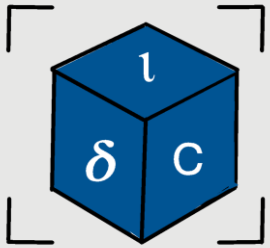
Reproducible Notebook Containers using Application Virtualization



[1]Raza Ahmad, [2]Naga Nithin Manne, [1]Tanu Malik

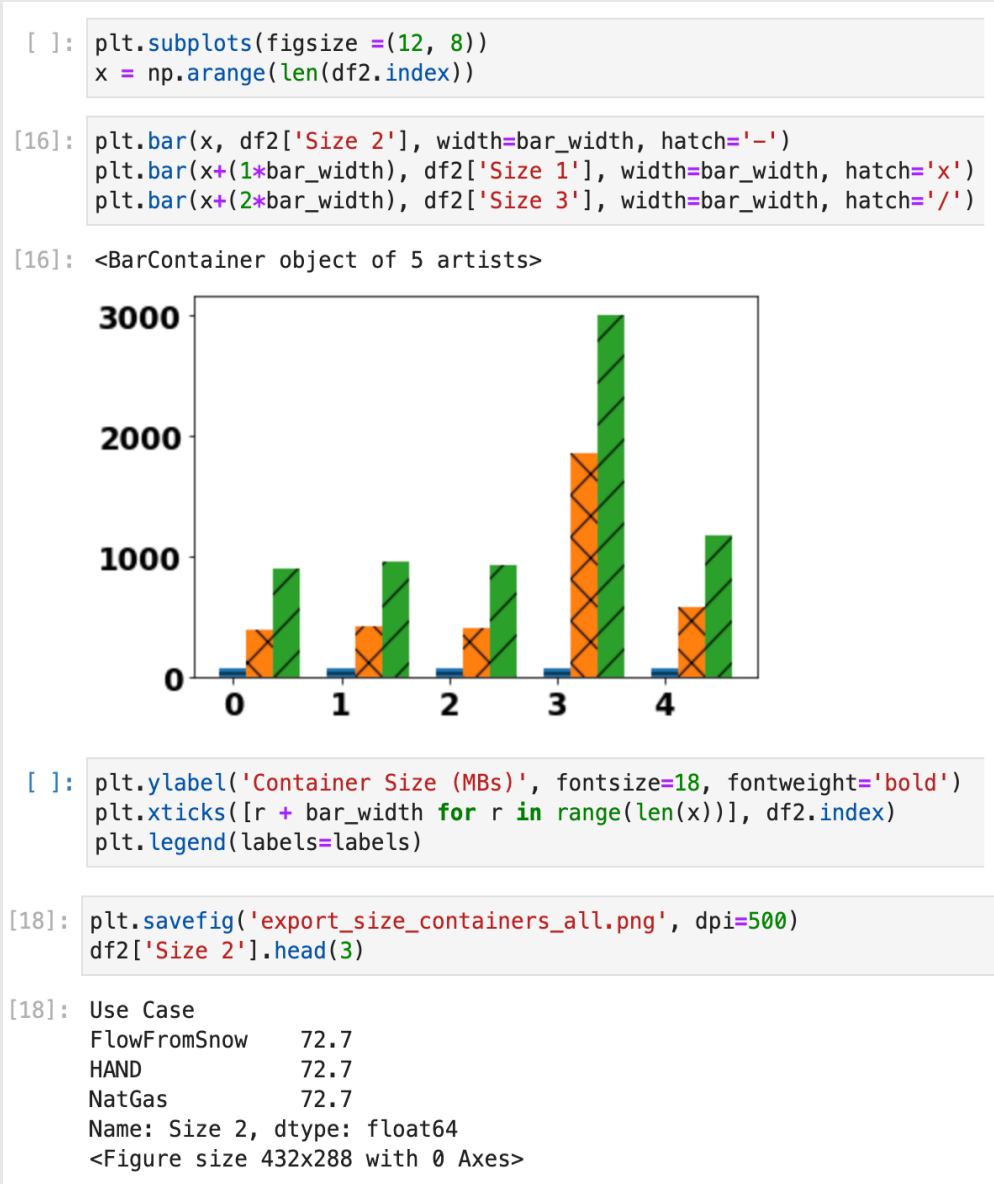
[1]School of Computing DePaul University,

[2]Argonne National Lab

Motivation

- Improve reproducibility of notebooks
- Notebooks are emerging programming paradigm in scientific computing.
  - Exploring data, executing models, visualizing results
- Reproducing notebooks is challenging
  - Hinders collaborative analytics, impacts data democratization
- We present FLINC, a system for notebook reproducibility using application virtualization
  - Enables notebook sharing using lighter weight containers
  - Provides flexible reproducibility

Notebook is Interactive and Shareable



```
[ ]: plt.subplots(figsize =(12, 8))
     x = np.arange(len(df2.index))

[16]: plt.bar(x, df2['Size 2'], width=bar_width, hatch='-')
      plt.bar(x+(1*bar_width), df2['Size 1'], width=bar_width, hatch='x')
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[16]: <BarContainer object of 5 artists>
```



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[ ]: 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)

[18]: plt.savefig('export_size_containers_all.png', dpi=500)
      df2['Size 2'].head(3)

[18]: Use Case
      FlowFromSnow    72.7
      HAND            72.7
      NatGas          72.7
      Name: Size 2, dtype: float64
      <Figure size 432x288 with 0 Axes>
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Notebook is like a "Container"

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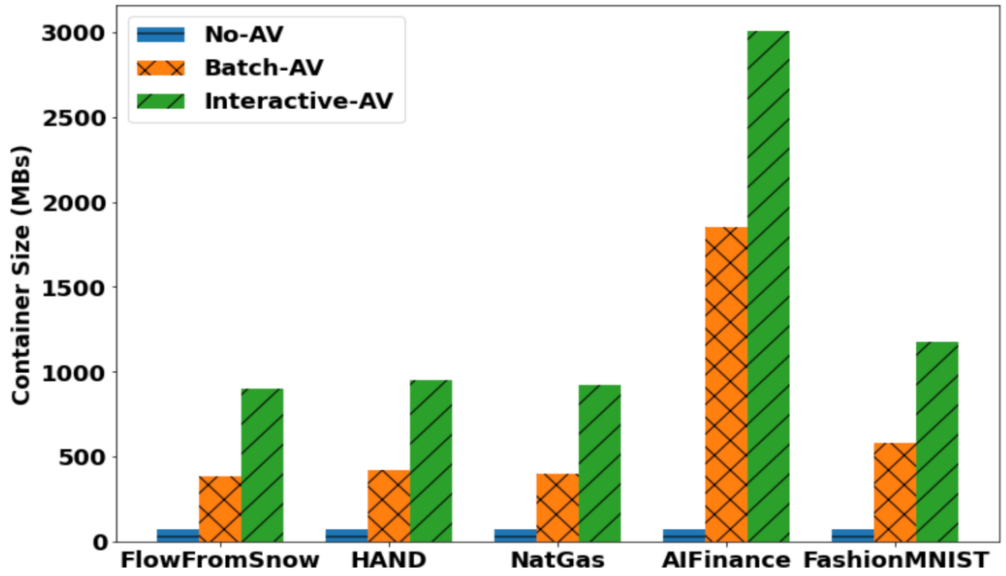

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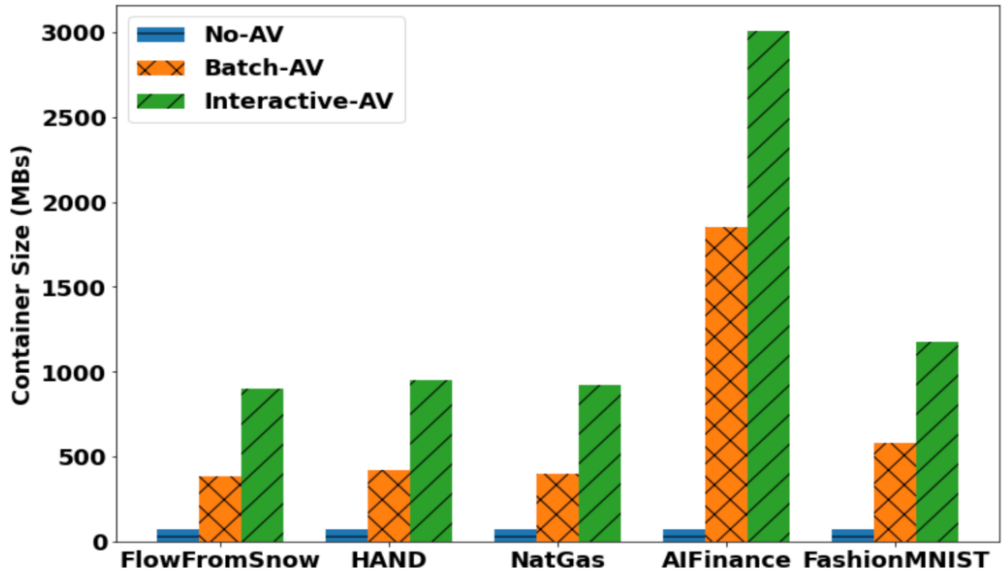

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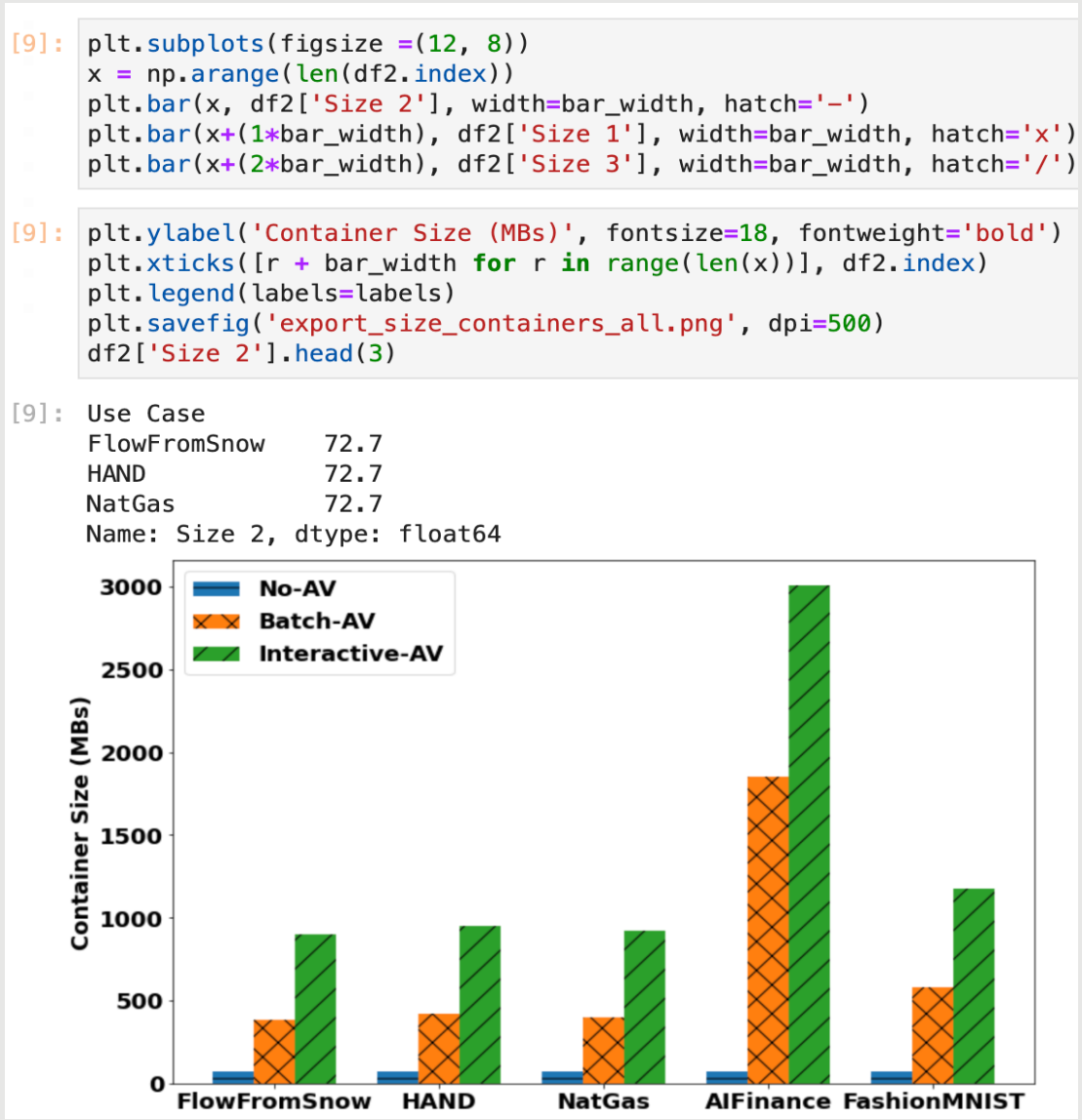

