Session 6.2 Scaling up Interactive Data Analysis in Jupyter Lab: From Laptop to HPC

SDSC Summer Institute 2023

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COMPUTING WITHOUT BOUNDARIES

EXPANSE

SAN DIEGO SUPERCOMPUTER CENTER

UNIVERSITY OF CALIFORNIA SAN DIEGO

Outline

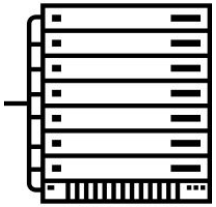
- When to run on Expanse
- Setup a portable and reproducible software environment
- Scale up calculations on CPU/GPU using Dataframes
- Run Jupyter Lab in Batch
- Best Practices for Authoring Jupyter Notebooks

When to run on Expanse

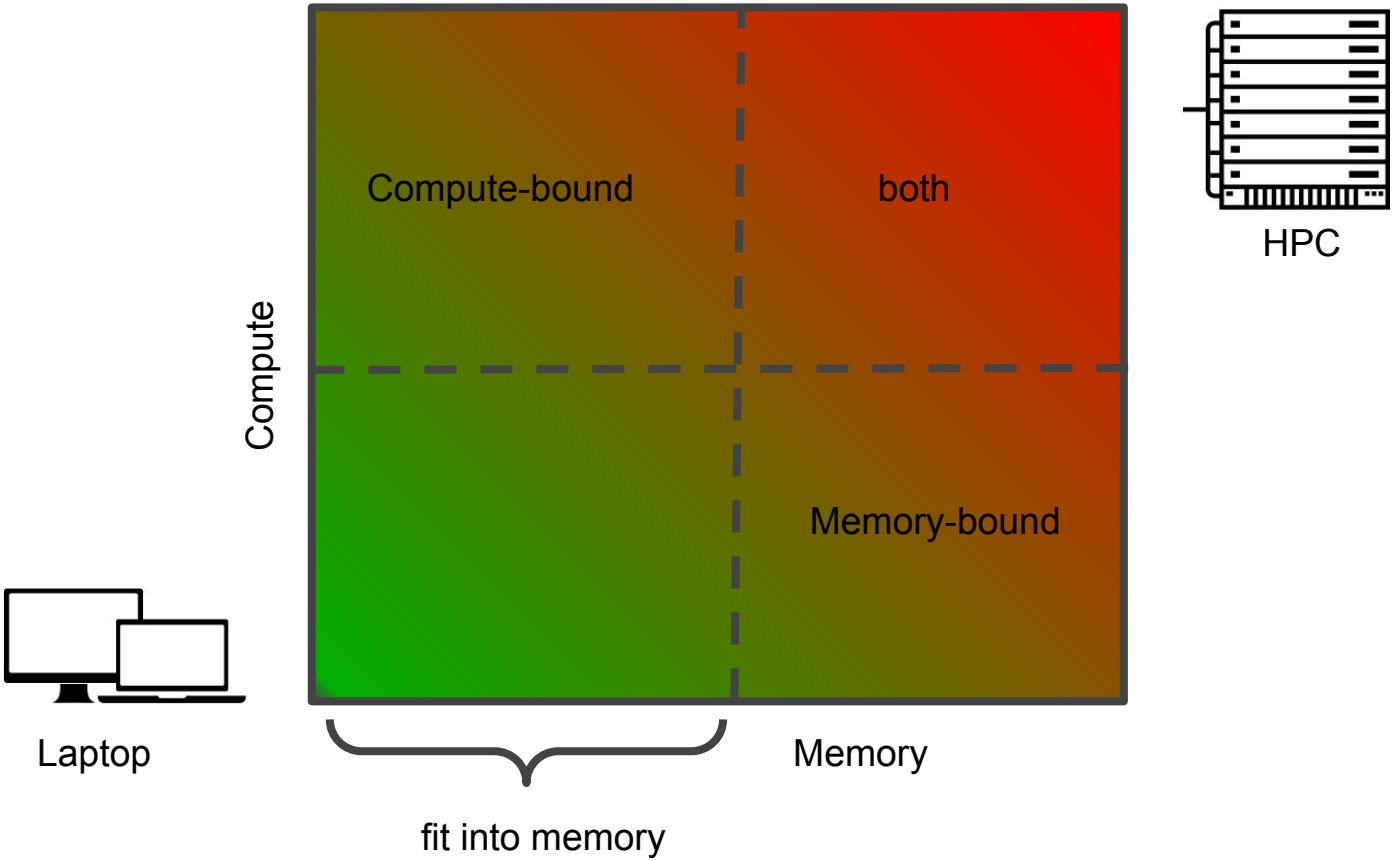
Laptop/Desktop

- Coding
- Exploratory phase
- Small datasets
- Run on single or few cores

Expanse



- Scaling up to
  - large datasets
  - long runtimes
- Run on many cores
- Run on GPUs


Compute-bound
both
Memory-bound
Compute
HPC
Laptop
Memory
fit into memory

Expanse Nodes

128 CPU cores/node

Compute Nodes	
CPU Type	*AMD EPYC 7742*
Nodes	728
Sockets	2
Cores/socket	64
Clock speed	2.25 GHz
Flop speed	4608 GFlop/s
Memory capacity	* 256 GB DDR4 DRAM
Local Storage	1TB Intel P4510 NVMe PCIe SSD
Max CPU Memory bandwidth	409.5 GB/s

4 GPUs, 40 CPU cores/node

GPU Nodes	
GPU Type	NVIDIA V100 SMX2
Nodes	52
GPUs/node	4
CPU Type	Xeon Gold 6248
Cores/socket	20
Sockets	2
Clock speed	2.5 GHz
Flop speed	34.4 TFlop/s
Memory capacity	*384 GB DDR4 DRAM
Local Storage	1.6TB Samsung PM1745b NVMe PCIe SSD
Max CPU Memory bandwidth	281.6 GB/s

