.groupby
               (["region","day"])
               .agg({"anomaly":["mean","std"],
                "precipitation":"sum"})
                .persist())
# Compute risk score
def risk_score(row):
    return 1.0*row[("anomaly", "mean")] + 0.1
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stats_ref = daily_stats
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[c_3]
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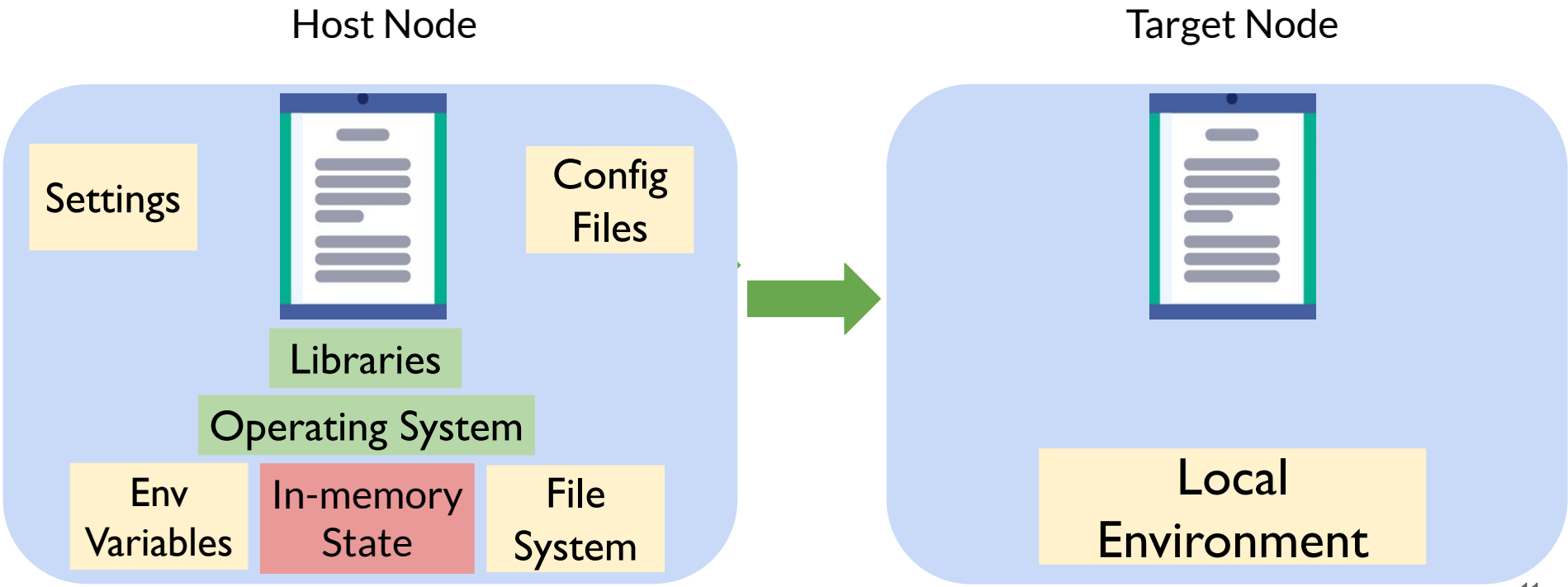
# large-scale distributed execution
result = high_risk.compute()
# Save summary for analysis and visualization
result.to_parquet("high_risk_24-06.parquet")
```

Only run part of distributed workflow in cell 2 

NBReplay