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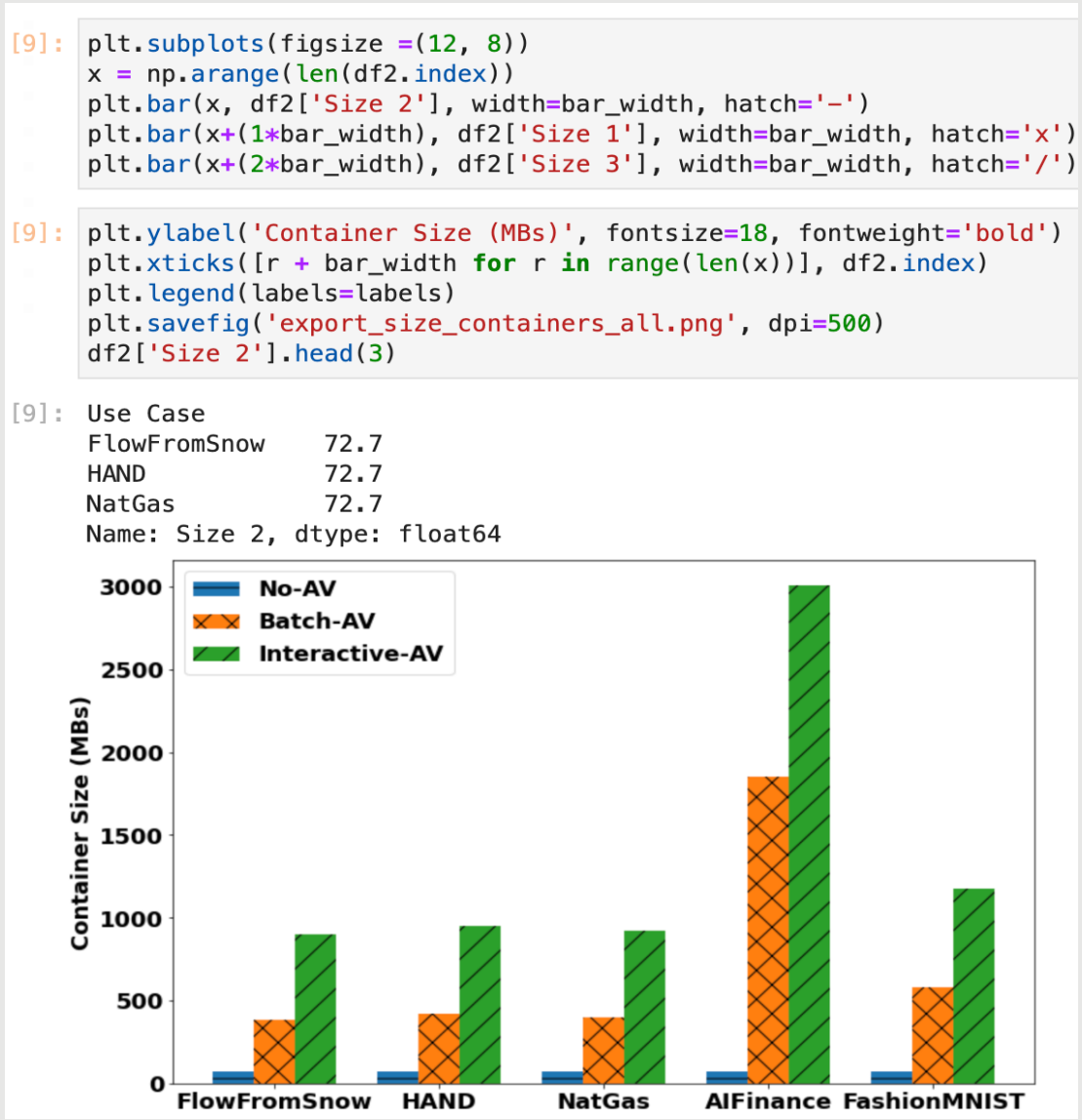

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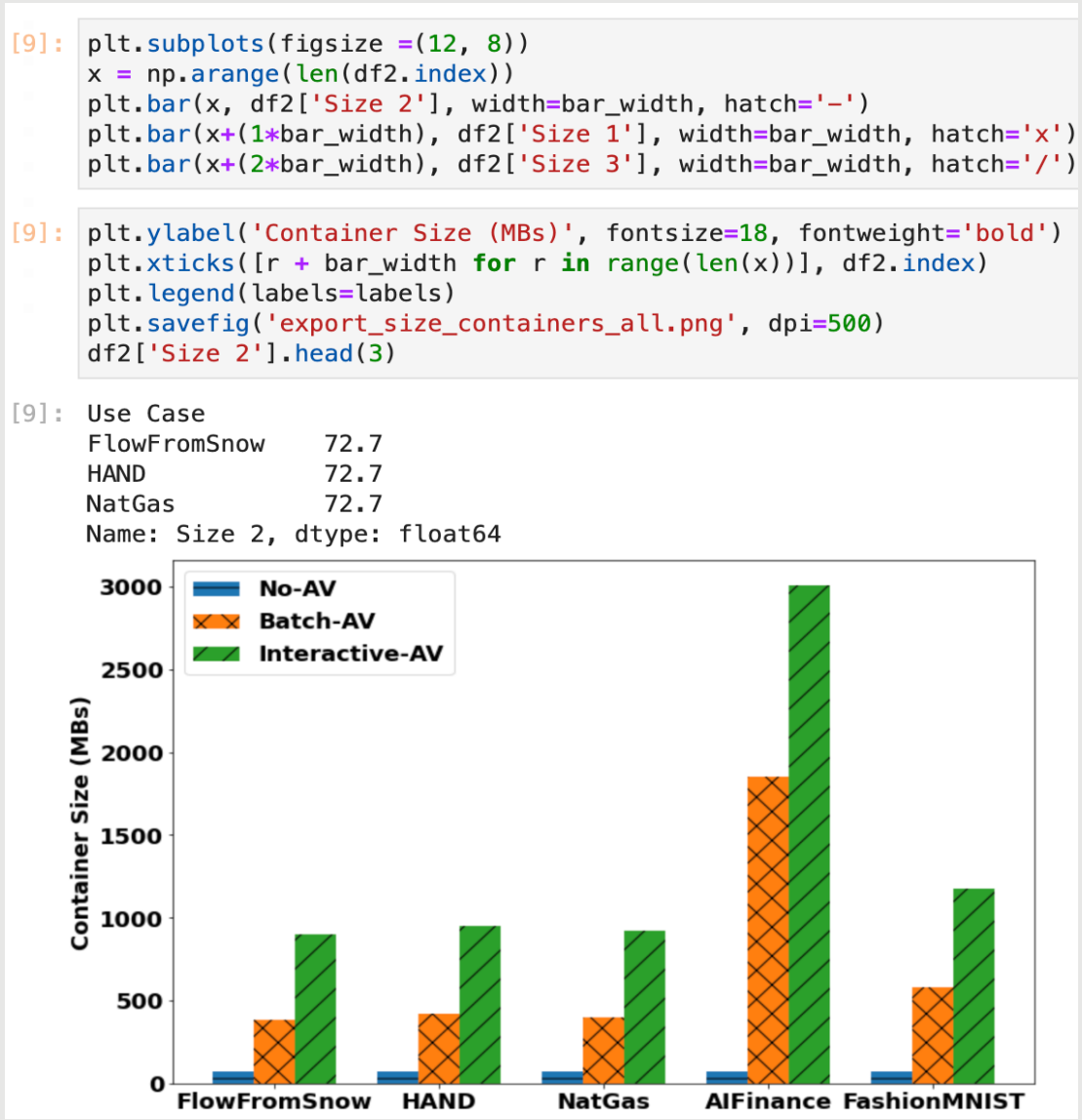

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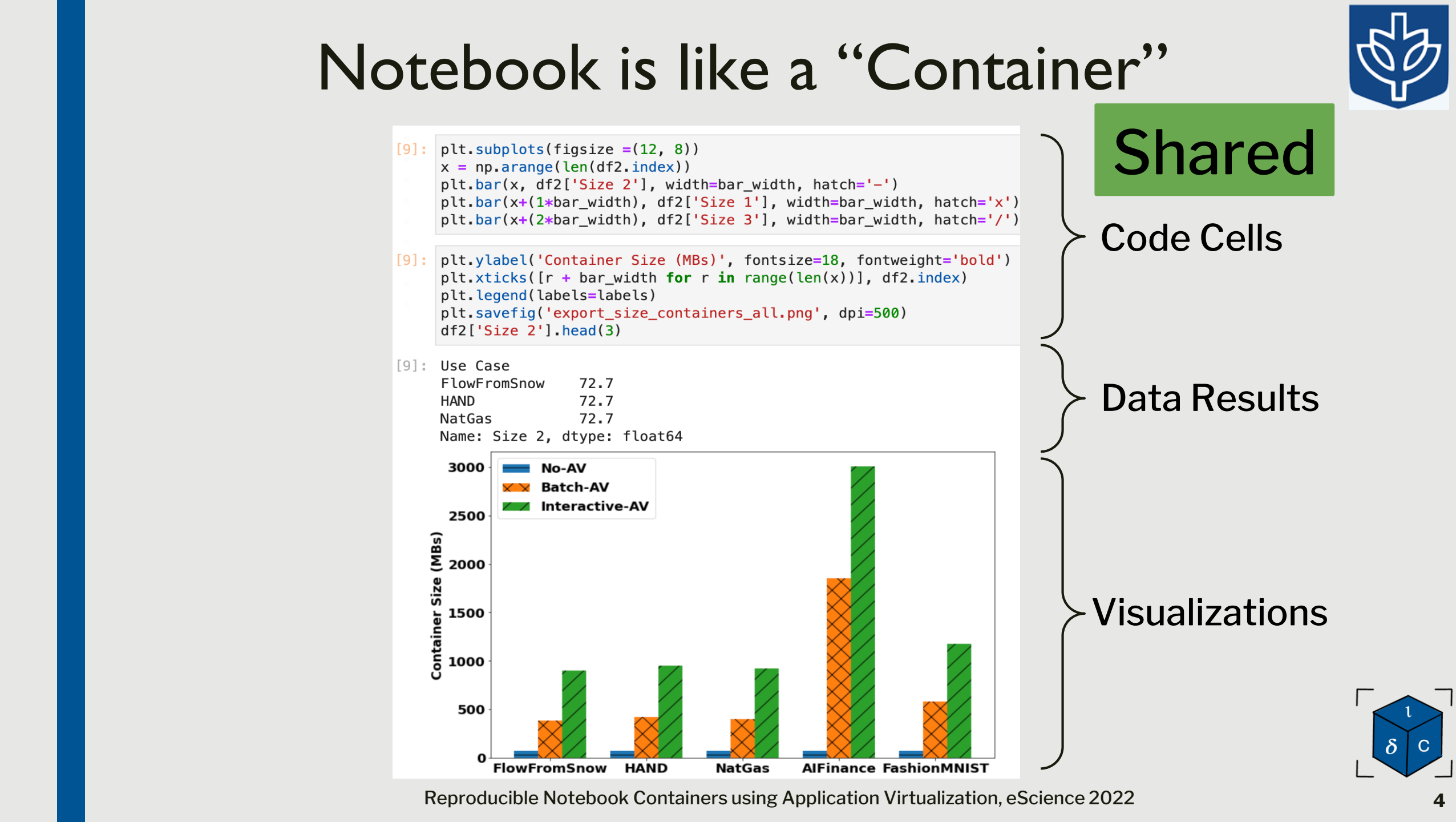
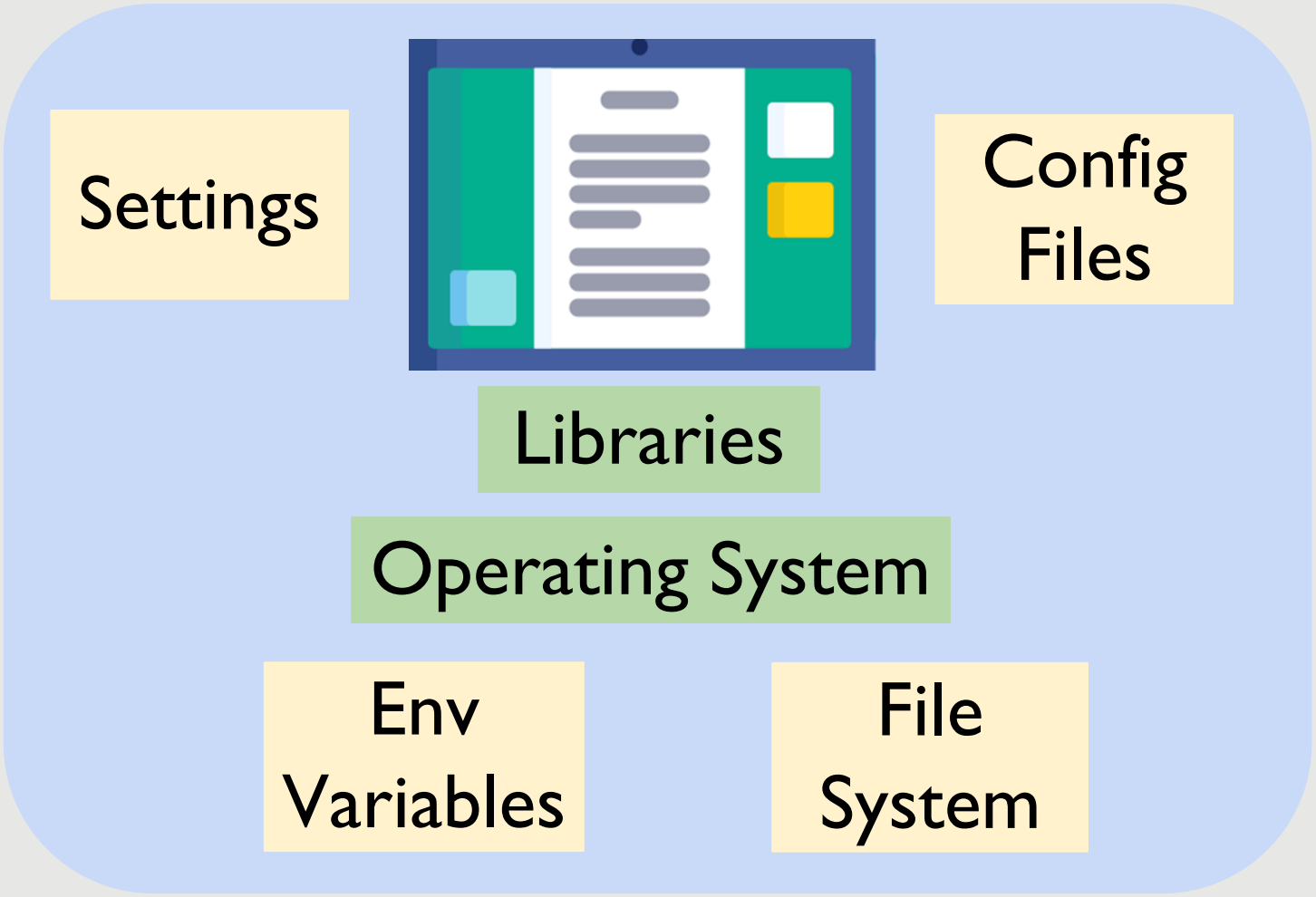


