Session 5.1 Scaling up Interactive Data Analysis in Jupyter Lab: From Laptop to HPC

SDSC Summer Institute 2024

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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
- Get ready to use Expanse: accounts, allocations
- Best Practices for Authoring Jupyter Notebooks

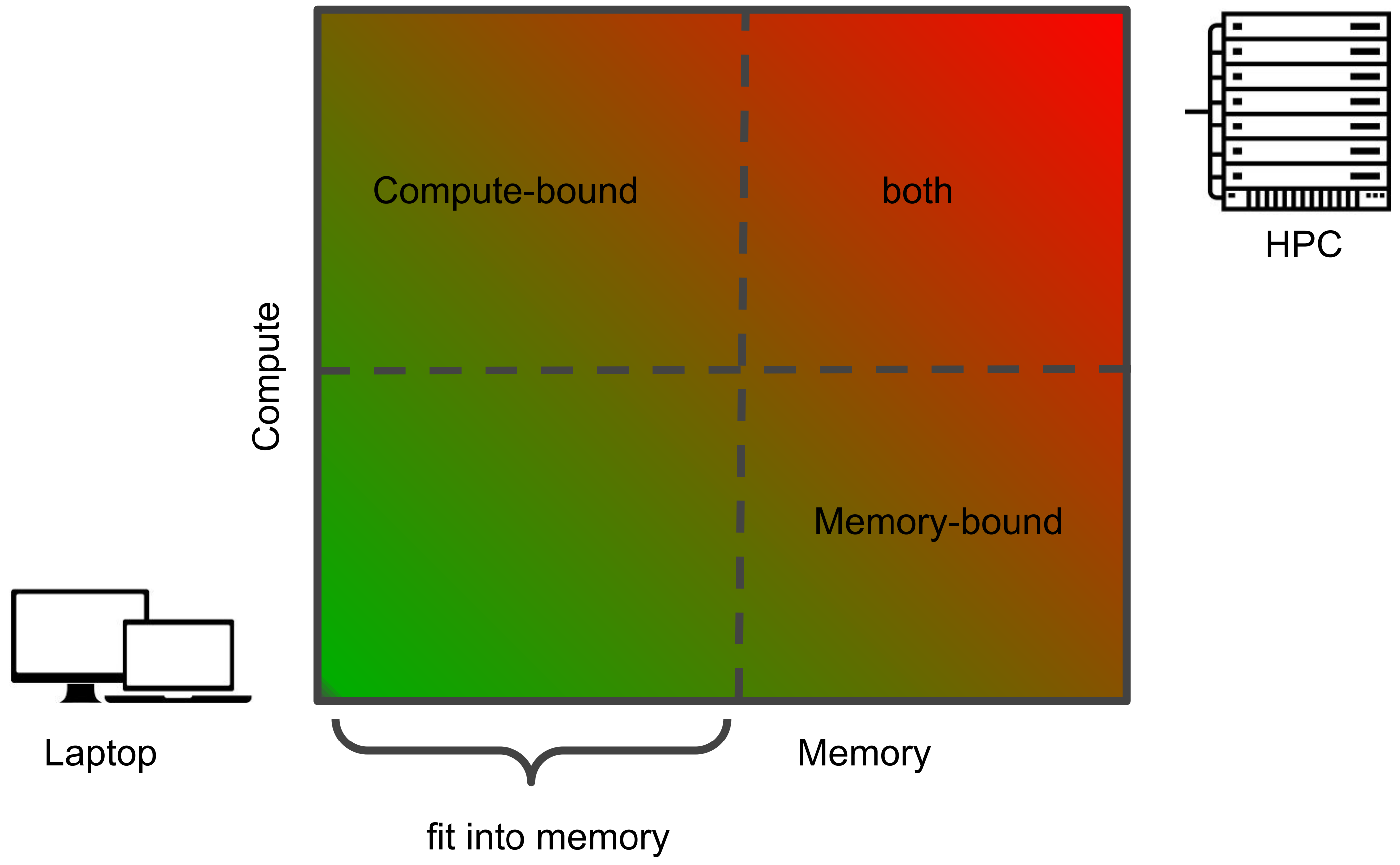
When to run on Expanse

Laptop/Desktop

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

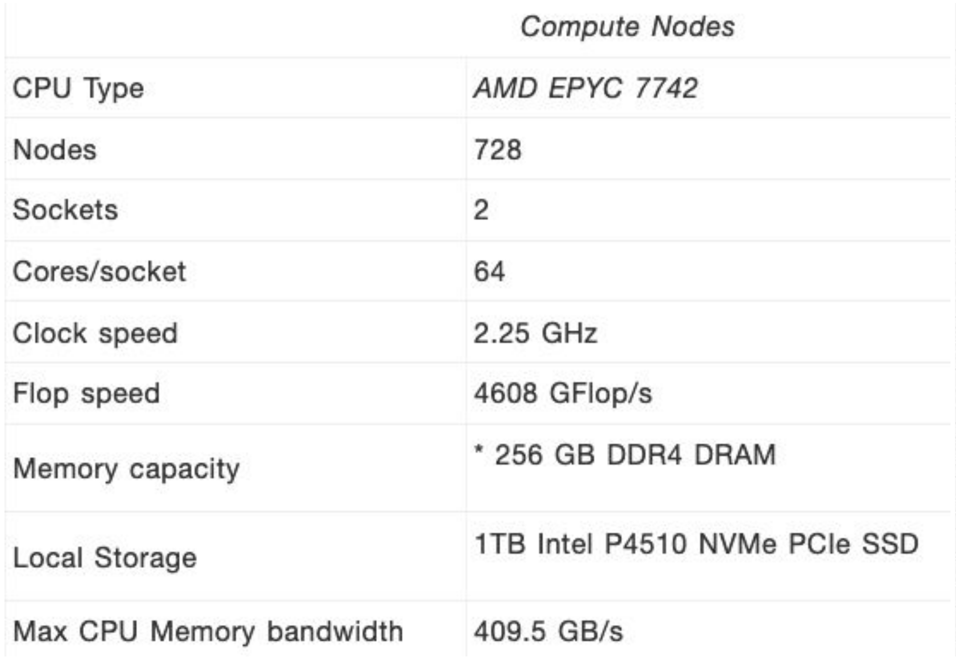
Expanse

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


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

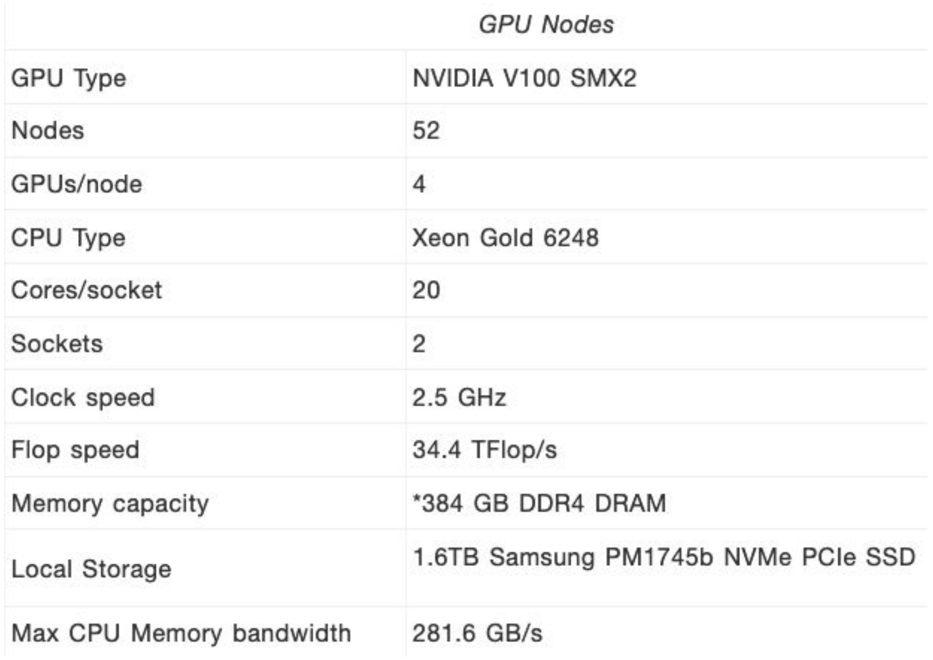
Expanse Nodes

128 CPU cores/node

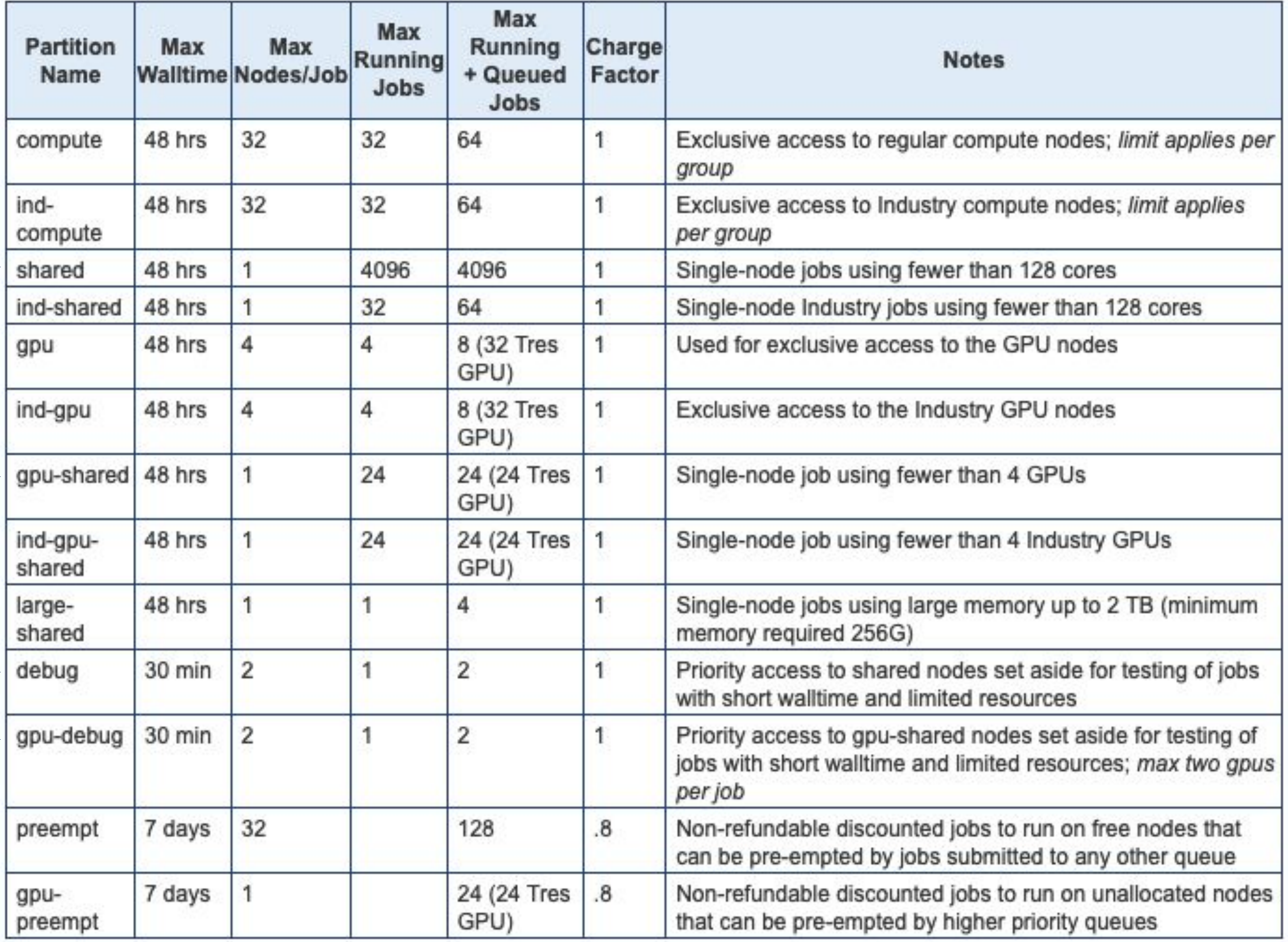


	Compute Nodes
CPU Type	*AMD EPYC 7742*
Nodes	728
Sockets	2
Cores/socket	64
Clock speed	2.25 GHz
Flop speed	4608 GFlop/s
Memory capacity	* 256 GB DDR4 DRAM
Local Storage	1TB Intel P4510 NVMe PCIe SSD
Max CPU Memory bandwidth	409.5 GB/s

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



	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*
Jupyter Notebook (CPU)	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
Jupyter Notebook (GPU)	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)
Testing (CPU)	debug	30 min	2	1	2	1	Priority access to shared nodes set aside for testing of jobs with short walltime and limited resources
Testing (GPU)	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*	**Reusability**	**Scalability**
obtaining **consistent** results using	obtaining **new** results using	obtaining **new** results using
same input data or parameters	**different** input data or parameters	**large** input data or parameter sets
same computational steps, methods, and code	**same** computational steps, methods, and code	**same** computational steps, methods, and code
same analysis conditions	**same** analysis conditions	**same** analysis conditions