- NBReplay is an end-to-end system to enable efficient and reproducible execution of distributed workflows:
  - Performs cell-level checkpointing to restore intermediate workflow state
  - Performs caching of distributed tasks to avoid redundant execution
- Creates two kernels:
  - **Audit** – for executing the notebook
  - **Repeat** – for repeating the notebook, on the same or different node

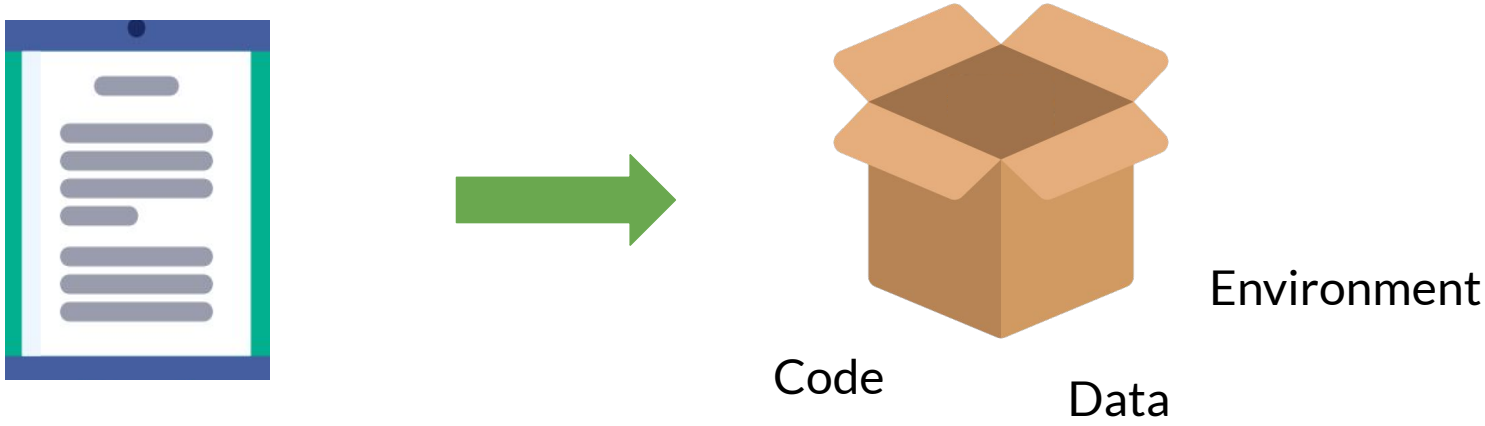
Scenario 1: Share and Repeat



Solution Scenario 1
Cell-level Checkpointing

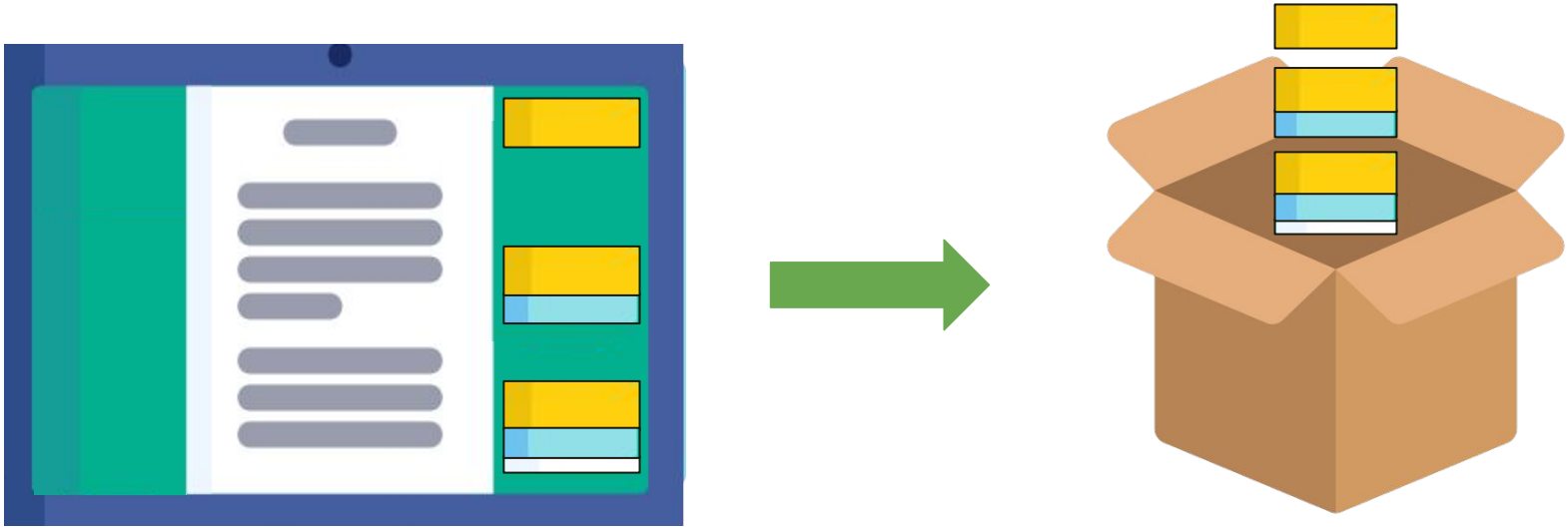
Notebook Containerization

- Audit kernel uses application virtualization to convert the notebook execution into self-contained package.