Details: https://portal.xsede.org/sdsc-expanse

Jupyter Notebook (CPU) →

Jupyter Notebook (GPU) →

Testing (CPU) →

Testing (GPU) →

Partition Name	Max Walltime	Max Nodes/Job	Max Running Jobs	Max Running + Queued Jobs	Charge Factor	Notes
compute	48 hrs	32	32	64	1	Exclusive access to regular compute nodes; *limit applies per group*
ind-compute	48 hrs	32	32	64	1	Exclusive access to Industry compute nodes; *limit applies per group*
shared	48 hrs	1	4096	4096	1	Single-node jobs using fewer than 128 cores
ind-shared	48 hrs	1	32	64	1	Single-node Industry jobs using fewer than 128 cores
gpu	48 hrs	4	4	8 (32 Tres GPU)	1	Used for exclusive access to the GPU nodes
ind-gpu	48 hrs	4	4	8 (32 Tres GPU)	1	Exclusive access to the Industry GPU nodes
gpu-shared	48 hrs	1	24	24 (24 Tres GPU)	1	Single-node job using fewer than 4 GPUs
ind-gpu-shared	48 hrs	1	24	24 (24 Tres GPU)	1	Single-node job using fewer than 4 Industry GPUs
large-shared	48 hrs	1	1	4	1	Single-node jobs using large memory up to 2 TB (minimum memory required 256G)
debug	30 min	2	1	2	1	Priority access to shared nodes set aside for testing of jobs with short walltime and limited resources
gpu-debug	30 min	2	1	2	1	Priority access to gpu-shared nodes set aside for testing of jobs with short walltime and limited resources; *max two gpus per job*
preempt	7 days	32		128	.8	Non-refundable discounted jobs to run on free nodes that can be pre-empted by jobs submitted to any other queue
gpu-preempt	7 days	1		24 (24 Tres GPU)	.8	Non-refundable discounted jobs to run on unallocated nodes that can be pre-empted by higher priority queues

Setup a portable and reproducible software environment

Reproducibility*

obtaining **consistent** results using

same input data or parameters

same computational steps, methods, and code

same analysis conditions

Reusability

obtaining **new** results using

different input data or parameters

same computational steps, methods, and code

same analysis conditions

Scalability

obtaining **new** results using

large input data or parameter sets

same computational steps, methods, and code

same analysis conditions

* L. Barba, https://figshare.com/articles/Next_in_Reproducibility_standards_policies_infrastructure_and_human_factors/8194328/1

Tools and Infrastructure

Computational notebooks: combine documentation, code, and results

Version-control system for tracking changes in source code

Source code repository

Open-source package and environment management system

Container that packages software and OS in a portable way

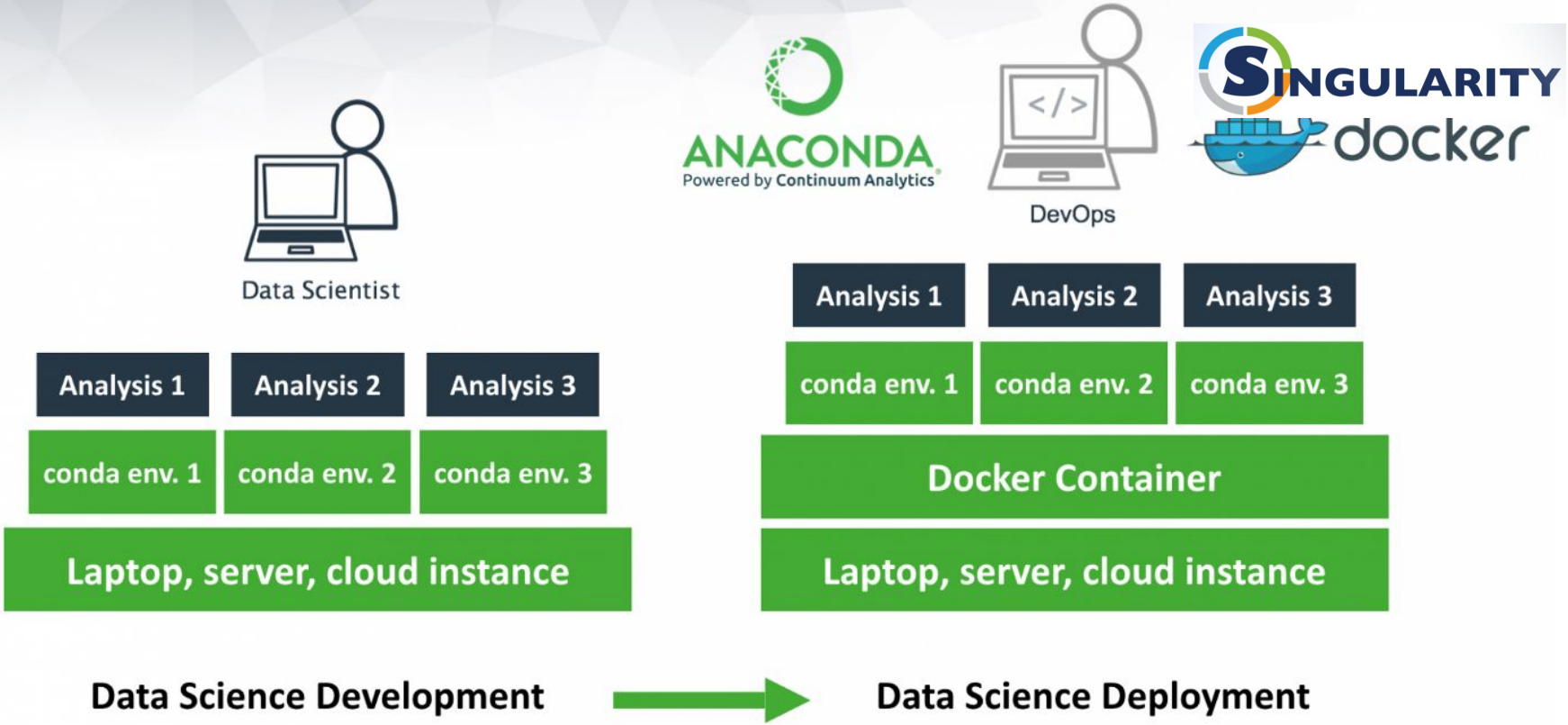
Scalable compute infrastructure

Reproducible Environments

CONDA

- Beginner
- Experience with Conda
- Exploratory development
- Frequently changing dependencies
- Easy to compose an environment with many dependencies
- Run on single node on Expanse
- Supported on Linux, Mac, Windows
- Run on native OS