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

Tools and Infrastructure

jupyter

Computational notebooks: combine documentation, code, and results

git

Version-control system for tracking changes in source code

GitHub

Source code repository

CONDA®

Open-source package and environment management system

SINGULARITY

Container that packages software and OS in a portable way

EXPANSE

Scalable compute infrastructure

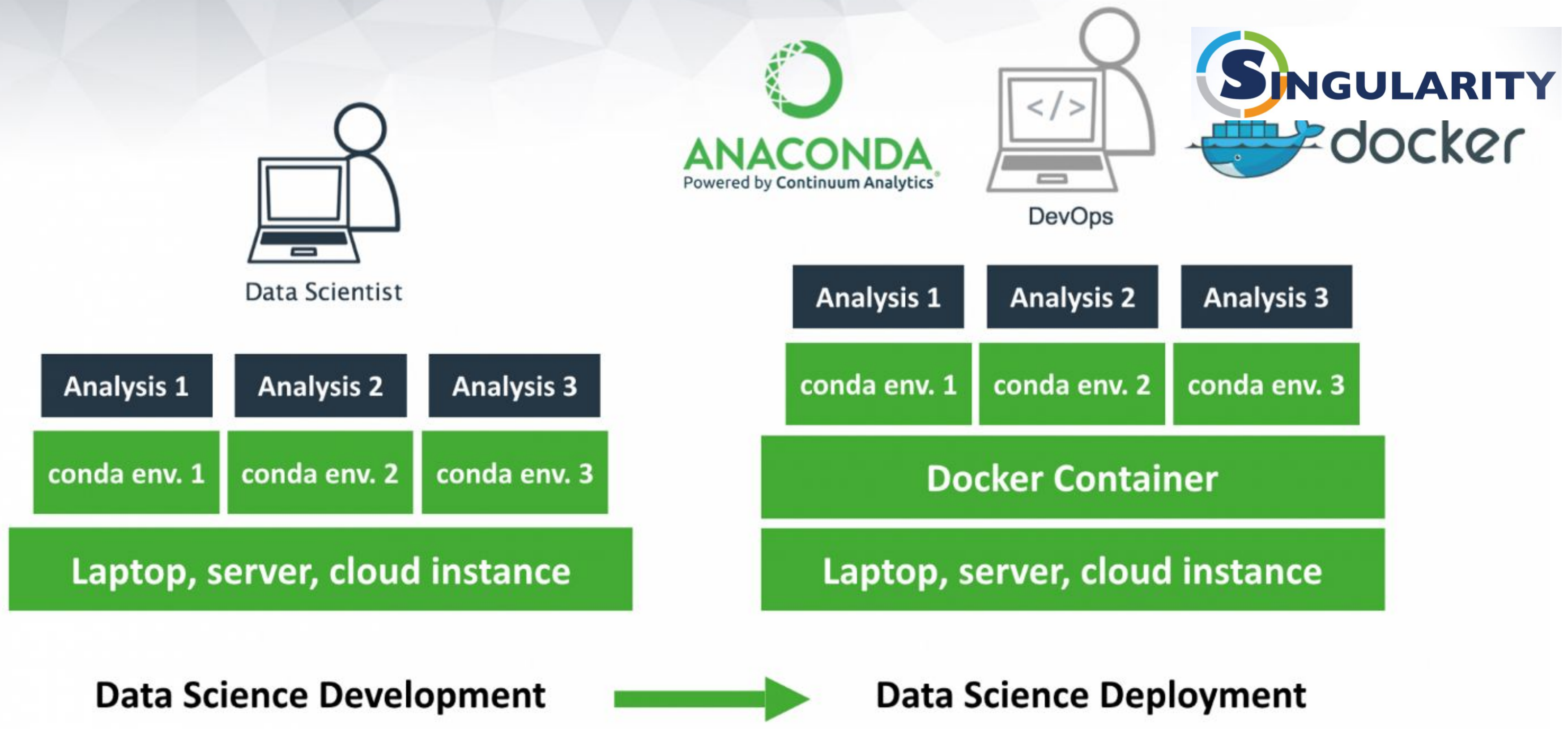
Reproducible Environments

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

SINGULARITY

- 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

CONDA®

- **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?

```
pip install pandas
pip install scikit-learn

Or

conda install pandas
conda install scikit-learn
```

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)

```
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)
```