Notebook Environment



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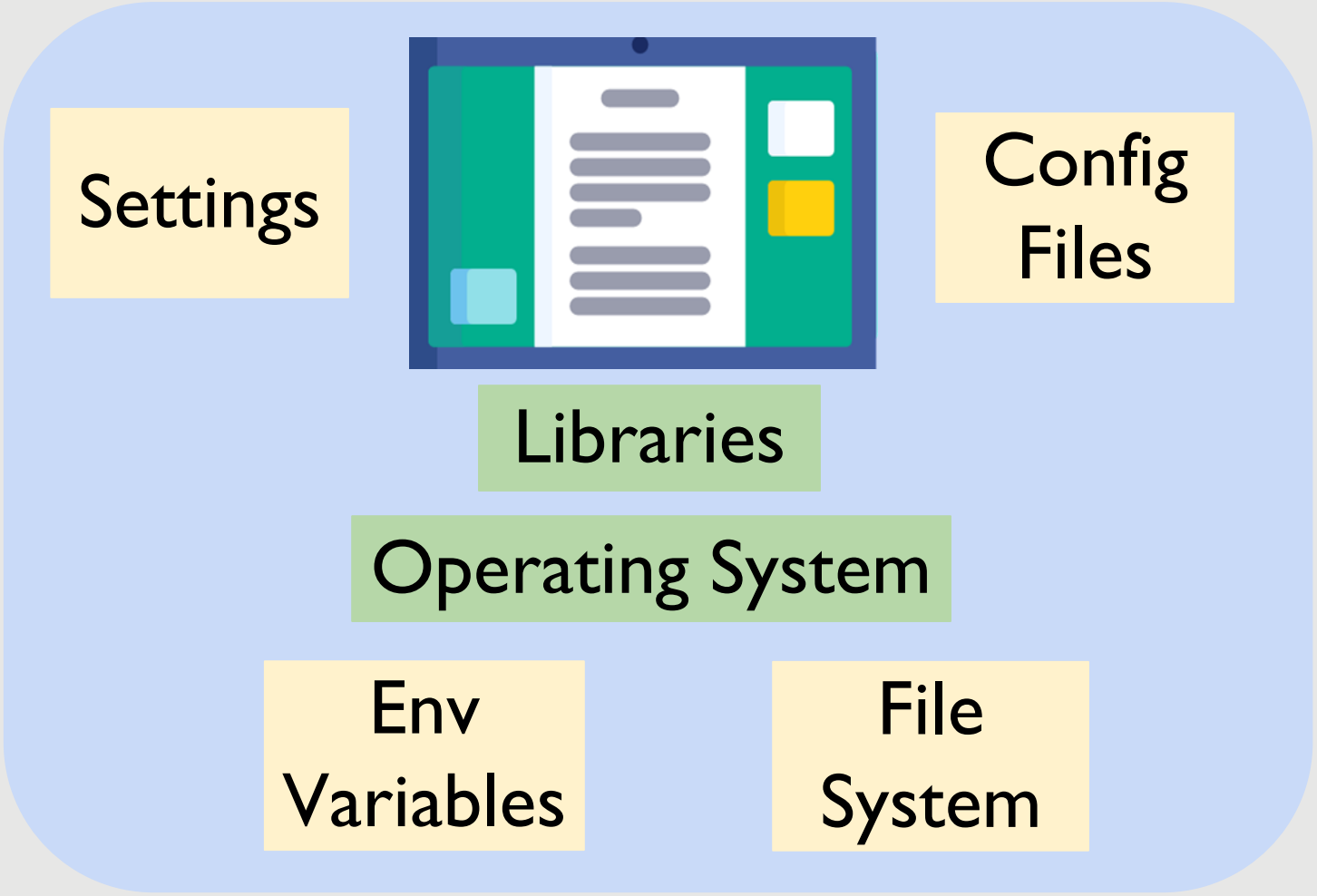

Not Shared

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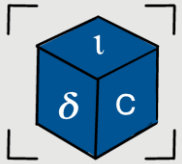

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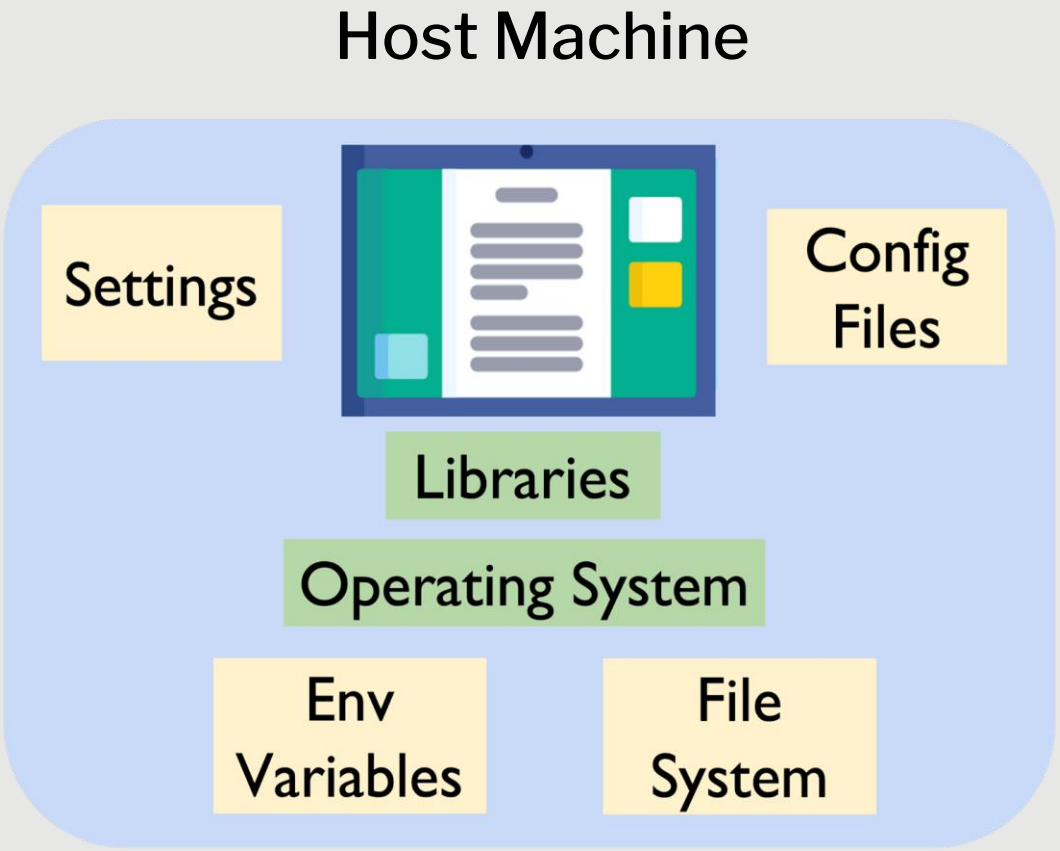

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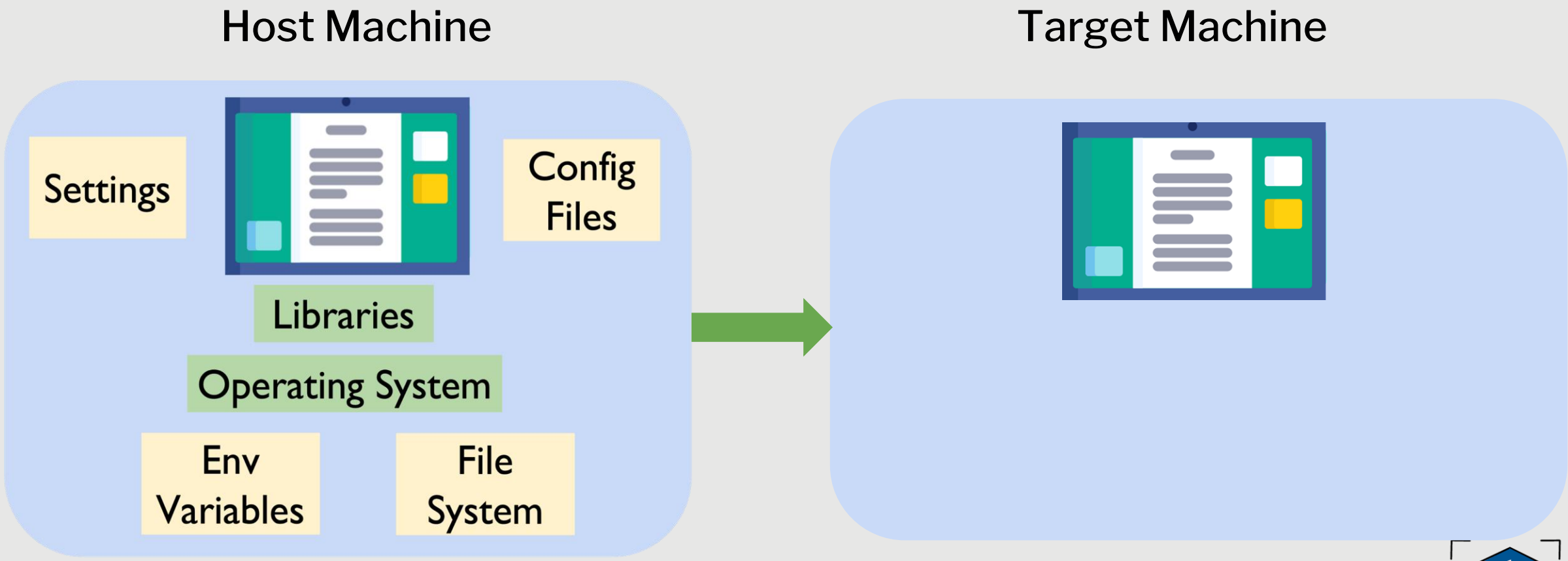

FLINC

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  - Preserves the interactive nature of notebooks
  - Guarantees reproducible execution
  - Supports flexibility to update and modify notebooks.