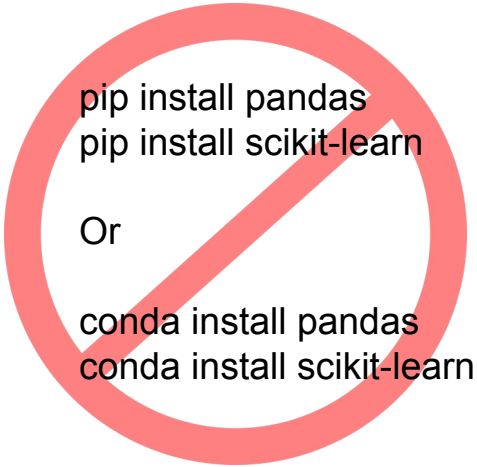
- Advanced user
- Experience with containers
- Production environment
- Often setup for a single tool
- Optimized containers for Expanse
  - pytorch, tensorflow, …
  - support for multi-node
- Supported on Linux
- Mac, Windows requires a VM
- Run on packaged OS, e.g. Ubuntu



Source: https://medium.com/@patrickmichelberger/getting-started-with-anaconda-docker-b50a2c482139

- **Package management system**
  - Conda installs, runs, and updates open source packages (e.g., NumPy, Pandas) and their dependencies, while checking compatibility with all preexisting packages.
- **Environment management system**
  - Conda allows you to create, save, load and switch between multiple environments on your local computer, as well as share instructions for how to recreate that environment on a different computer.
- **Multi-platform (Windows, MacOS, and Linux)**
- **Multi-language (Python, R, Ruby, Scala, Java, JavaScript, C/ C++, etc.)**

Why Conda Environments?



Directly installing packages into your base environment will lead to version conflicts, errors, and non-reproducible results.

environment_1

python=3.7
pandas=0.25.0
scikit-learn=0.20.0

environment_2

python=3.9
pandas=1.2.4
scikit-learn=0.24.2

By creating conda environments, multiple versions of software packages can co-exists without interference.

Conda environments are portable and can be installed on multiple platforms.

Define a Conda Environments

Create an **environment.yml** file in the top level of a Git Repository (https://github.com/sbl-sdsc/df-parallel)

```yaml
name: df-parallel

channels:
  - conda-forge
  - anaconda

dependencies:
  - python=3.10
  - jupyterlab=4.0.1
  - ipywidgets=8.0.6
  - matplotlib=3.7.1
  - seaborn=0.12.2
  - papermill=2.3.4
  - dask=2023.3.2
  - pyspark=3.4.0
  - pyarrow=10.0.1
  - openjdk=17.0.3

variables:
  # SPARK conf directory with logging configuration
  SPARK_CONF_DIR: ../conf
  SPARK_DRIVER_MEMORY: 16G
  SPARK_DRIVER_MAXRESULTSIZE: 4G
  SPARK_WORKER_MEMORY: 4G
```

Use the same name as your Git repository

Specify the channels where to look for packages. Order matters! The conda-forge channel has newer versions than anaconda.

Specify (**"pin"**) version number to ensure reproducibility and compatibility.

Specify non-Python packages (e.g., Java).

Set environment variables (e.g., configuration options).

Create a Conda Environment

Prerequisite: Miniconda3 (light-weight, preferred) or Anaconda3 installed

https://docs.conda.io/en/latest/miniconda.html

Create a Conda environment

```
conda env create -f environment.yml
```

or

```
mamba env create -f environment.yml (faster)
```

Mac, Windows, Linux

Activate a Conda environment

```
conda activate <environment_name>
```

Run Jupyter Lab

```
jupyter lab
```

Expanse: **Do not** create a Conda environment in your home directory (network file system)
-> Use the **galyleo** script!

Deactivate conda environment

```
conda deactivate
```

Example of using a Conda Environment on Expanse

Clone the Git repo

```
git clone https://github.com/sbl-sdsc/df-parallel.git
cd df-parallel
```

Run on CPU (Pandas, Dask, Spark dataframes)

```
galyleo launch --account <account_number> --partition shared --cpus 10 --memory 20
--time-limit 01:00:00 --conda-env df-parallel --conda-yml environment.yml --mamba
```

Run on GPU (cuDF, Dask-cuDF dataframes)

```
galyleo launch --account <account_number> --partition gpu-shared --cpus 10
--memory 92 --gpus 1 --time-limit 01:00:00 --conda-env df-parallel-gpu
--conda-yml environment-gpu.yml --mamba
```

1 GPU + 10 CPUs + 92 GB = ¼ of a GPU node

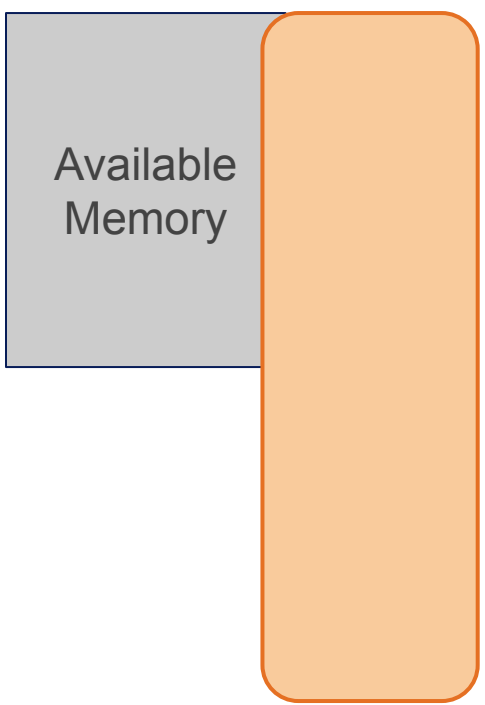
Task 1 - Launch Jupyter Lab on Expanse using a Conda environment