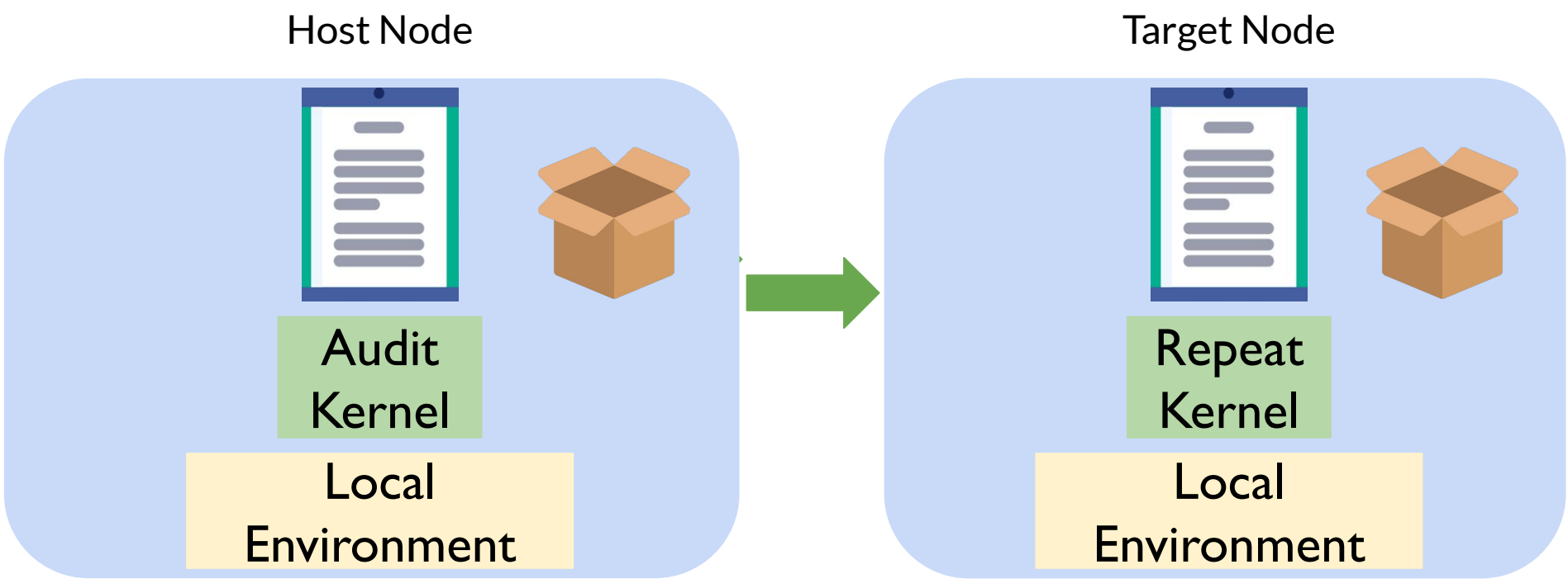
Cell-level Checkpointing

- Program state at each cell is stored in incremental checkpoints



- Checkpoints are added to the container for sharing

Sharing Checkpoints with the Notebook



Restoring Checkpoints during Repeat

- To explore the impact of **risk_score**, restore all checkpoints up to cell 2

- Re-execute cell 3 ONLY

[c_1]
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import dask.dataframe as ddf
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client = Client("tcp://scheduler:8786")
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df = ddf.read_parquet("run_24-06.parquet")
# Lazy preprocessing
df = df[df["temperature"].notnull()]
df = df.assign(anomaly = df["temperature"]-