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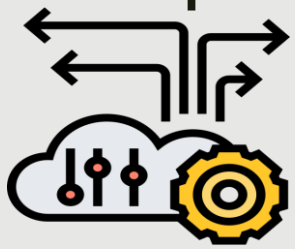

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Preserve Interactivity

Flexible for Modifications

Efficient and Easy to Use

Notebook Reproducibility

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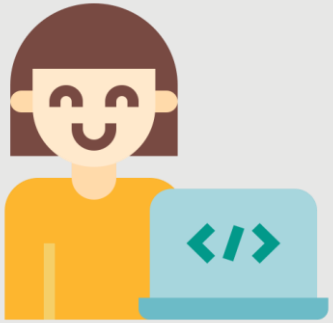
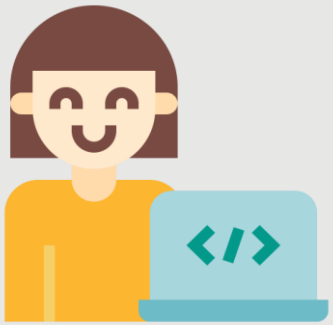


Alice

Notebook Reproducibility



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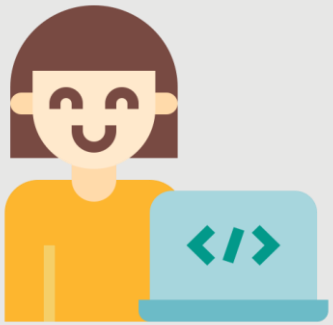

Alice

execute

modify

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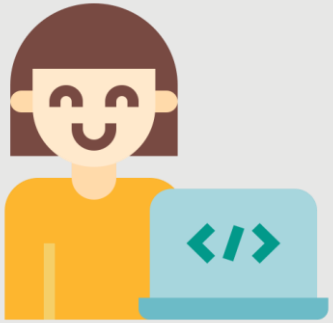

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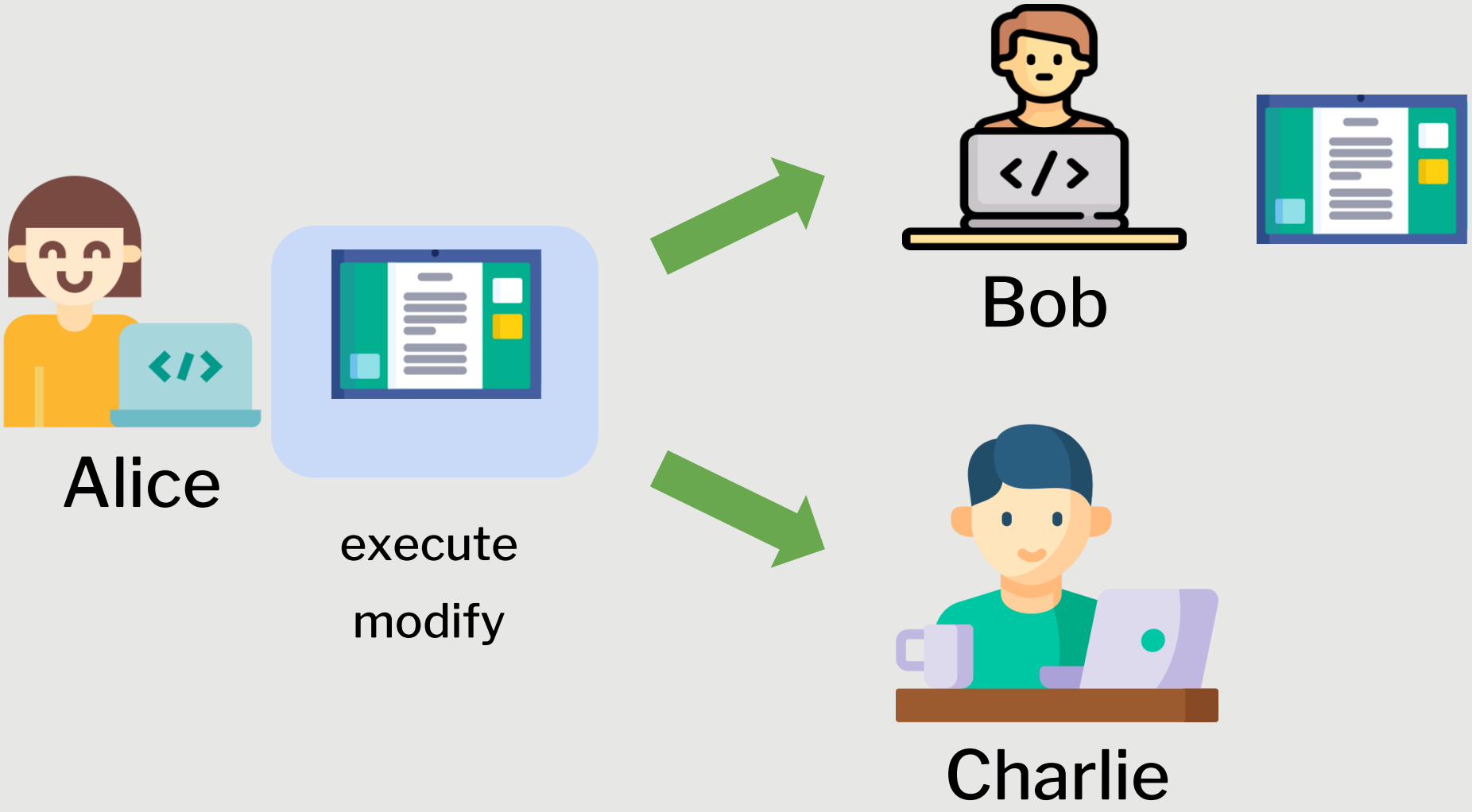

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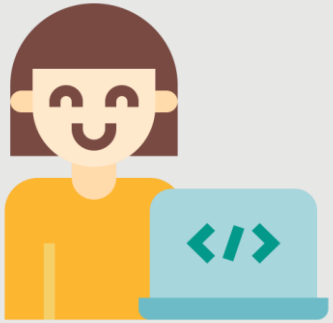

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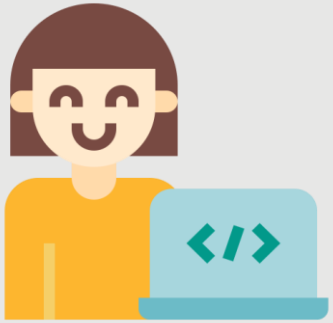

Alice

execute

modify

Bob

~~execute~~

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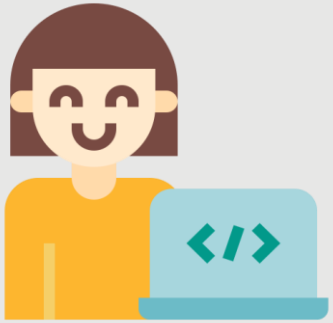

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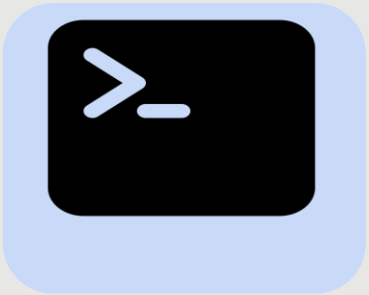

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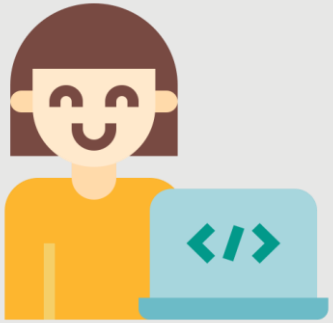

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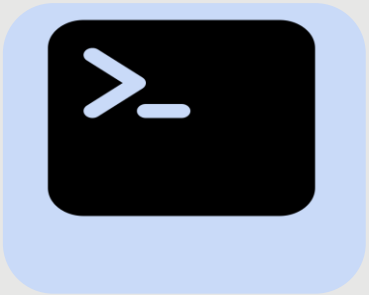

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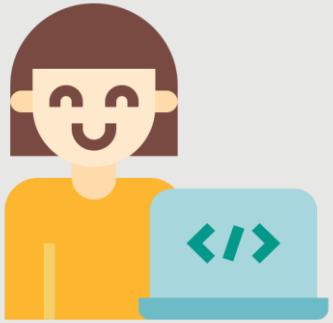

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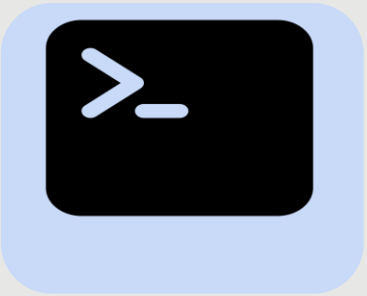

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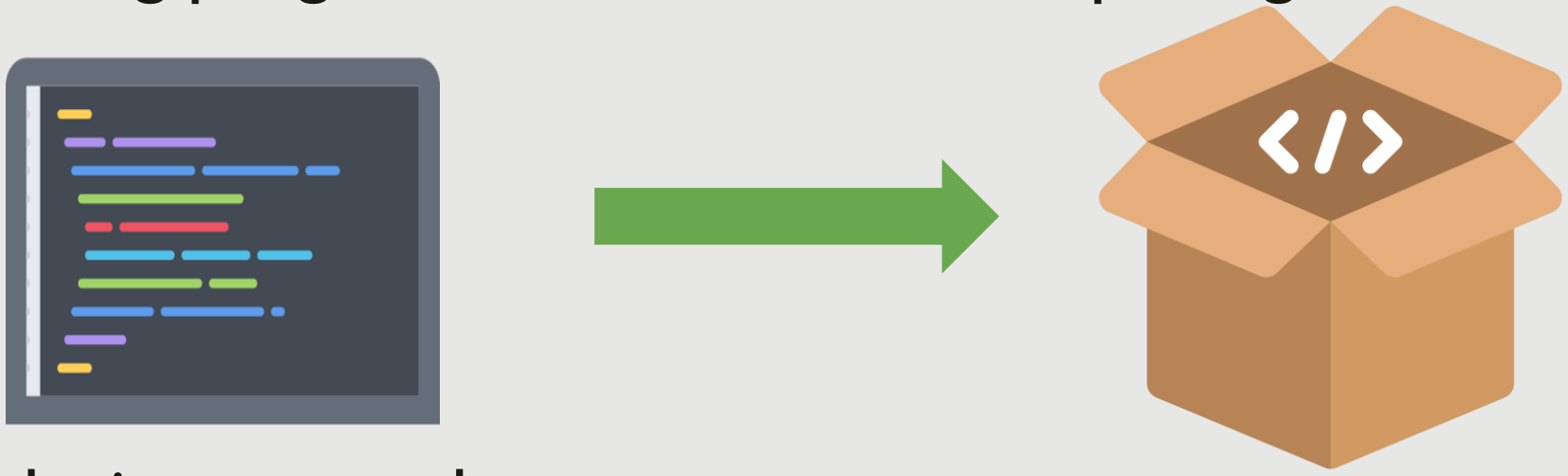
Problem

- Manual and time consuming.
- Requires technical knowledge.
- Conflict with existing environment.

Another Solution: Application Virtualization

- Application Virtualization(AV) is a method to convert executing programs into self-contained packages.