Mamba

✓ Mac, Windows, Linux

Activate a Conda environment

```
conda activate <environment_name>
```

Run Jupyter Lab

```
jupyter lab
```

Deactivate conda environment

```
conda deactivate
```

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

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

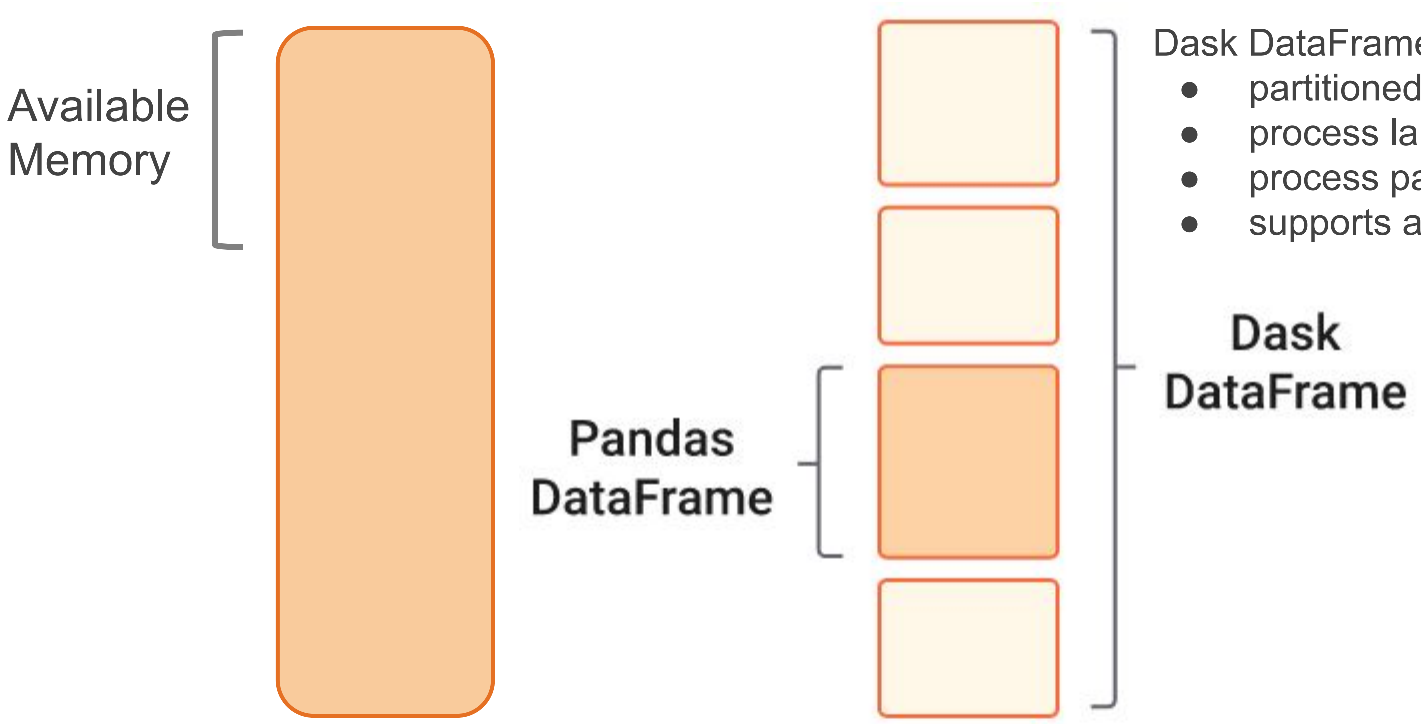
Task 1 - Launch Jupyter Lab on Expanse using a Conda environment