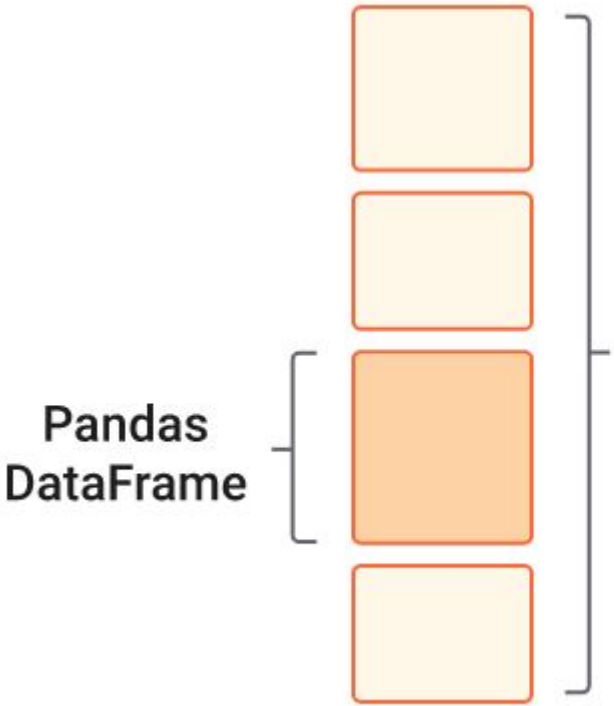
- Clone df-parallel Git repository
- Start galyleo on a GPU node
- Paste the URL for your Jupyter Lab session into your browser

- Follow the instructions for Task 1

Scale up Calculations on CPU/GPU using Dataframes

Processing large Datasets on CPU





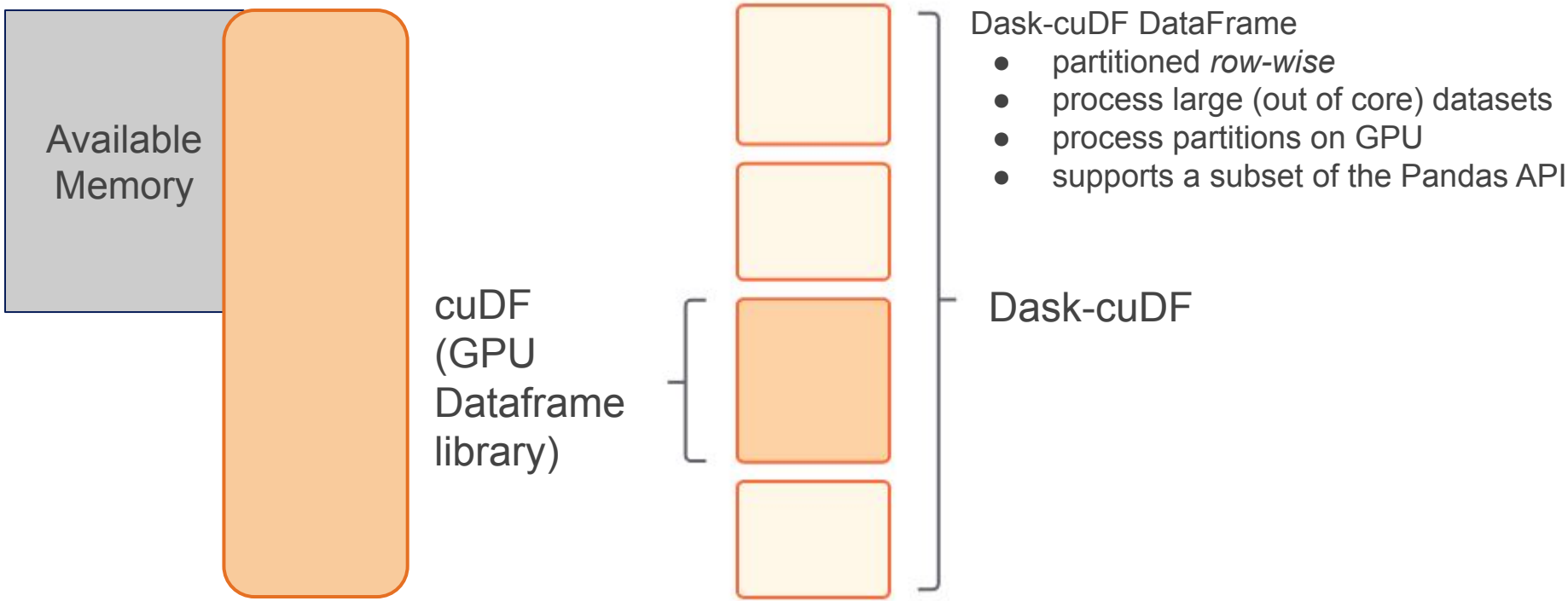
Dask DataFrame

- partitioned *row-wise*
- process large (out of core) datasets
- process partitions in parallel on CPU
- supports a subset of the Pandas API

https://pandas.pydata.org/docs/index.html

https://docs.dask.org/en/stable/dataframe.html

Processing large Datasets on GPU



Dask-cuDF DataFrame

- partitioned *row-wise*
- process large (out of core) datasets
- process partitions on GPU
- supports a subset of the Pandas API

https://docs.rapids.ai/api

Example Notebooks

https://github.com/sbl-sdsc/df-parallel

Dataframe Library	Parallel	Out-of-core	CPU/GPU	Evaluation
Pandas	no	no [1]	CPU	eager
Dask	yes	yes	CPU	lazy
Spark	yes	yes	CPU	lazy
cuDF	yes	no	GPU	eager
Dask-cuDF	yes	yes	GPU	lazy

[1] Pandas can read data in chunks, but they have to be processed independently.