- Works in two modes:
  - Audit Mode - capture and encapsulate execution
  - Repeat Mode - repeat the captured execution

Limitations of AV

- Most AV systems assume batch workflows.
  - Not suited to capturing interactive notebooks.
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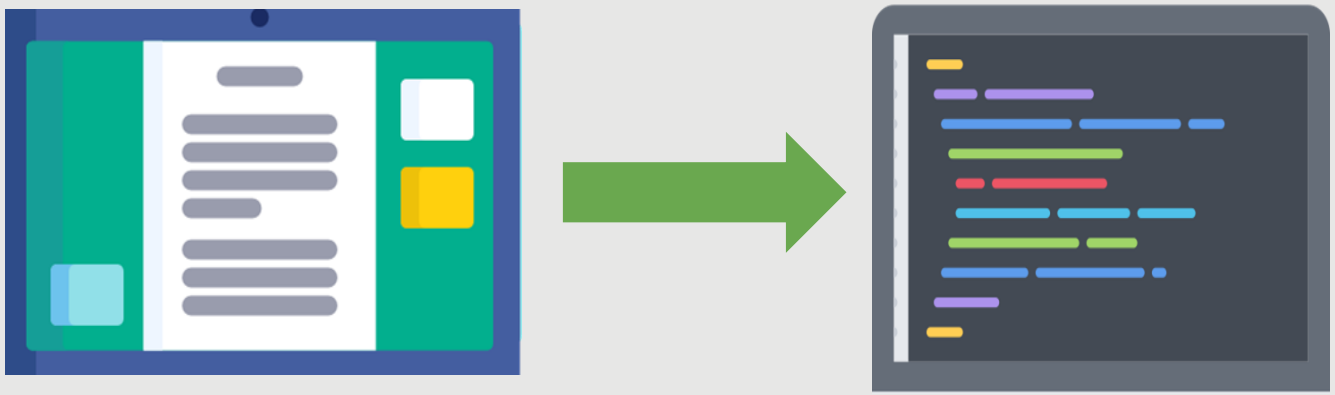

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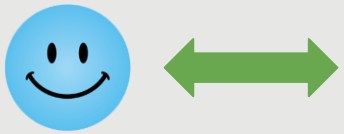

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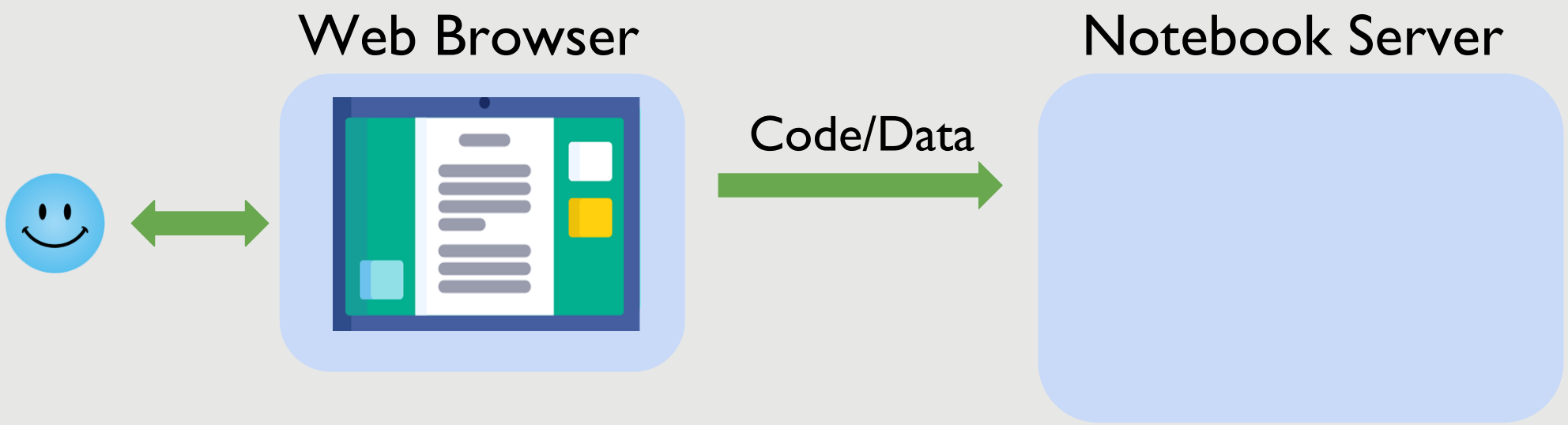

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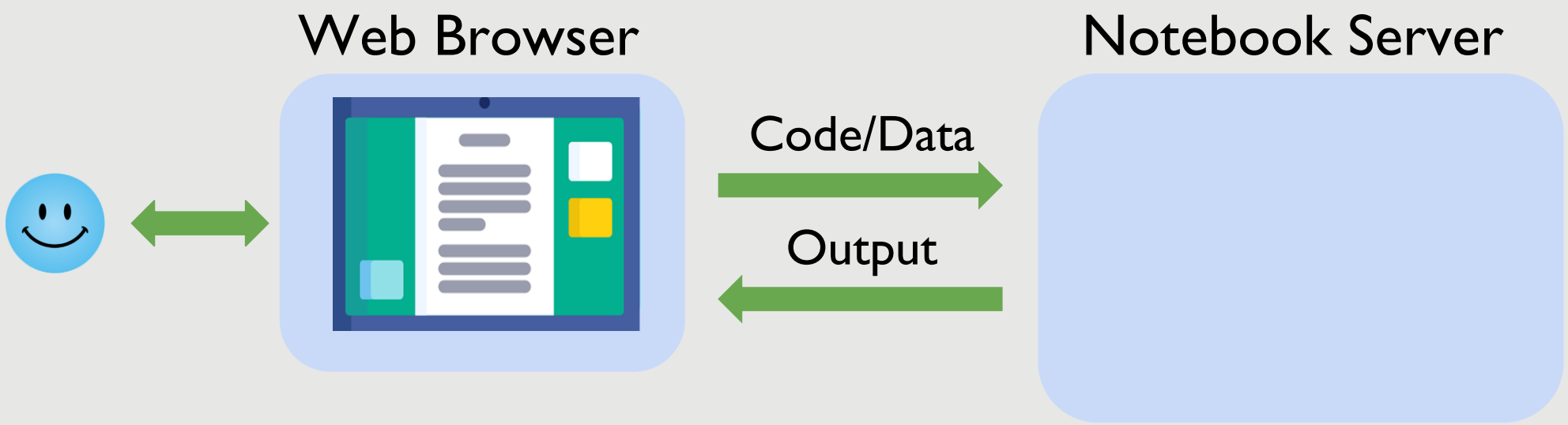

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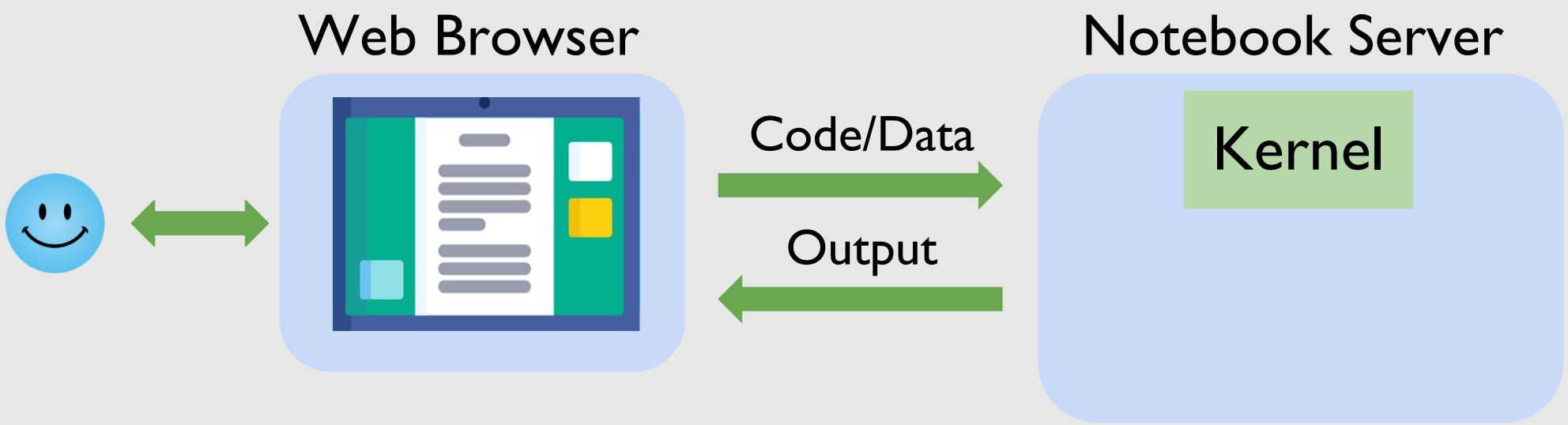

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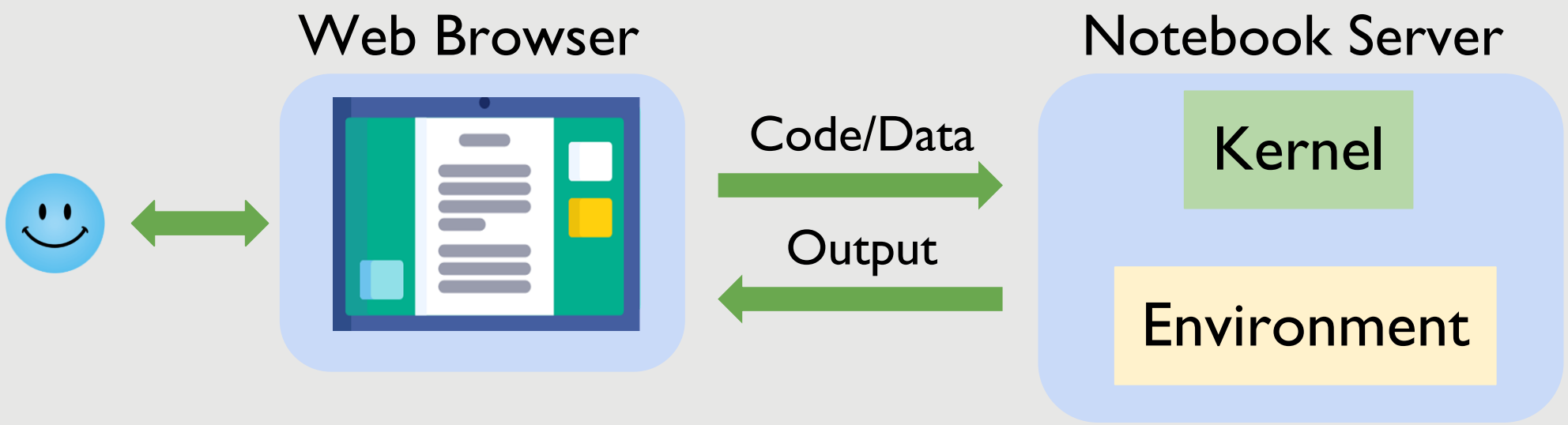

Extend AV to Notebook Client-Server Architecture

- Creates two additional kernels:
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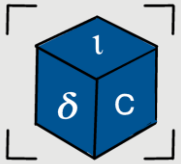
  - *Repeat kernel – repeats the containerized code*



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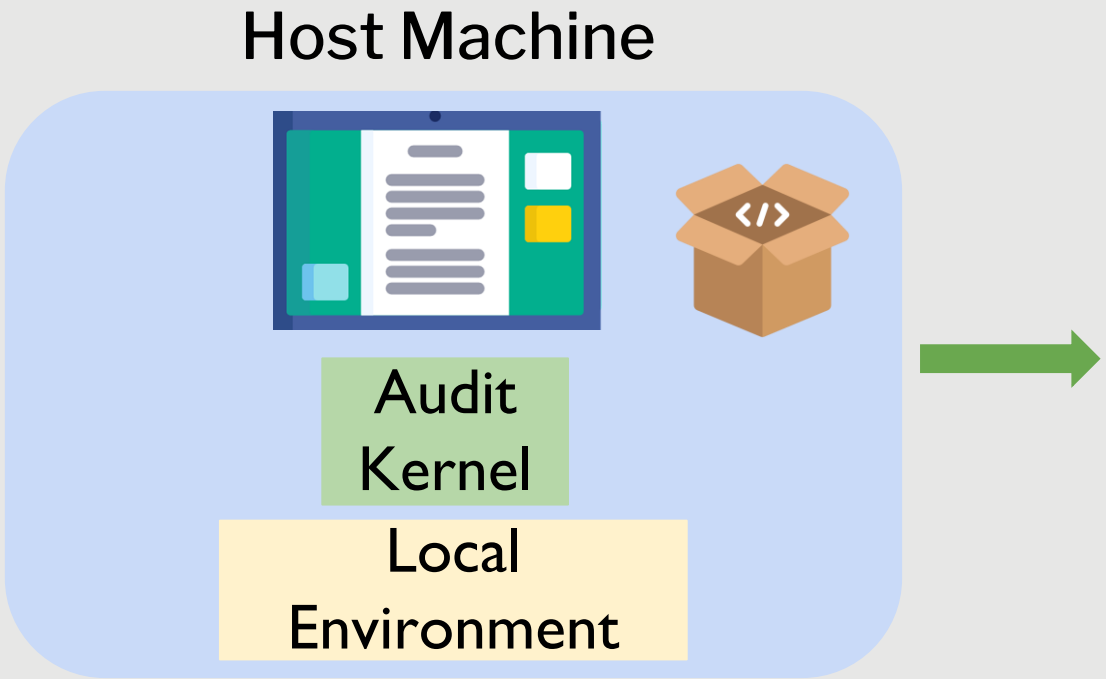