- 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

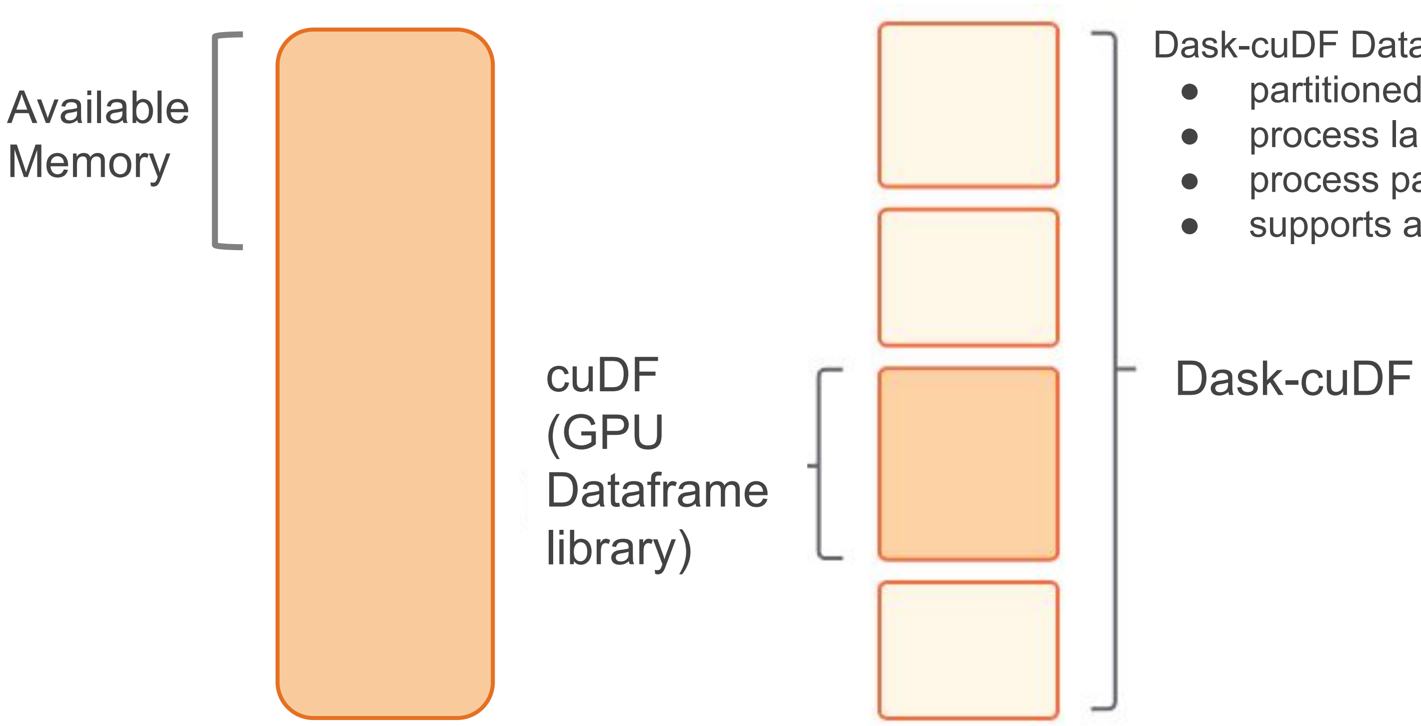


Dask DataFrame
- partitioned *row-wise*
- process large (out of core) datasets
- process partitions in parallel on CPU
- supports a subset of the Pandas API