Efficient File Formats

Columnar Storage Format - Parquet

@EmrgencyKittens

Query and space efficient file format (default: Snappy compression)

Vertical partitioning (projection push down) + Horizontal partitioning (predicate push down) = Read only the data you need!

a	b	c
a1	b1	c1
a2	b2	c2
a3	b3	c3
a4	b4	c4
a5	b5	c5

+

a	b	c
a1	b1	c1
a2	b2	c2
a3	b3	c3
a4	b4	c4
a5	b5	c5

=

a	b	c
a1	b1	c1
a2	b2	c2
a3	b3	c3
a4	b4	c4
a5	b5	c5

Horizontal partitioning uses column min/max statistics from Parquet metadata.

https://www.slideshare.net/julienledem/if-you-have-your-own-columnar-format-stop-now-and-use-parquet

Creating Parquet "Files" with Dask

```
genes = dd.read_csv(input, dtype=str, sep="\t")

genes.to_parquet(output, write_index=False,
write_metadata_file=True, engine="pyarrow")
```

```
genes = dd.read_csv(input, dtype=str, sep="\t")

genes.to_parquet(output, write_index=False,
write_metadata_file=True, engine="pyarrow",
partition_on=["type_of_gene"])
```

```
[xdtr104@login02 ~]$ ls -lh gene_info.parquet/
total 1.2G
-rw-r--r-- 1 xdtr104 uic157 6.9K Aug  4 10:14 _common_metadata
-rw-r--r-- 1 xdtr104 uic157 161K Aug  4 10:14 _metadata
-rw-r--r-- 1 xdtr104 uic157 9.9M Aug  4 10:14 part.0.parquet
-rw-r--r-- 1 xdtr104 uic157 9.8M Aug  4 10:14 part.1.parquet
-rw-r--r-- 1 xdtr104 uic157  16M Aug  4 10:14 part.10.parquet
-rw-r--r-- 1 xdtr104 uic157  18M Aug  4 10:14 part.11.parquet
-rw-r--r-- 1 xdtr104 uic157  20M Aug  4 10:14 part.12.parquet
-rw-r--r-- 1 xdtr104 uic157  17M Aug  4 10:14 part.13.parquet
-rw-r--r-- 1 xdtr104 uic157  19M Aug  4 10:14 part.14.parquet
-rw-r--r-- 1 xdtr104 uic157  18M Aug  4 10:14 part.15.parquet
-rw-r--r-- 1 xdtr104 uic157  20M Aug  4 10:14 part.16.parquet
-rw-r--r-- 1 xdtr104 uic157  21M Aug  4 10:14 part.17.parquet
-rw-r--r-- 1 xdtr104 uic157  19M Aug  4 10:14 part.18.parquet
-rw-r--r-- 1 xdtr104 uic157  20M Aug  4 10:14 part.19.parquet
```

```
[xdtr104@login02 ~]$ ls -lh gene_info.parquet/
total 698K
-rw-r--r-- 1 xdtr104 uic157 6.9K Aug  4 16:16  _common_metadata
-rw-r--r-- 1 xdtr104 uic157 1.5M Aug  4 16:16  _metadata
drwxr-xr-x 2 xdtr104 uic157    4 Aug  4 16:16 'type_of_gene=biological-region'
drwxr-xr-x 2 xdtr104 uic157   68 Aug  4 16:15 'type_of_gene=miscRNA'
drwxr-xr-x 2 xdtr104 uic157   87 Aug  4 16:15 'type_of_gene=ncRNA'
drwxr-xr-x 2 xdtr104 uic157   87 Aug  4 16:15 'type_of_gene=other'
drwxr-xr-x 2 xdtr104 uic157   87 Aug  4 16:15 'type_of_gene=protein-coding'
drwxr-xr-x 2 xdtr104 uic157   87 Aug  4 16:15 'type_of_gene=pseudo'
drwxr-xr-x 2 xdtr104 uic157   87 Aug  4 16:15 'type_of_gene=rRNA'
drwxr-xr-x 2 xdtr104 uic157    5 Aug  4 16:16 'type_of_gene=scRNA'
drwxr-xr-x 2 xdtr104 uic157   85 Aug  4 16:15 'type_of_gene=snRNA'
drwxr-xr-x 2 xdtr104 uic157   85 Aug  4 16:16 'type_of_gene=snoRNA'
drwxr-xr-x 2 xdtr104 uic157   87 Aug  4 16:15 'type_of_gene=tRNA'
drwxr-xr-x 2 xdtr104 uic157   62 Aug  4 16:16 'type_of_gene=unknown'
```

- Parquet files are typically directories of files.

- Parquet files can be partitioned by one or more columns for query efficiency.

Vertical & Horizontal Partitioning

```
# vertical partitioning
column_names = ["GeneID", "Symbol", "Synonyms", "description", "type_of_gene", "#tax_id", "chromosome"]

# horizontal partitioning (conditions can be nested for complex filters)
filters=[[("type_of_gene", "==", "protein-coding")]]

# Pandas
genes = pd.read_parquet(filename, columns=column_names, filters=filters)
# Dask
genes = dd.read_parquet(filename, columns=column_names, filters=filters)
# cuDF
genes = cudf.read_parquet(filename, columns=column_names, filters=filters)
# Dask-cuDF
genes = dask_cudf.read_parquet(filename, columns=column_names, filters=filters)

# Spark
genes = spark.read.parquet(filename)
genes = genes.select(column_names)
genes = genes.filter("type_of_gene == 'protein-coding'")
```

Benchmark Dataframe Libraries

- TASK 2: Benchmark Dataframe Libraries using a csv Input File
- TASK 3: Benchmark Dataframe Libraries using a Parquet Input File
- TASK 4: Measure Parallel Efficiency