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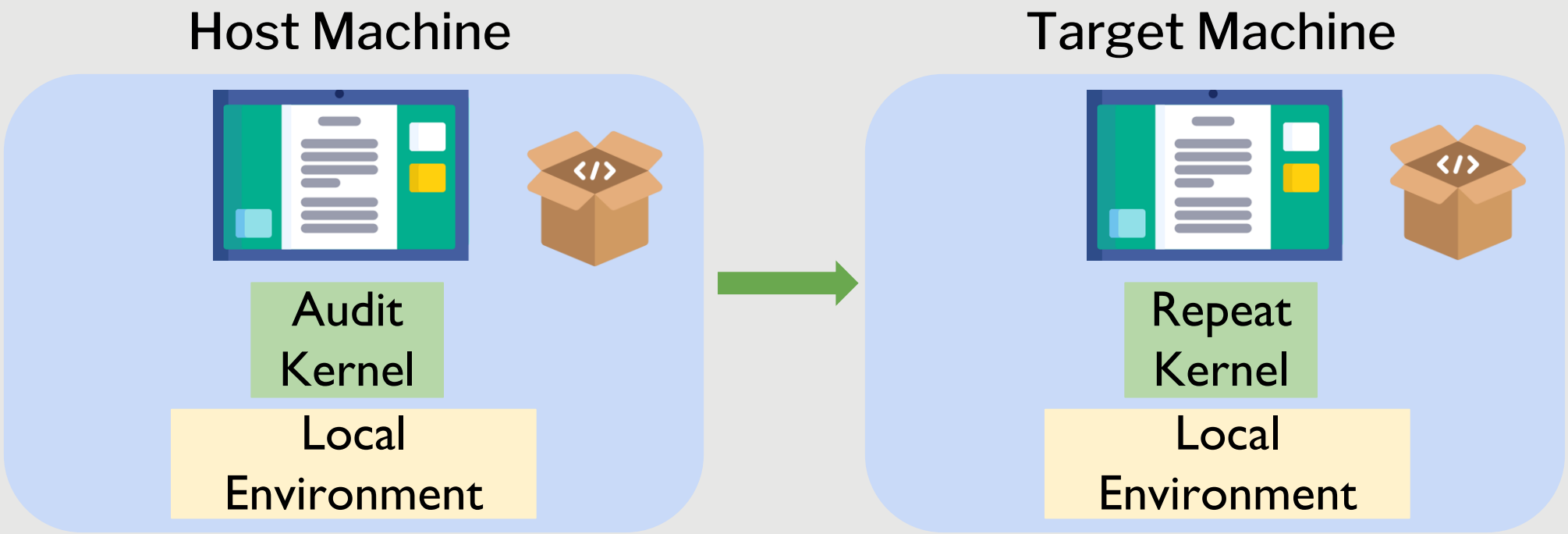

But, is Extending AV Enough? NO!

Bob

~~execute~~
modify

1. No Guarantee of Reproducible Execution
   - Notebook and container are separately shared

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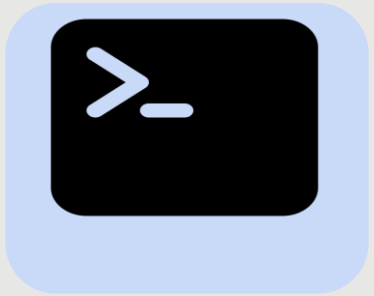
Bob

~~execute~~
modify

Charlie



execute
~~modify~~

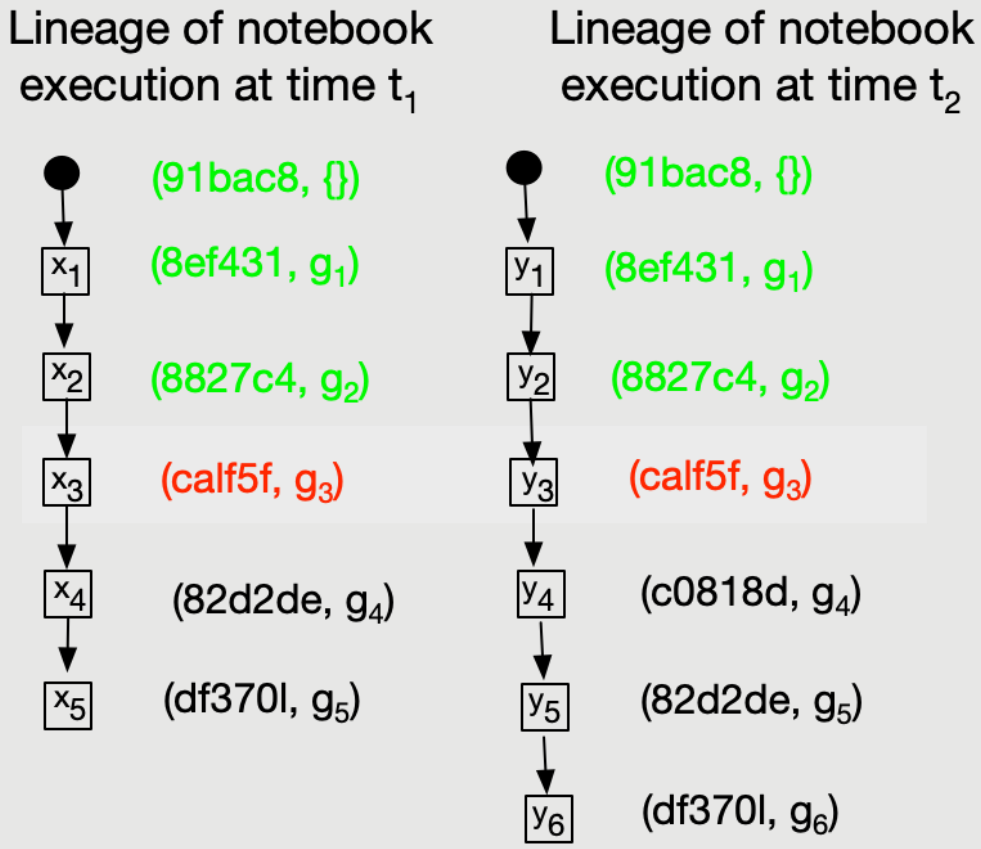
1. No Guarantee of Reproducible Execution
   - Notebook and container are separately shared

2. No Flexibility with Reproducible Execution
   a. No way to export dependencies

Ensuring Reproducible Execution

- **Key Idea: Lineage-based notebook cell equivalence**
- Compare *per cell* lineage during audit time with repeat time
  - Cell lineage = cell code hashes and state lineage
  - State lineage =
    - the predecessor cell's lineage
    - the sequence of system events triggered by program instructions in the cell, and
    - the hashes of the associated external data dependencies.

Lineage Equivalence



E_3 in L_1	E_3 in L_2
4183 fork 4184 4184 exec '/usr/torch/dataloader.py' 4184 open '/home/alice/new_fashion' 4183 mem 567894567 4184 read b2e1772	6254 fork 6255 6255 exec '/usr/torch/dataloader.py' 6255 open '/home/alice/new_fashion' 6255 read 6789b34 6254 mem 589715363

Given two notebook executions E_1 and E_2, cell state ps_i in E_1 is equal to cell state ps_j in E_2, denoted $ps_i = ps_j$, iff

(i) $h_i = h_j$, and

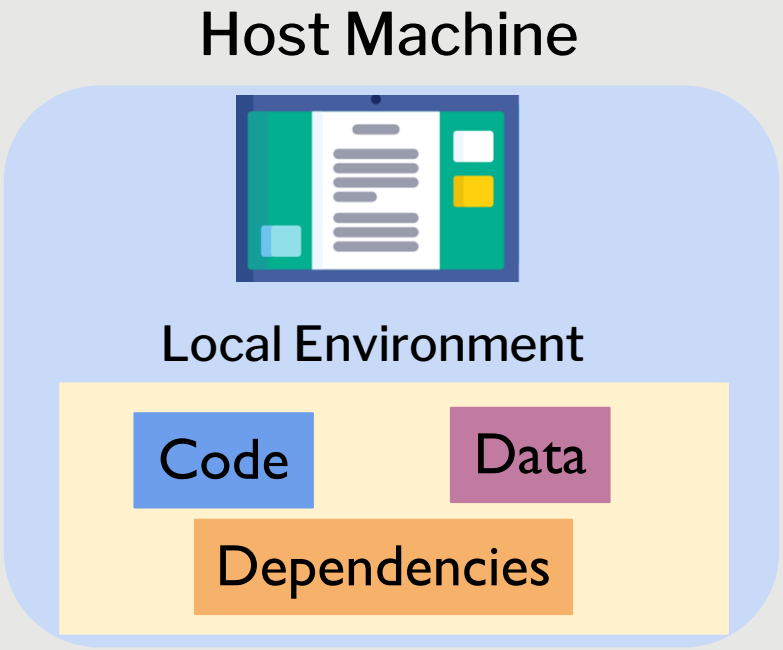
(ii) $g_i = g_j$

Flexible Reproducibility

Flexible Reproducibility

Export
Functionality

Flexible Reproducibility



Export
Functionality

Flexible Reproducibility

Host Machine

Local Environment

Code

Data

Dependencies

Export Functionality

Generates

Provenance Log

```
CLOSE /lib/x86_64-linux-gnu/libpthread.so.0
EXECVE 28567 /data/software/GLib/2.62.0-GCCcore-8.3.
EXECVE 28567 /data/software/GDAL/3.0.2-foss-2019b/bi
EXECVE 28567 /data/software/libiconv/1.16-GCCcore-8.
EXECVE 28567 /data/software/netCDF-C++4/4.3.1-gompi-
EXECVE 28567 /data/software/libdap/3.20.6-GCCcore-8.
EXECVE 28567 /data/software/netCDF-Fortran/4.5.2-gom
EXECVE 28567 /data/software/GRASS/7.8.3-foss-2019b/b
EXECVE 28567 /data/software/Java/11.0.2/ip /data/con
READ /data/lib/python3.7/site-packages/matplotlib-3.
CLOSE /data/lib/python3.7/site-packages/rasterio-1.2
READ /data/lib/python3.7/site-packages/xarray-0.16.2
READ /data/lib/python3.7/site-packages/numpy-1.20.1.
READ /data/lib/python3.7/site-packages/geopandas-0.1
READ /data/lib/python3.7/site-packages/pandas-1.2.2.
```

Flexible Reproducibility

Host Machine

Local Environment

Code

Data

Dependencies

Export Functionality

Generates

Provenance Log

```
CLOSE /lib/x86_64-linux-gnu/libpthread.so.0
EXECVE 28567 /data/software/GLib/2.62.0-GCCcore-8.3.
EXECVE 28567 /data/software/GDAL/3.0.2-foss-2019b/bi
EXECVE 28567 /data/software/libiconv/1.16-GCCcore-8.
EXECVE 28567 /data/software/netCDF-C++4/4.3.1-gompi-
EXECVE 28567 /data/software/libdap/3.20.6-GCCcore-8.
EXECVE 28567 /data/software/netCDF-Fortran/4.5.2-gom
EXECVE 28567 /data/software/GRASS/7.8.3-foss-2019b/b
EXECVE 28567 /data/software/Java/11.0.2/ip /data/con
READ /data/lib/python3.7/site-packages/matplotlib-3.
CLOSE /data/lib/python3.7/site-packages/rasterio-1.2
READ /data/lib/python3.7/site-packages/xarray-0.16.2
READ /data/lib/python3.7/site-packages/numpy-1.20.1.
READ /data/lib/python3.7/site-packages/geopandas-0.1
READ /data/lib/python3.7/site-packages/pandas-1.2.2.
```

Extract

```
numpy==1.19.1
memory_profiler==0.57.0
mccabe==0.6.1
pyzmq==19.0.1
pyepsg==0.4.0
decorator==4.4.2
pycparser==2.20
astroid==2.4.2
sklearn==0.0
pysumma==3.0.0
MarkupSafe==1.1.1
PyYAML==5.3.1
```

Notebook Dependencies

Flexible Reproducibility

Host Machine

Local Environment

Code

Data

Dependencies

Export Functionality

Target Machine

Local Env

Virtual Environment

Code

Data

Dependencies

Generates

Installs

Provenance Log

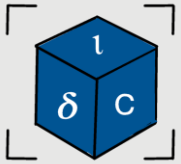
```
CLOSE /lib/x86_64-linux-gnu/libpthread.so.0
EXECVE 28567 /data/software/GLib/2.62.0-GCCcore-8.3.
EXECVE 28567 /data/software/GDAL/3.0.2-foss-2019b/bi
EXECVE 28567 /data/software/libiconv/1.16-GCCcore-8.
EXECVE 28567 /data/software/netCDF-C++4/4.3.1-gompi-
EXECVE 28567 /data/software/libdap/3.20.6-GCCcore-8.
EXECVE 28567 /data/software/netCDF-Fortran/4.5.2-gom
EXECVE 28567 /data/software/GRASS/7.8.3-foss-2019b/b
EXECVE 28567 /data/software/Java/11.0.2/ip /data/con
READ /data/lib/python3.7/site-packages/matplotlib-3.
CLOSE /data/lib/python3.7/site-packages/rasterio-1.2
READ /data/lib/python3.7/site-packages/xarray-0.16.2
READ /data/lib/python3.7/site-packages/numpy-1.20.1.
READ /data/lib/python3.7/site-packages/geopandas-0.1
READ /data/lib/python3.7/site-packages/pandas-1.2.2.
```