     df["temperature_baseline"])
raw_df = df
```

checkpoint cell 1

[c_2]
```
# Compute summary stats across worker nodes
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# Compute risk score
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stats_ref = daily_stats
daily_stats = daily_stats.map_partitions(
              lambda part: part.assign(
              risk_score = part.apply(
              risk_score, axis=1)))
```

checkpoint cell 2

[c_3]
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# large-scale distributed execution
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# Save summary for analysis and visualization
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```

Scenario 2: Repeat Part of a Cell

Update **risk_score** function definition in cell 2

[c_2]
```
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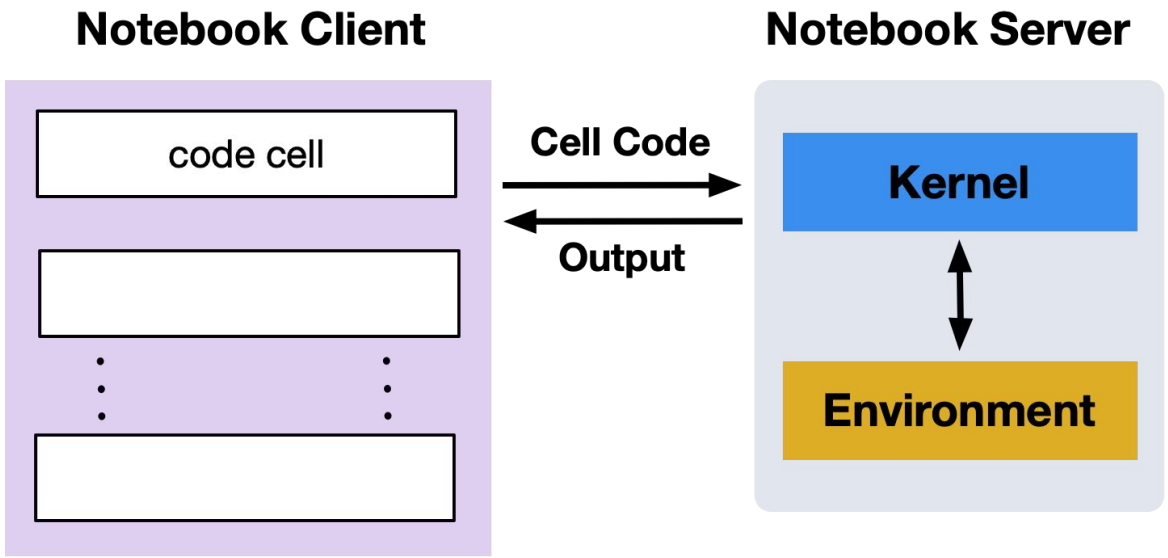
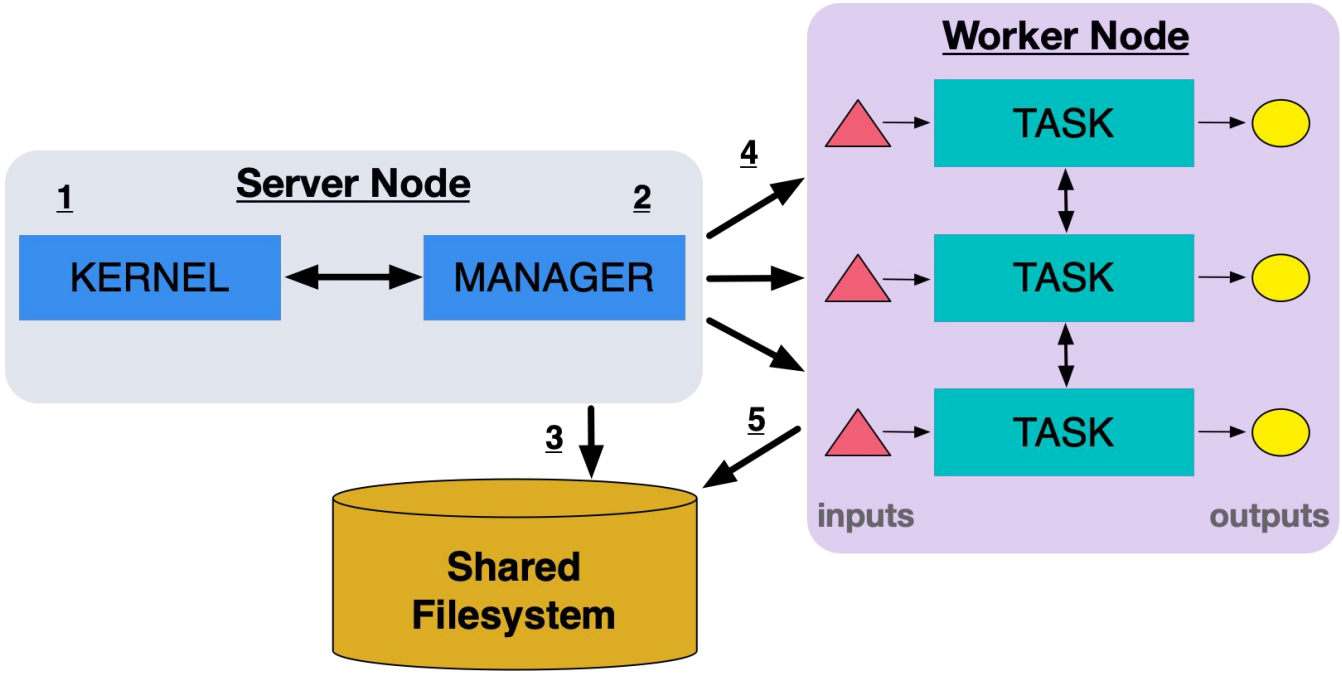
Only run part of distributed workflow in cell 2 

Execution in Notebook Environment



Distributed Execution in Notebooks



Distributed Task Generation

[c_1]
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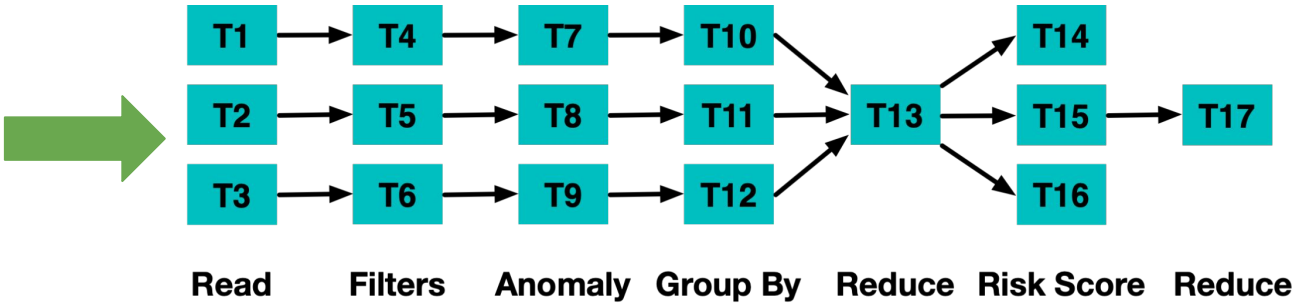
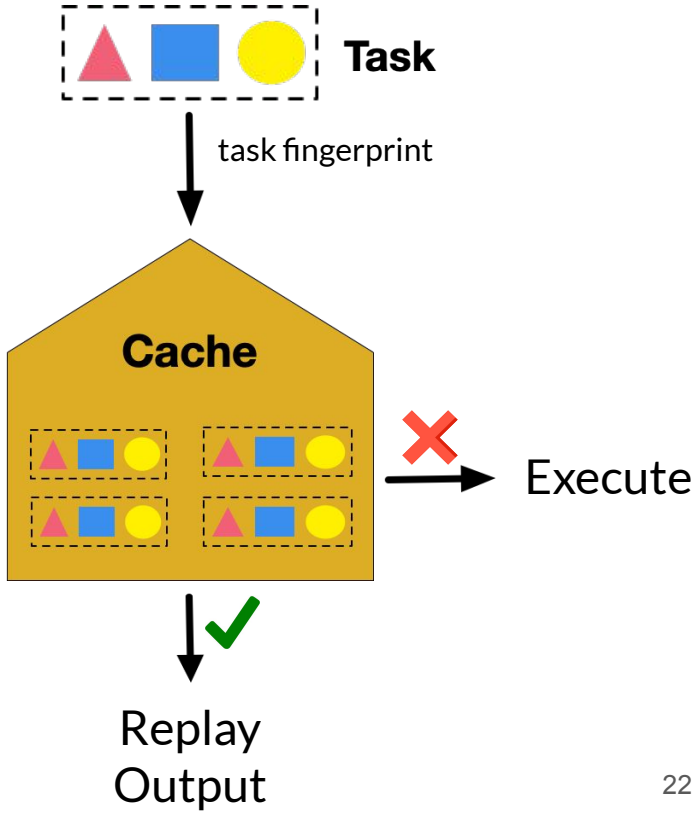


DAG of Parallel Tasks

Solution Scenario 2
Partial Re-execution with Caching

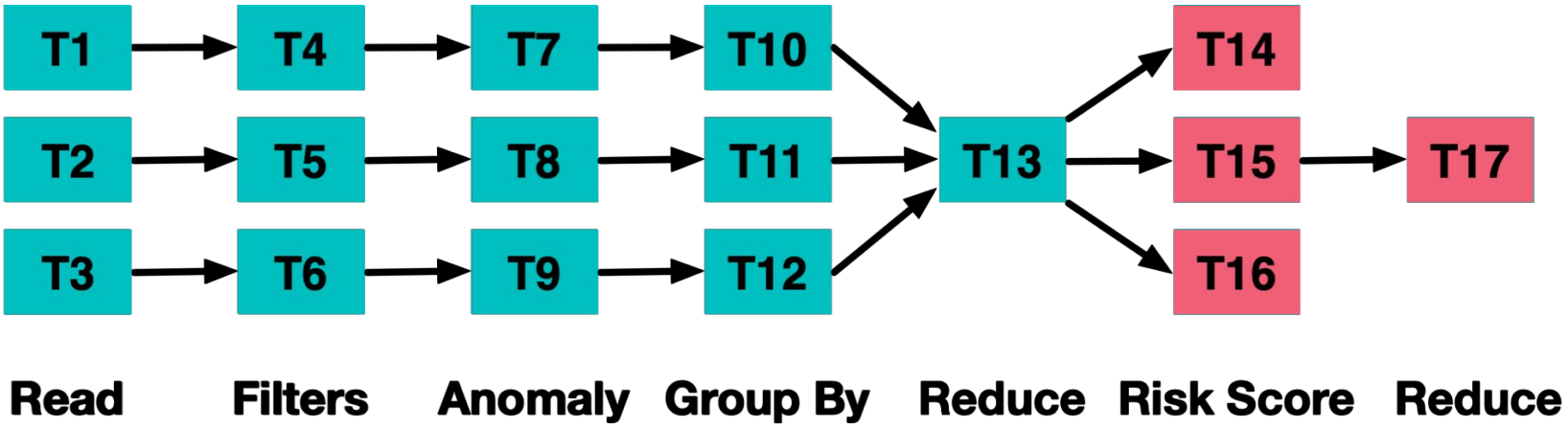
Task Fingerprinting and Caching

- Maintain a cache of tasks including their code, inputs, and outputs
- Incoming tasks are compared with the cache using a task fingerprint.