Dataframe Benchmark

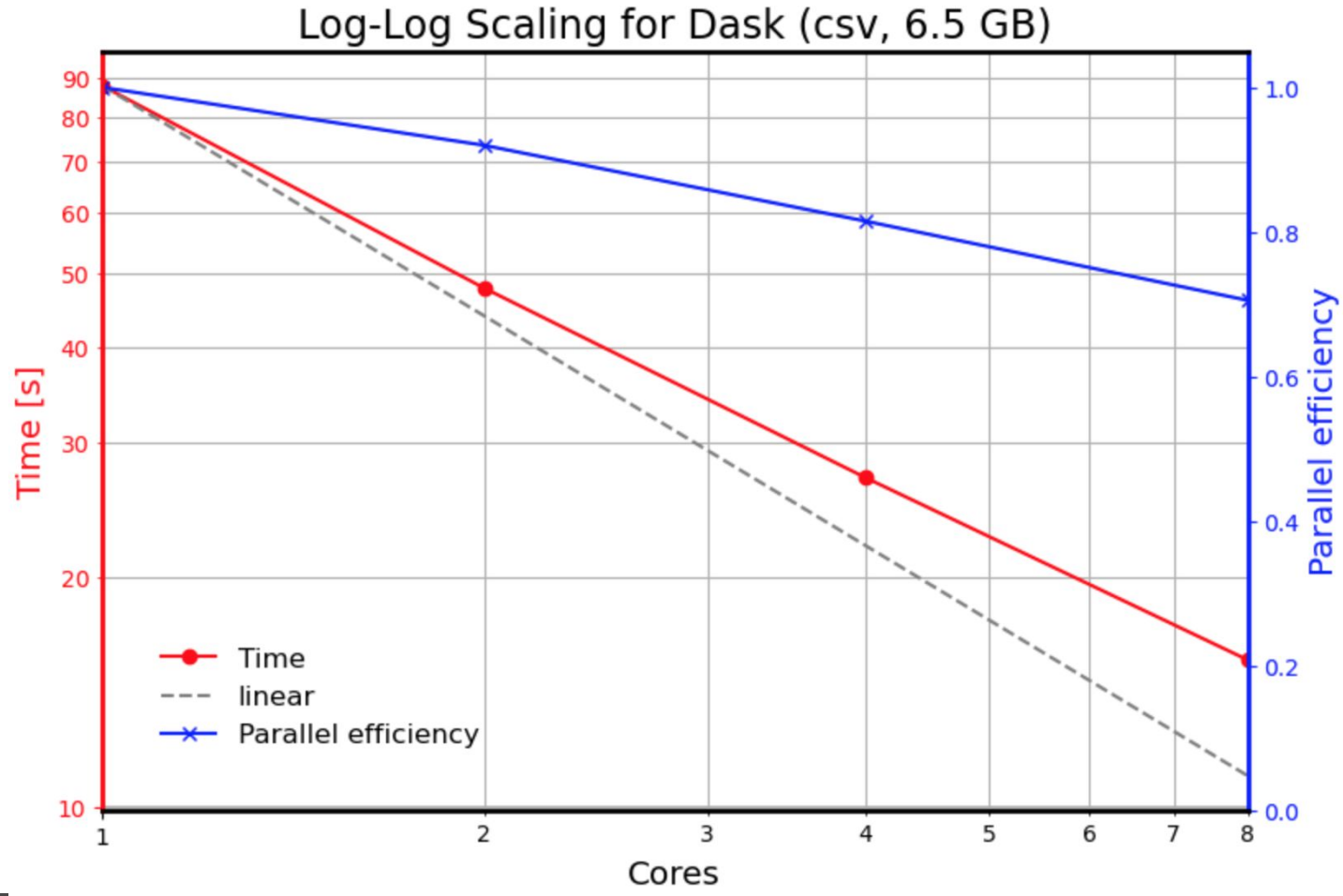
Results for running on SDSC Expanse GPU node with 10 CPU cores (Intel Xeon Gold 6248 2.5 GHz), 1 GPU (NVIDIA V100 SMX2), and 92 GB of memory (DDR4 DRAM), local storage (1.6 TB Samsung PM1745b NVMe PCIe SSD).

Datafile size (gene_info.tsv):

- Dataset 1: 5.4 GB (18 GB in Pandas)
- Dataset 2: 21.4 GB (4 x Dataset 1) (62.4 GB in Pandas)
- Dataset 3: 43.7 GB (8 x Dataset 1)

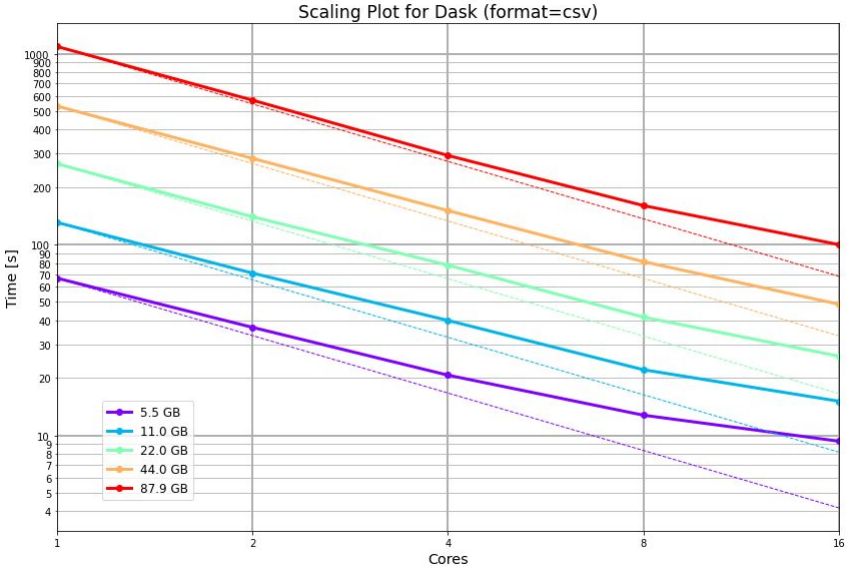
Dataframe Library	time(5.4 GB) (s)	time(21.4 GB) (s)	time(43.7 GB) (s)	Parallel	Out-of-core	CPU/GPU
Pandas	56.3	222.4	-- [2]	no	no	CPU
Dask	15.7	42.1	121.8	yes	yes	CPU
Spark	14.2	31.2	56.5	yes	yes	CPU
cuDF	3.2	-- [2]	-- [2]	yes	no	GPU
Dask-cuDF	7.3	11.9	19.0	yes	yes	GPU