Extract

```
numpy==1.19.1
memory_profiler==0.57.0
mccabe==0.6.1
pyzmq==19.0.1
pyepsg==0.4.0
decorator==4.4.2
pycparser==2.20
astroid==2.4.2
sklearn==0.0
pysumma==3.0.0
MarkupSafe==1.1.1
PyYAML==5.3.1
```

Notebook Dependencies

Experiments



Experiments

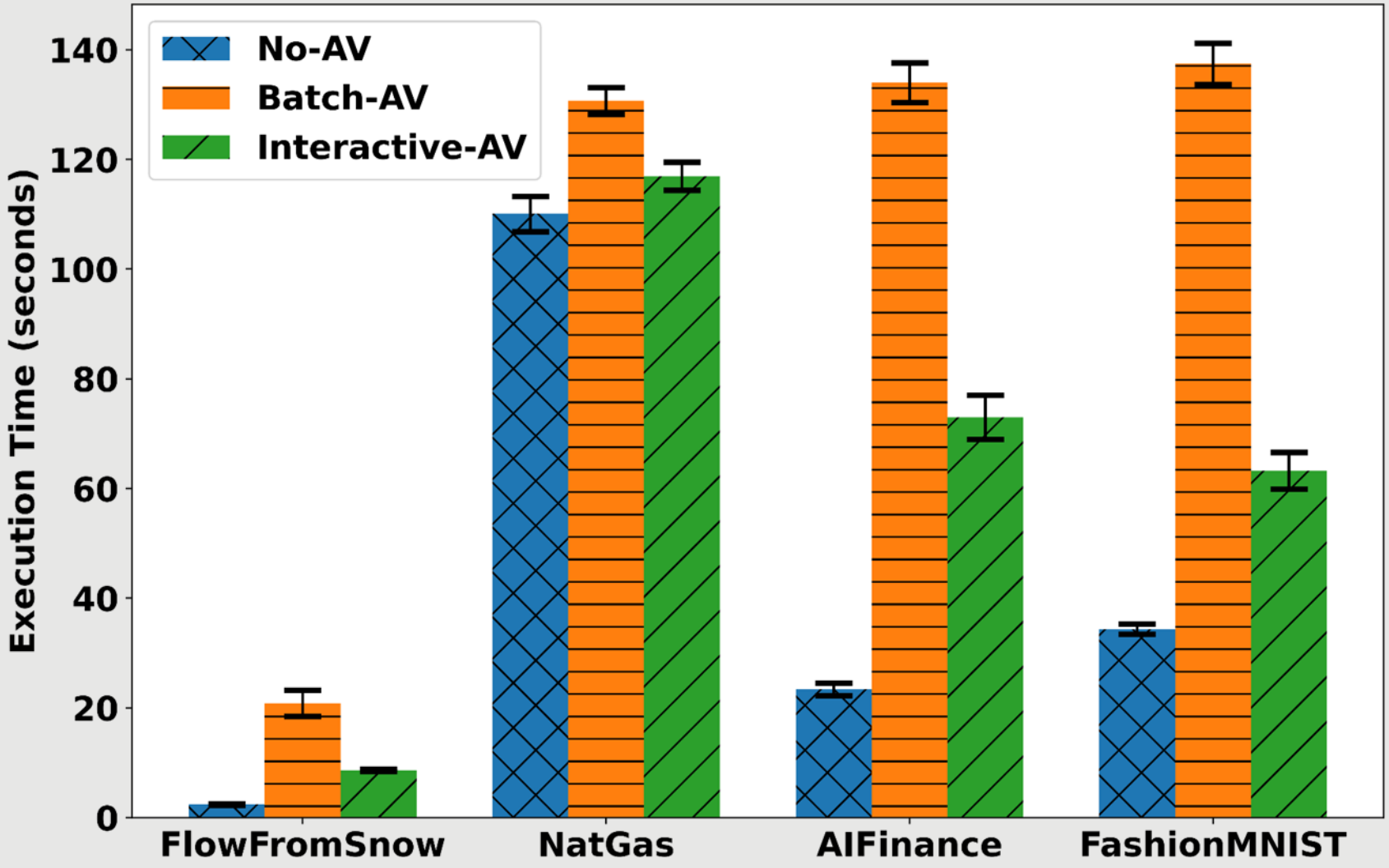
- Analyze storage and running time for AV and export.
- Experiment using 4 Python notebooks.
- Compare three methods for AV performance.

  1. Interactive-AV: FLINC notebook auditing

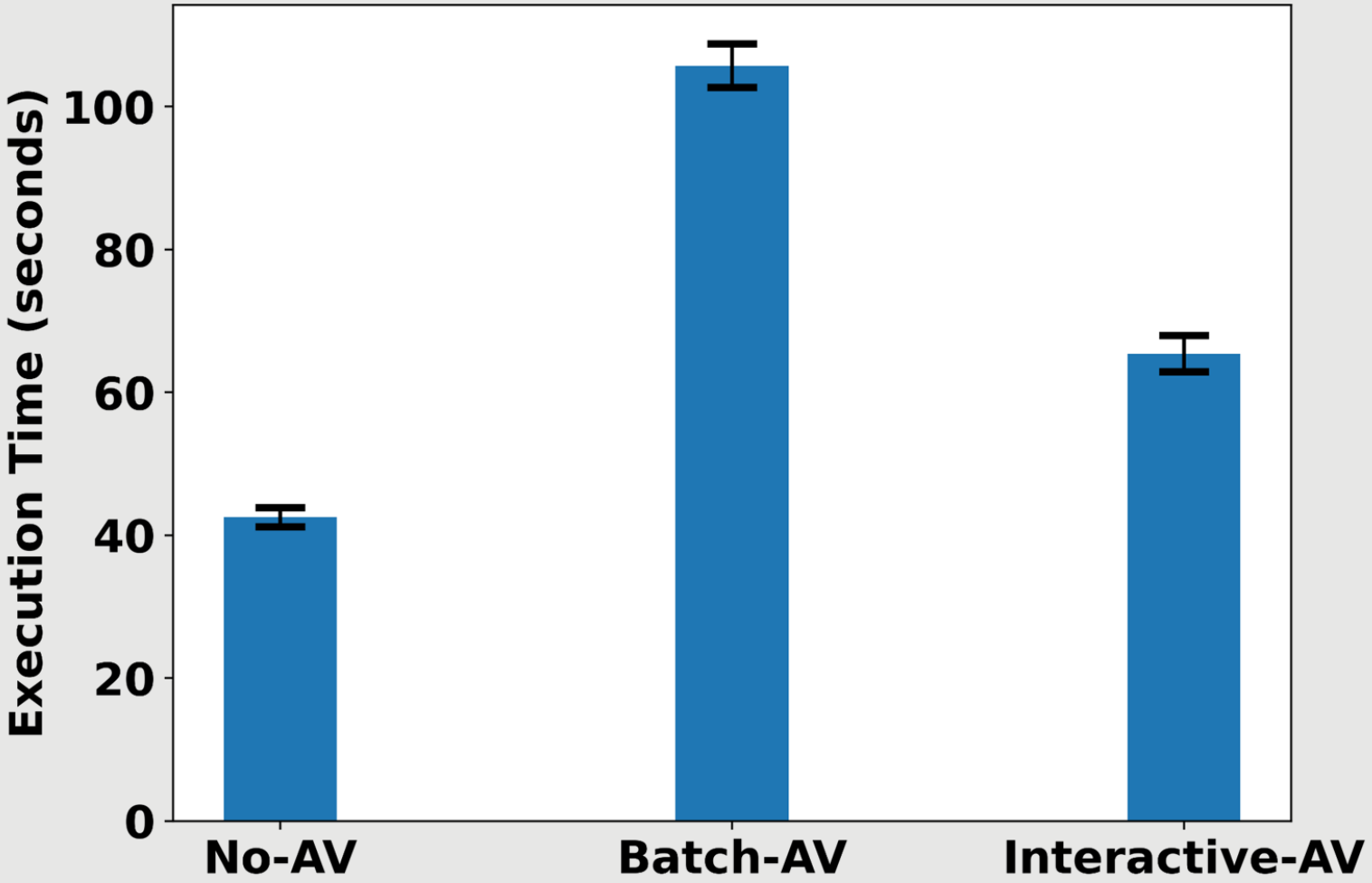
  2. Batch-AV: Python file of notebook audited using AV