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

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

Processing large Datasets on GPU



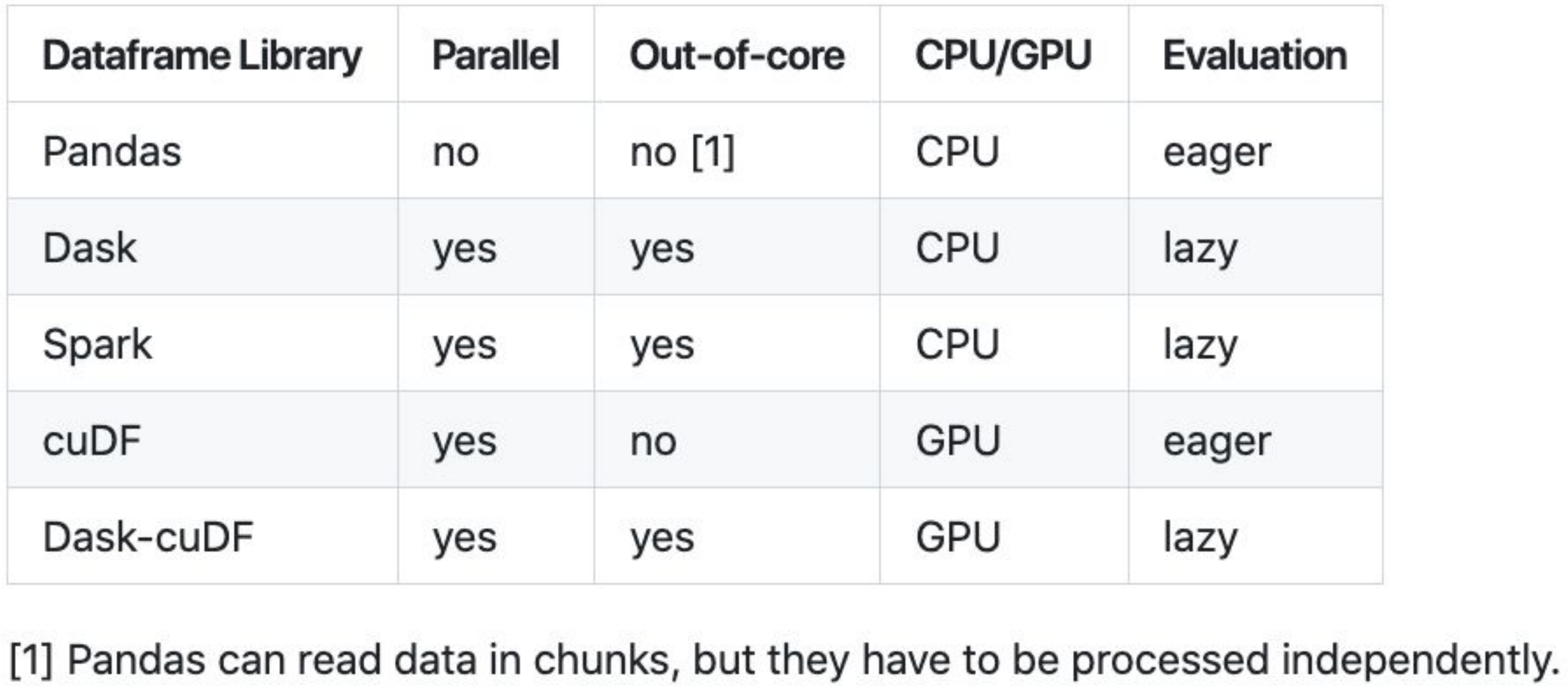
Dask-cuDF DataFrame

- 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

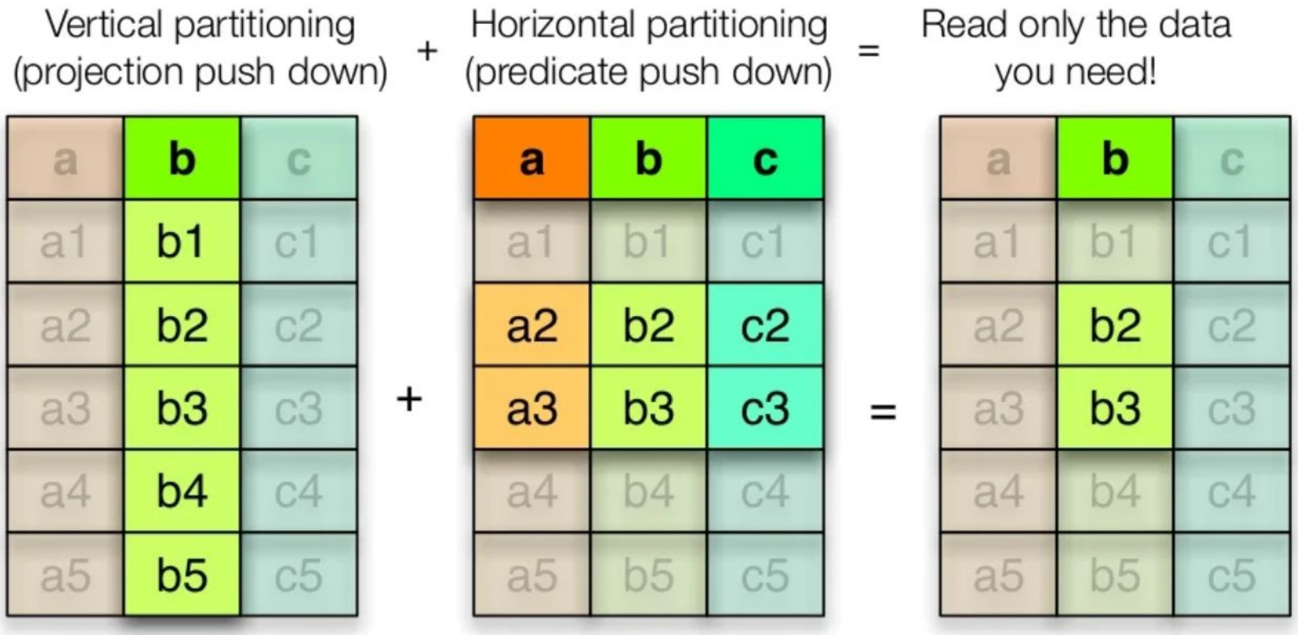
[1] Pandas can read data in chunks, but they have to be processed independently.

Efficient File Formats

Columnar Storage Format - Parquet