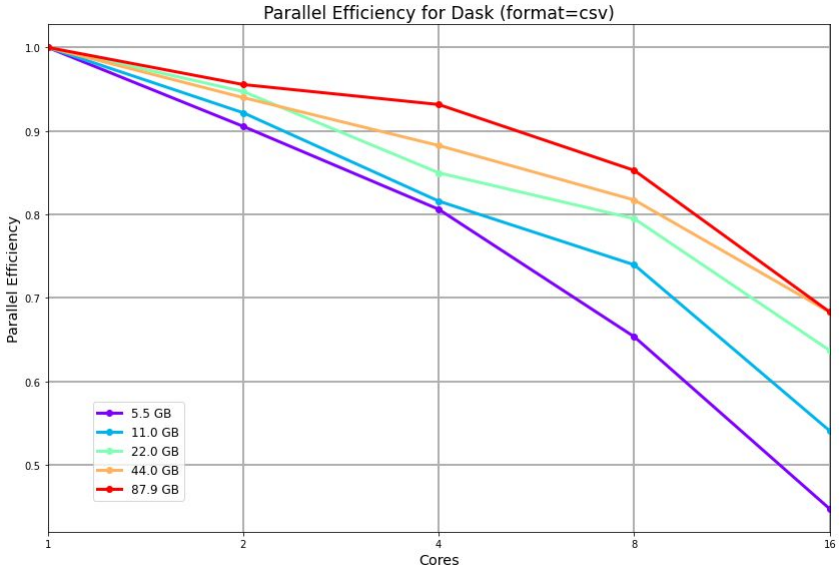
[2] out of memory


Log-Log Scaling for Dask (csv, 6.5 GB)
Time [s]
Parallel efficiency
Cores
Time
linear
Parallel efficiency
90
80
70
60
50
40
30
20
10
1.0
0.8
0.6
0.4
0.2
0.0
1
2
3
4
5
6
7
8

Scaling for Dask Dataframe

Runtime as function of dataset size and number of cores





Batch benchmark: slurm script: benchmark.sb notebook: 8-BenchmarkSummary.ipynb

Run Jupyter Lab in Batch

Run Jupyter Lab in Batch

Example batch file

https://github.com/sbl-sdsc/df-parallel/blob/main/solution.sh

Submit job

```
sbatch solution.sh
```

Papermill (https://papermill.readthedocs.io/en/latest/)

- execute notebook on the command line

```
papermill input.ipynb output.ipynb
```

- execute notebook in Python

```
import papermill as pm
pm.execute_notebook("input.ipynb", "output.ipynb")
```

- parameterize notebook (pass arguments to Jupyter Notebooks)

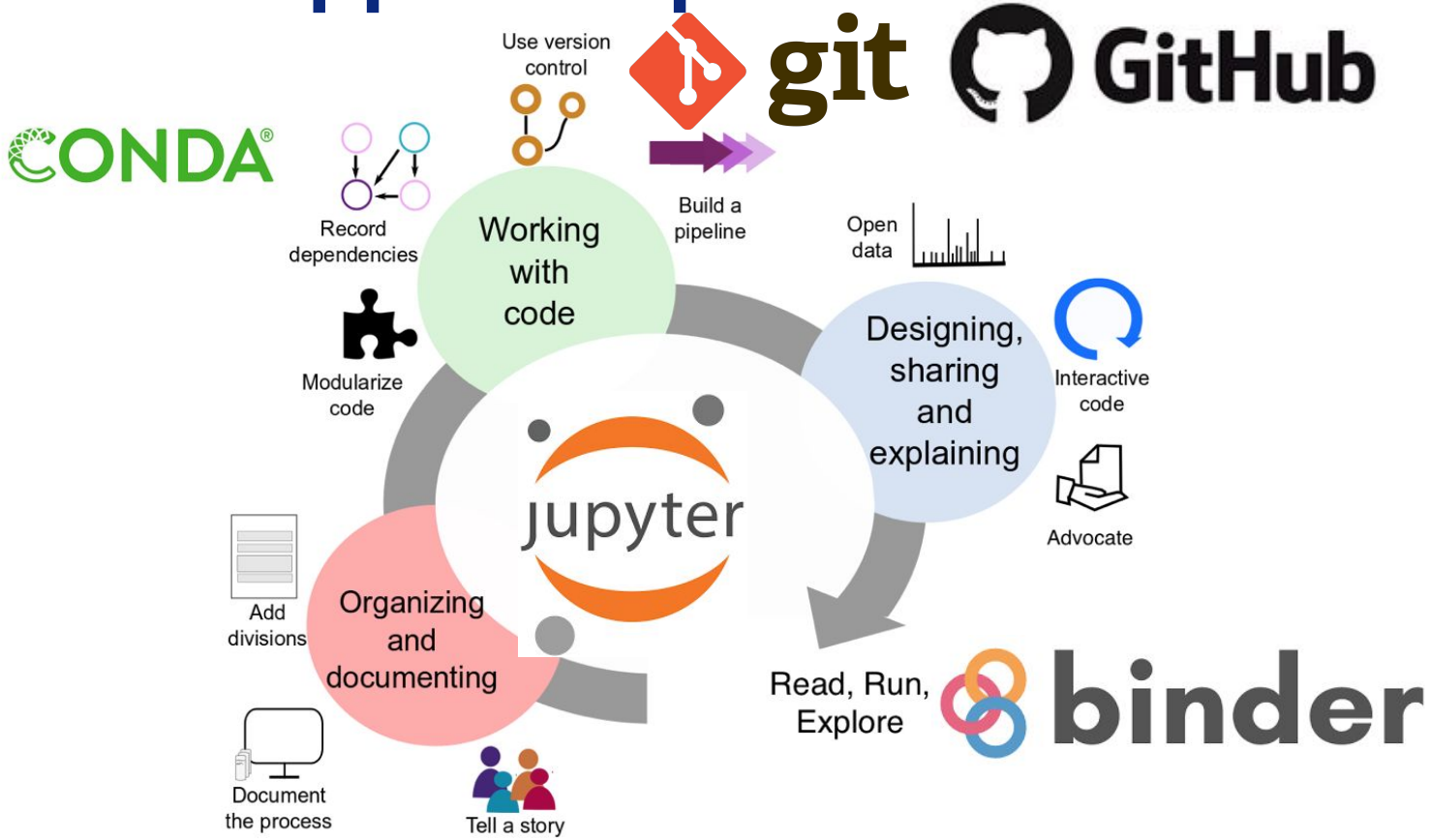
```
papermill input.ipynb output.ipynb -p variable1 value1 -p variable2 value2
```