  3. Baseline: No-AV: Regular notebook execution

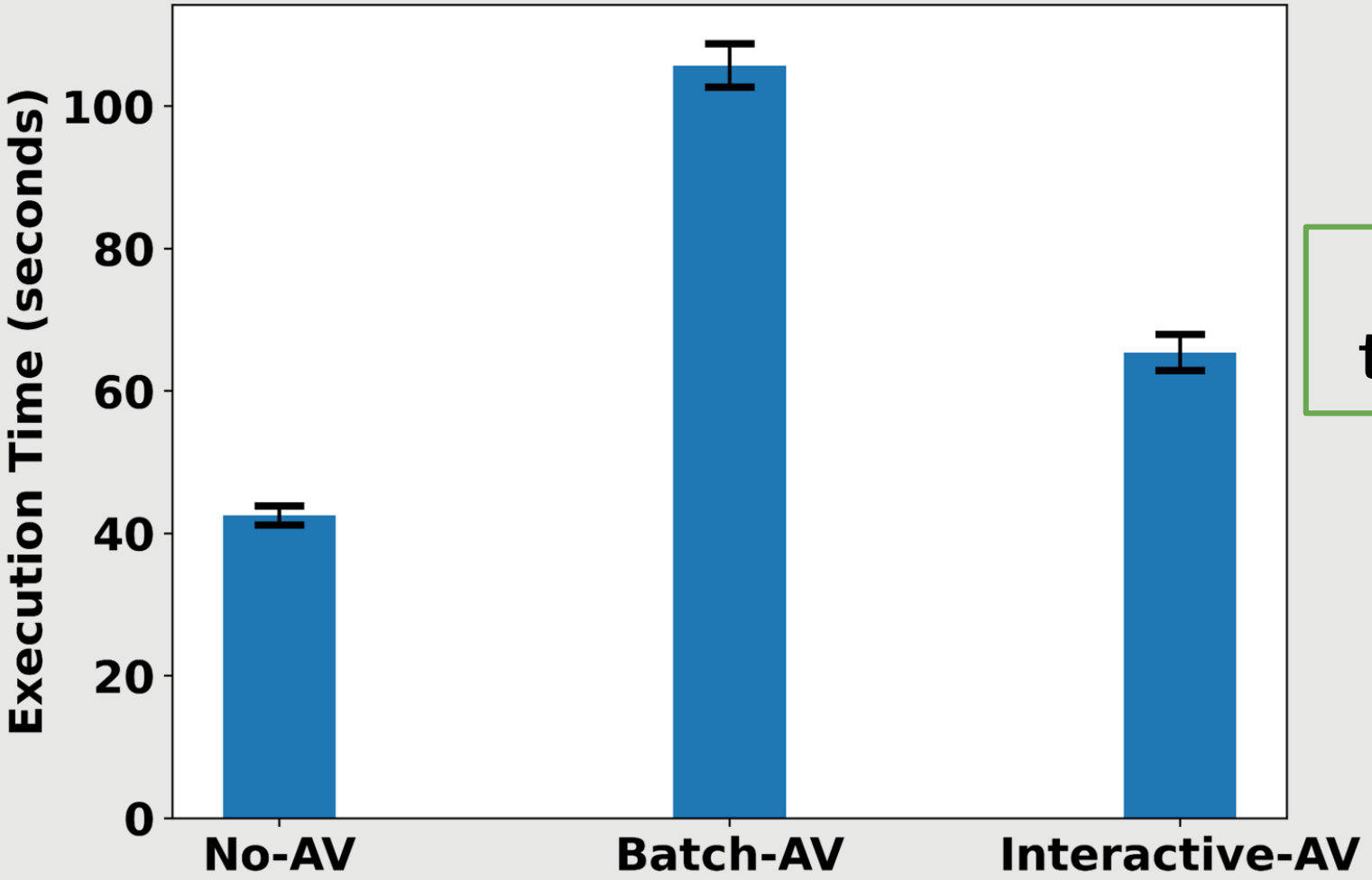
Notebook Execution Time



Average Execution Time

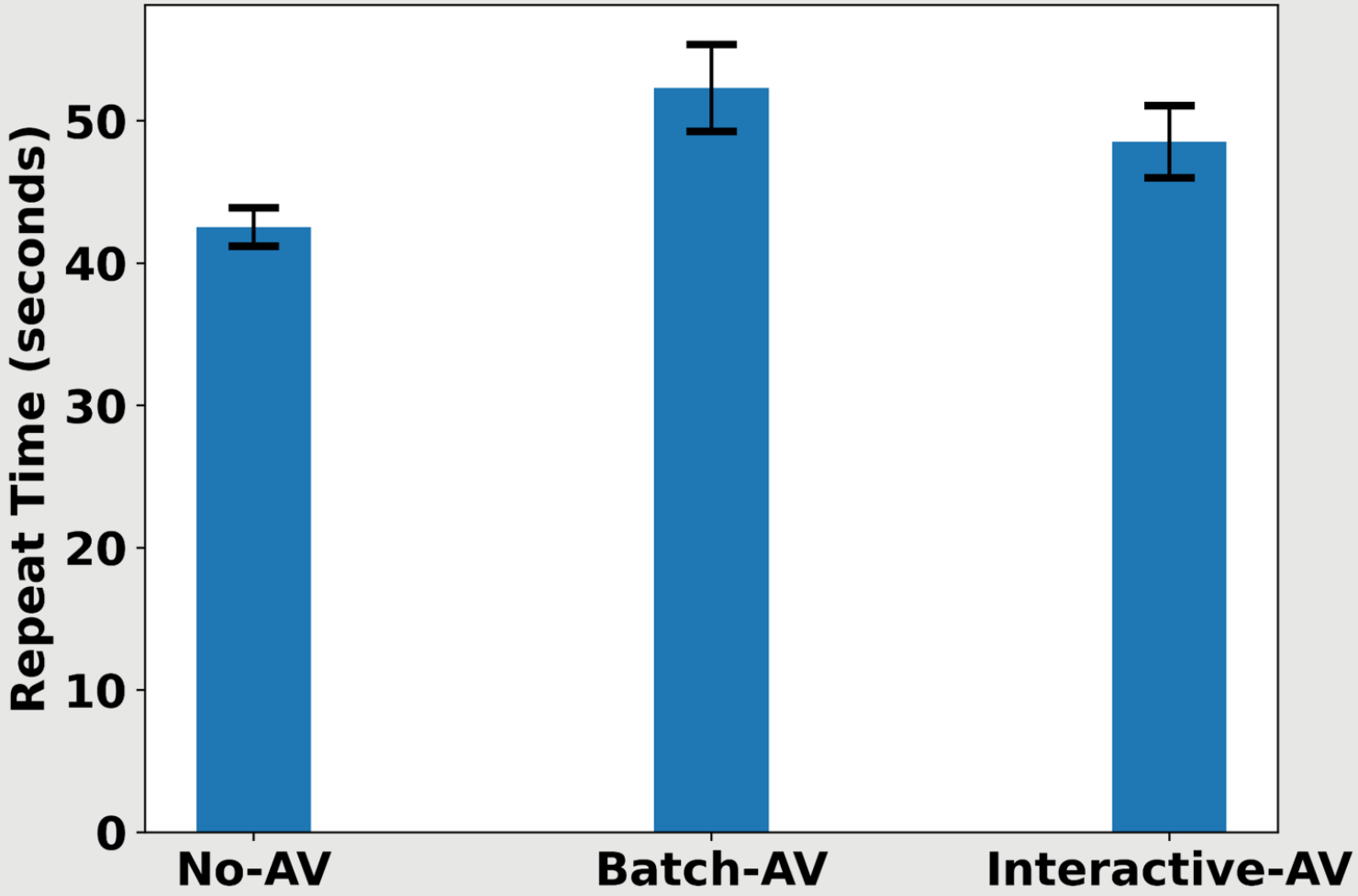


Average Execution Time



38% less than Batch-AV

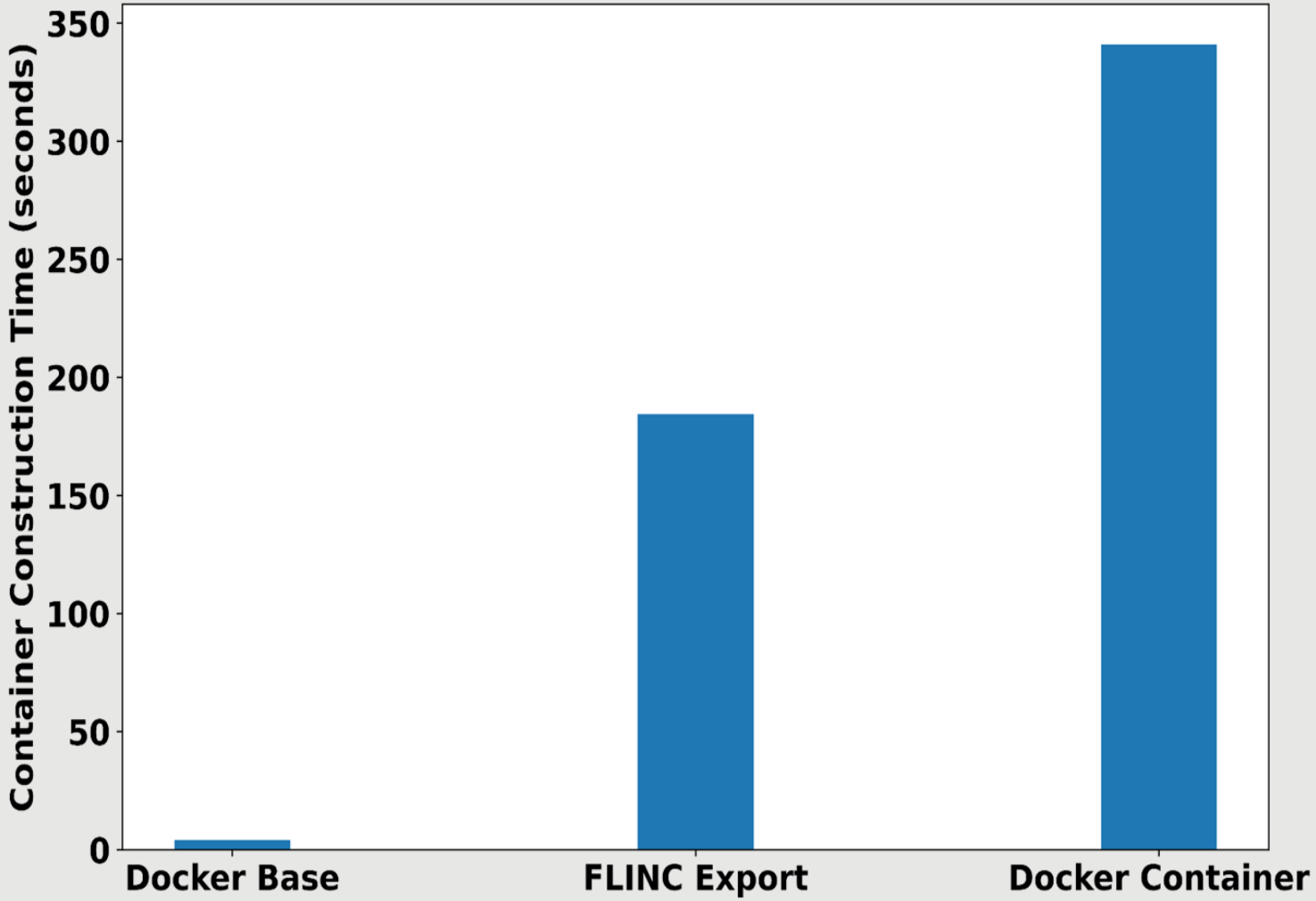
Average Repeat Time



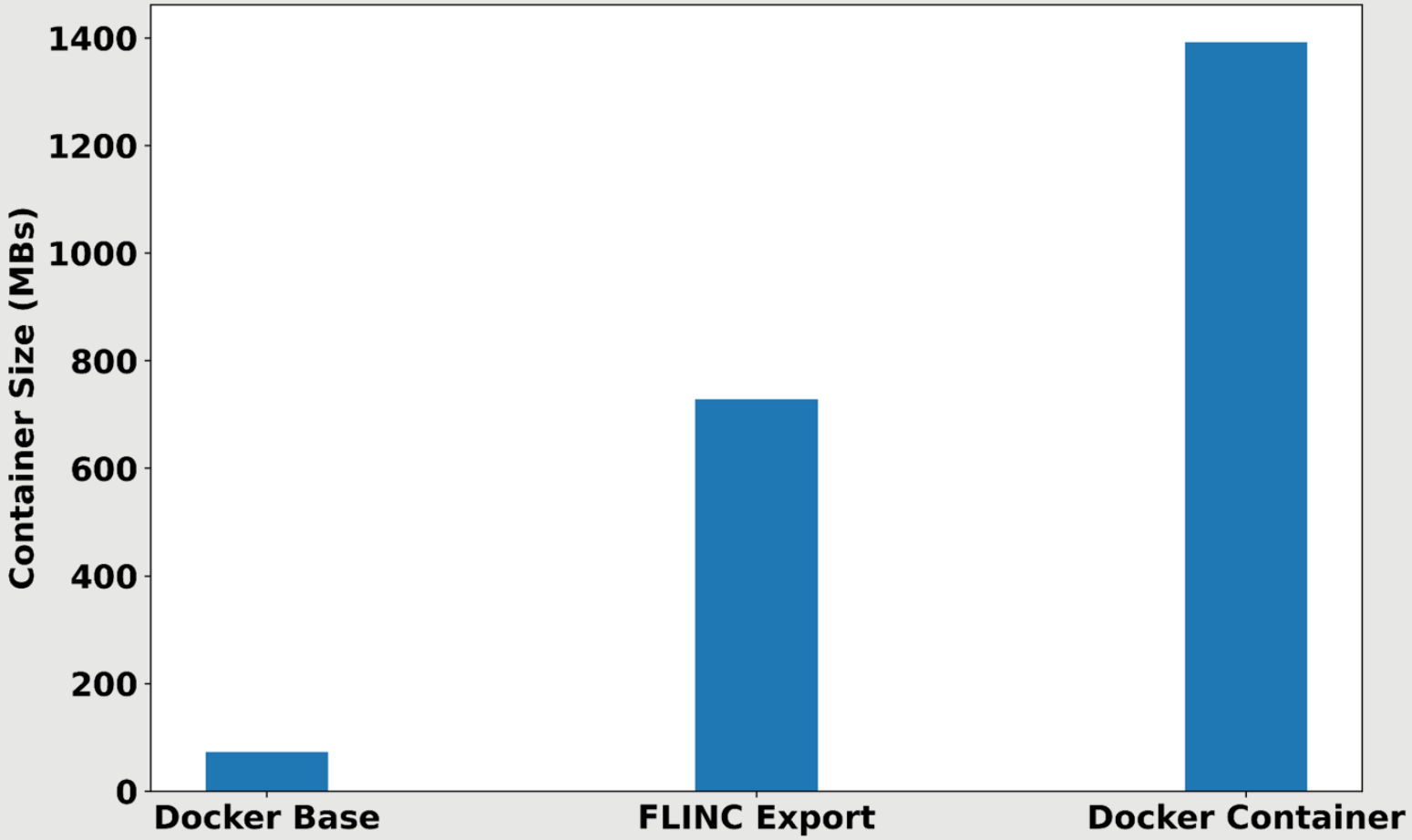
FLINC Export Overhead

- Compare three methods for export functionality.
  1. FLINC Export
     - FLINC virtual environment with dependencies
  2. Docker Container
     - Docker container with same dependencies
  3. Docker Base
     - Docker base Ubuntu image

Export Execution Time



Export Size


Container Size (MBs)
0
200
400
600
800
1000
1200
1400
Docker Base
FLINC Export
Docker Container

Future Work

- Detailed analysis on the performance of FLINC.
- Beyond current reliance on Linux *strace* for auditings.
- Extendible to other event tracing systems like ETW/procmon for Windows and OpenBSM/dtrace for MacOS.
- Extendible to other packaging formats such as Flatpak or MacOS Bundles.

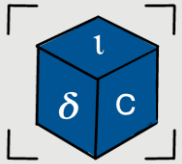
Conclusion

- Motivate the need for sharing and reproducing notebooks successfully.
- Elaborate reproducibility of notebooks for different scenarios.
- Introduce FLINC to create reproducible notebook containers that work across multiple environments.
- Experiments on notebooks using FLINC.

Acknowledgements

- NSF CNS-1846418, NSF ICER-1639759, ICER-1661918.

- David Tarboton, Jonathan L. Goodall, Shilvi Satpati, YoungDon Choi, Ayman Nassar, Binata Roy, Iman Maghami, Zhiyu Li, and Anthony Castronova.



THANK YOU!

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