- If the task is found in cache, it is NOT executed and its cached output is replayed.

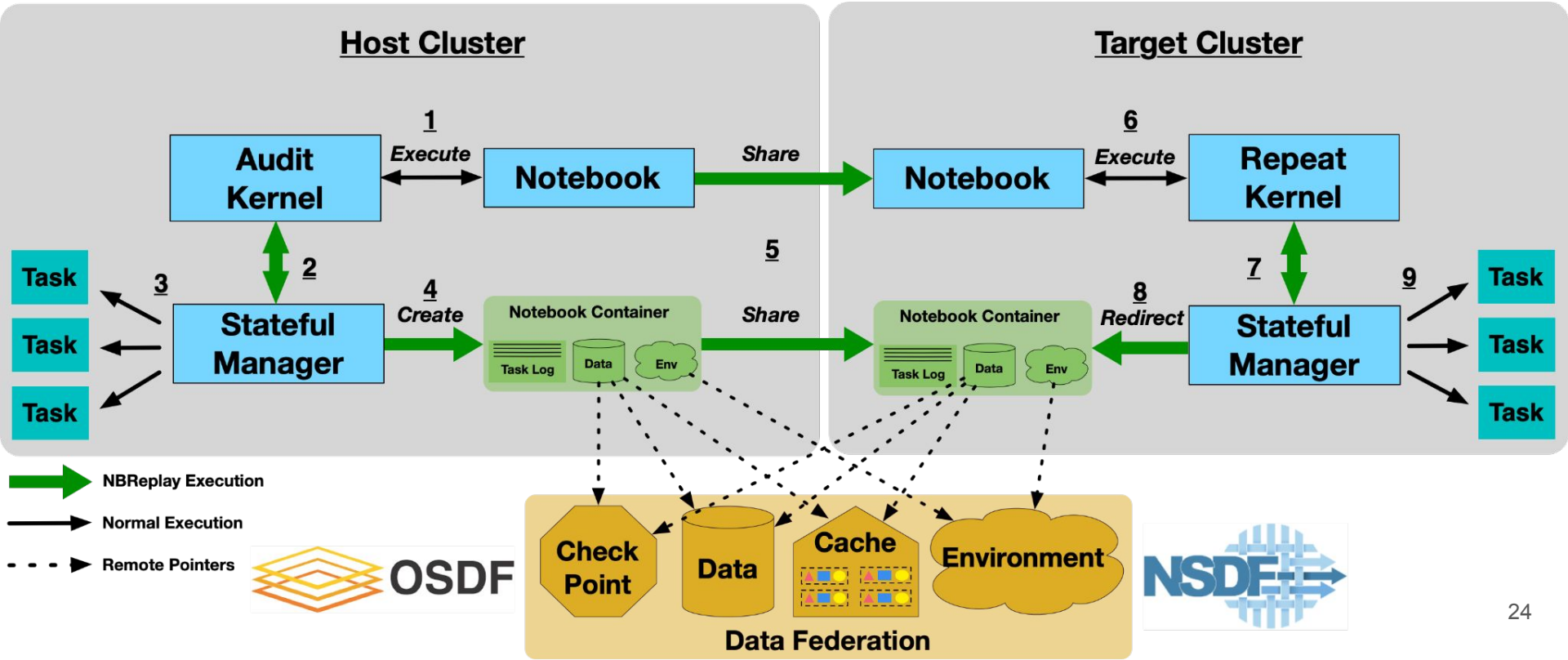


Partial Re-execution

- When **risk_score** function is updated, only the updated tasks are re-executed, shown in red.