Best Practices for Authoring Jupyter Notebooks

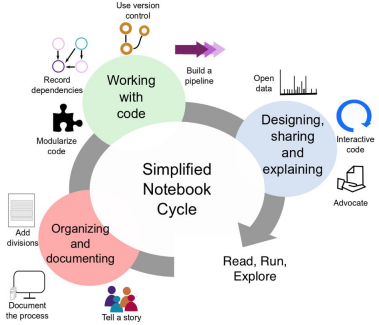
Paper: https://doi.org/10.1371/journal.pcbi.1007007

Git repo: https://github.com/jupyter-guide/ten-rules-jupyter

Tools to Support Reproducible Workflows

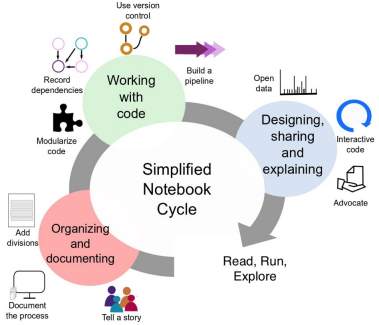


Organizing and Documenting



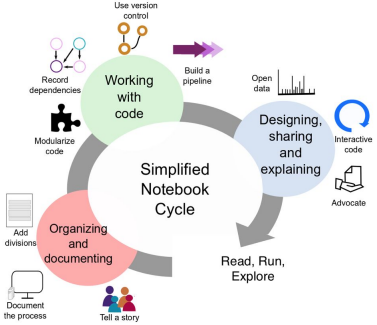
- **Rule 1: Tell a Story for an Audience**
  - Beginning - introduce topic
  - Middle - describe steps
  - End - interprets results
  - Describe not just what you did, by why you did it, how the steps are connected, and what it all means.
  - Adjust your description depending on the intended audience
- **Rule 2: Document the process, not just the results**
  - Add descriptive notes, e.g., why a particular parameter was chosen
- **Rule 3: Use cell divisions to make steps clear**
  - Avoid long cells
  - Limit each cell to one meaningful step
  - Split long notebooks into a series of notebooks
  - Keep a top-level index notebook with links to the individual notebooks

Working with Code



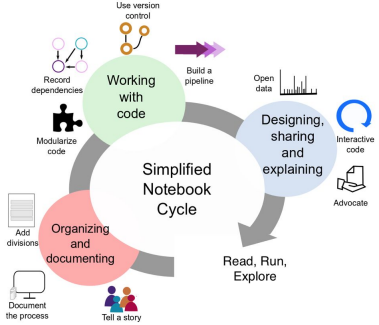
- **Rule 4: Modularize Code**
  - Use functions instead of duplicating code cells
- **Rule 5: Record Dependencies**
  - Manage your dependencies explicitly from the start using a tool such as
    - Conda's environment.yml
    - pip's requirements.txt
- **Rule 6: Use Version Control**
  - Consider using a public repository from the beginning of a project
  - Tie research results to specific software versions
- **Rule 7: Build a Pipeline**
  - Design notebooks with reuse in mind (different input data and parameters)
  - Define key input data and parameters at the top of each notebook
  - Break long notebooks into smaller notebooks that focus on one or a few analysis steps.

Sharing, explaining



- **Rule 8: Share and Explain Your Data**
  - Share your data in a repository with a persistent identifier, e.g., DOI or ARK
    - Bio repositories, e.g., NCBI, Ensemble, PDB
    - General repositories, e.g., Zenodo https://zenodo.org/
  - Small datasets can be stored in GitHub with your source code (< 50MB)
    - E.g., in a /data folder
  - Very large datasets
    - Consider using a sample of the data and a link to the original data
  - Save intermediate data after data processing
    - E.g., in /intermediate_data folder
    - Can be used to verify each step in a workflow

Sharing, explaining cont



- **Rule 9: Design your notebooks to be read, run, and explored**
  - Git repository
    - Add a descriptive README file
    - Add a LICENCE file (liberal licence, e.g., MIT, Apache 2)
    - Add a static HTML/PDF file of your notebooks for long-term preservation
    - Add Binder badge/link to launch notebooks in the cloud (https://mybinder.org/)
  - Consider using ipywidgets to add menus or sliders to enable interactive exploration of parameters

Sharing, explaining cont.

- **Rule 10: Advocate for open research**
  - Apply what you learned in this tutorial in your own research and be an advocate for open and reproducible research in your lab or workplace
  - Publish a fully reproducible paper! Create all figures, data tables, and all other computational results using Jupyter Notebook and deposit in Github.

Brad Voytek @bradleyvoytek · 20 Apr 2018

Our lab's moving to this model: publish "static PDF" papers as expected, but also a shadow, interactive @ProjectJupyter version alongside that has all code to process, analyze, and visualize data.

"The Scientific Paper Is Obsolete" featuring @fperez_org

The Scientific Paper Is Obsolete

Here's what's next.

theatlantic.com

Summary

- When to run on Expanse
- Setup a portable and reproducible software environment
- Scale up calculations on CPU/GPU using Dataframes
- Run Jupyter Lab in Batch
- Best Practices for Authoring Jupyter Notebooks

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