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

@EmrgencyKittens

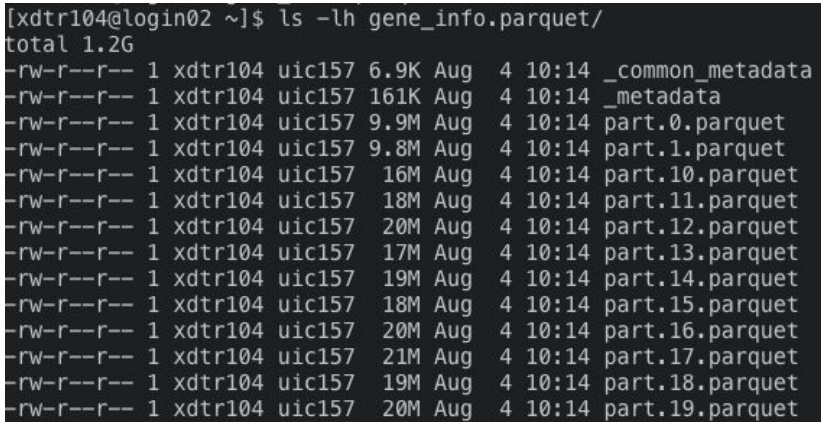

Vertical partitioning (projection push down)
+
Horizontal partitioning (predicate push down)
=
Read only the data you need!
a b c
a1 b1 c1
a2 b2 c2
a3 b3 c3
a4 b4 c4
a5 b5 c5
+
=

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

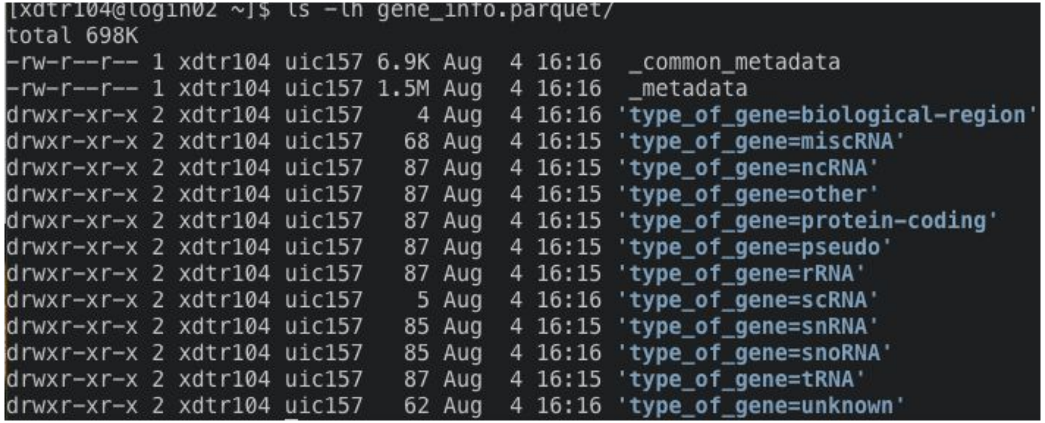
```
genes = dd.read_csv(input, dtype=str, sep="\t")

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