NBReplay Architecture and Workflow



Dataset

Dataset of 5 notebooks from different domains with distributed workflows

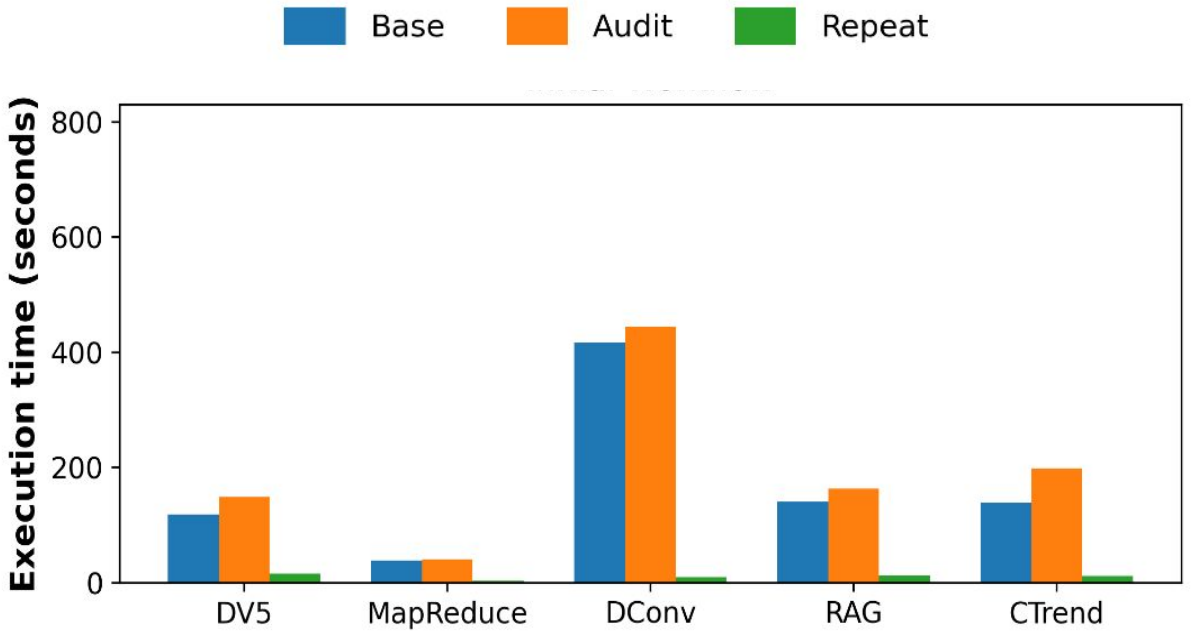
Notebook	Distributed Tasks	Domain
DV5	4	High Energy Physics
MapReduce	13	NLP
DConv	1024	Image Processing
RAG	4	ML
CTrend	120	Climate Analysis

Experiments

- **Audit – Create Checkpoints and Cache Tasks**
- **Repeat – Restore Checkpoints and Replay Tasks**
  - Repeat with change
  - Repeat without change
- **Baseline**
  - Plain notebook execution with change
  - Plain notebook execution without change

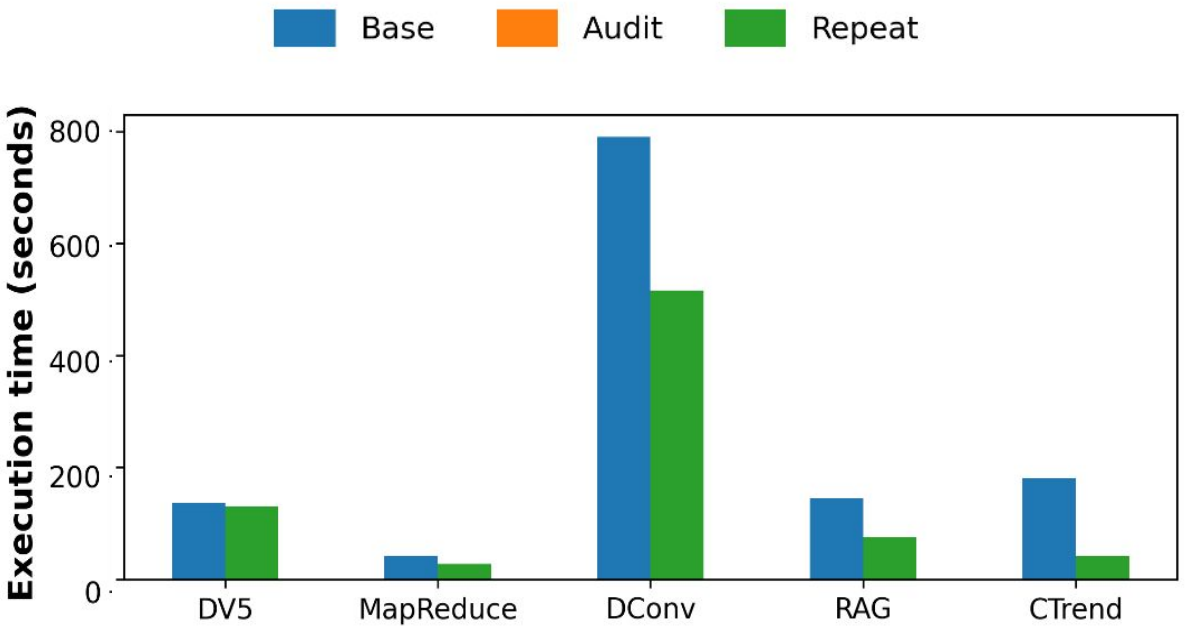
Audit vs. Repeat With Change

- An average gain of more than 2.08x on repeat with change.



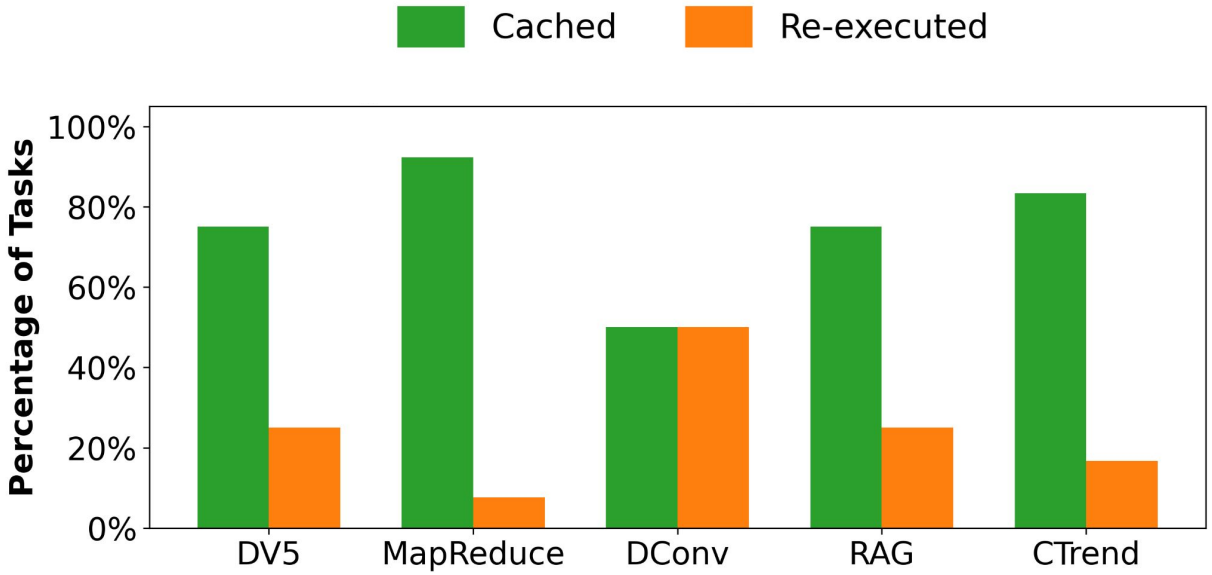
Audit vs. Repeat Without Change

- An average gain of more than 18.4x on repeat without change.



Cache Effectiveness in Partial Re-execution

- Average hit rate of 75%



Limitations & Future Work

- Overhead of auditing in compute and storage
- Assumes deterministic workflows
- Integration with data federations for data-intensive workflows
- Integretion with backpack-like mechanisms for improved collaboration
- Support a broader range of parallel and distributed computing frameworks

Conclusion

- Motivate the need for sharing and reproducing distributed workflows in notebooks successfully.
- Elaborate need for reproducibility of notebooks through different scenarios.
- Introduce NBReplay for efficient, reproducible execution for distributed workflows. It uses checkpoint and restore mechanism and avoid redundant execution through selective task caching and replay
- Experiments on notebooks using NBReplay which show good performance gains and cache effectiveness.

floability

floability.github.io

Sciunit

FLINC

github.com/radiant-systems-lab

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