```
[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
```

- Parquet files are typically directories of files.

```
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 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 can be partitioned by one or more columns for query efficiency.

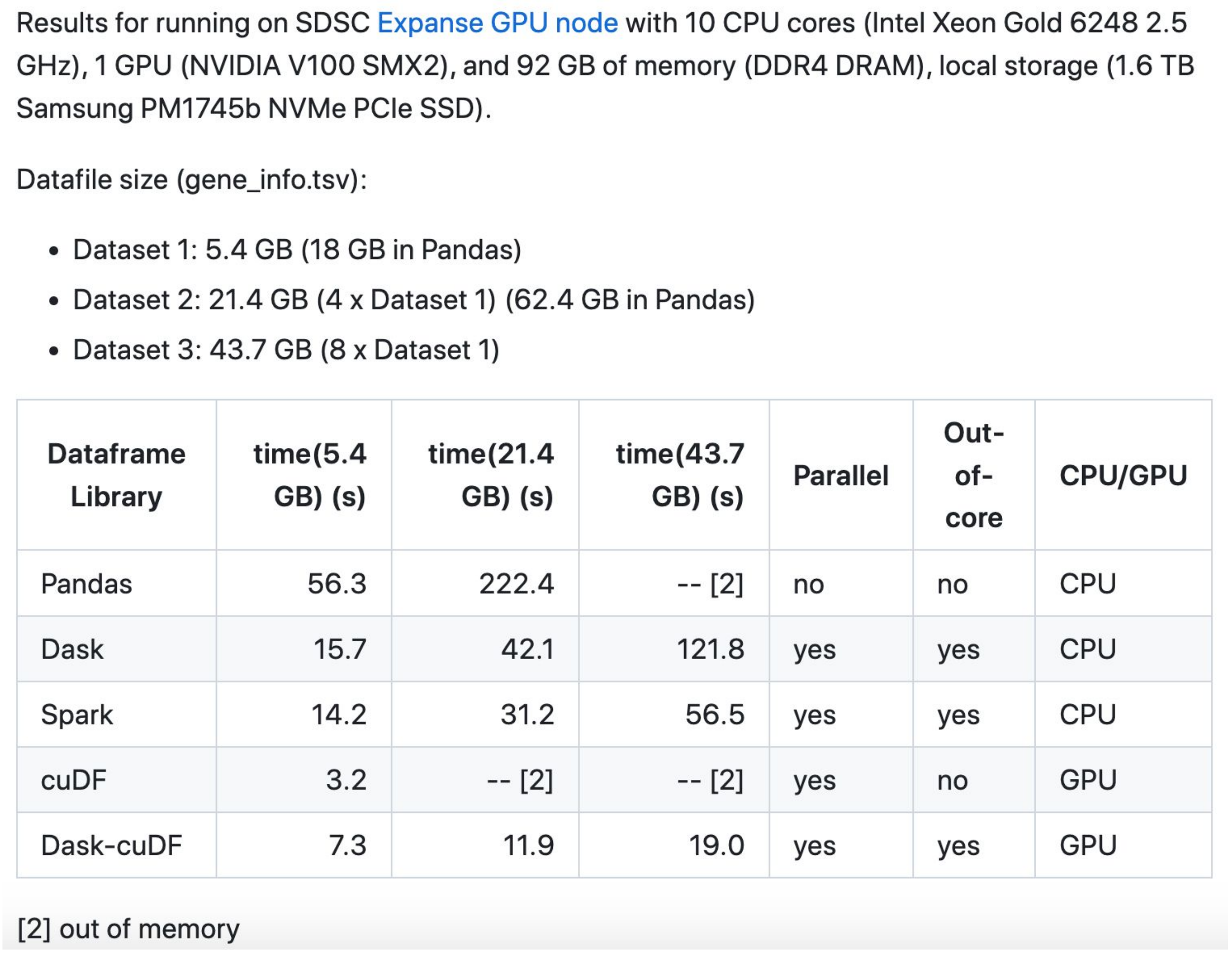
Vertical & Horizontal Partitioning

```
# 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



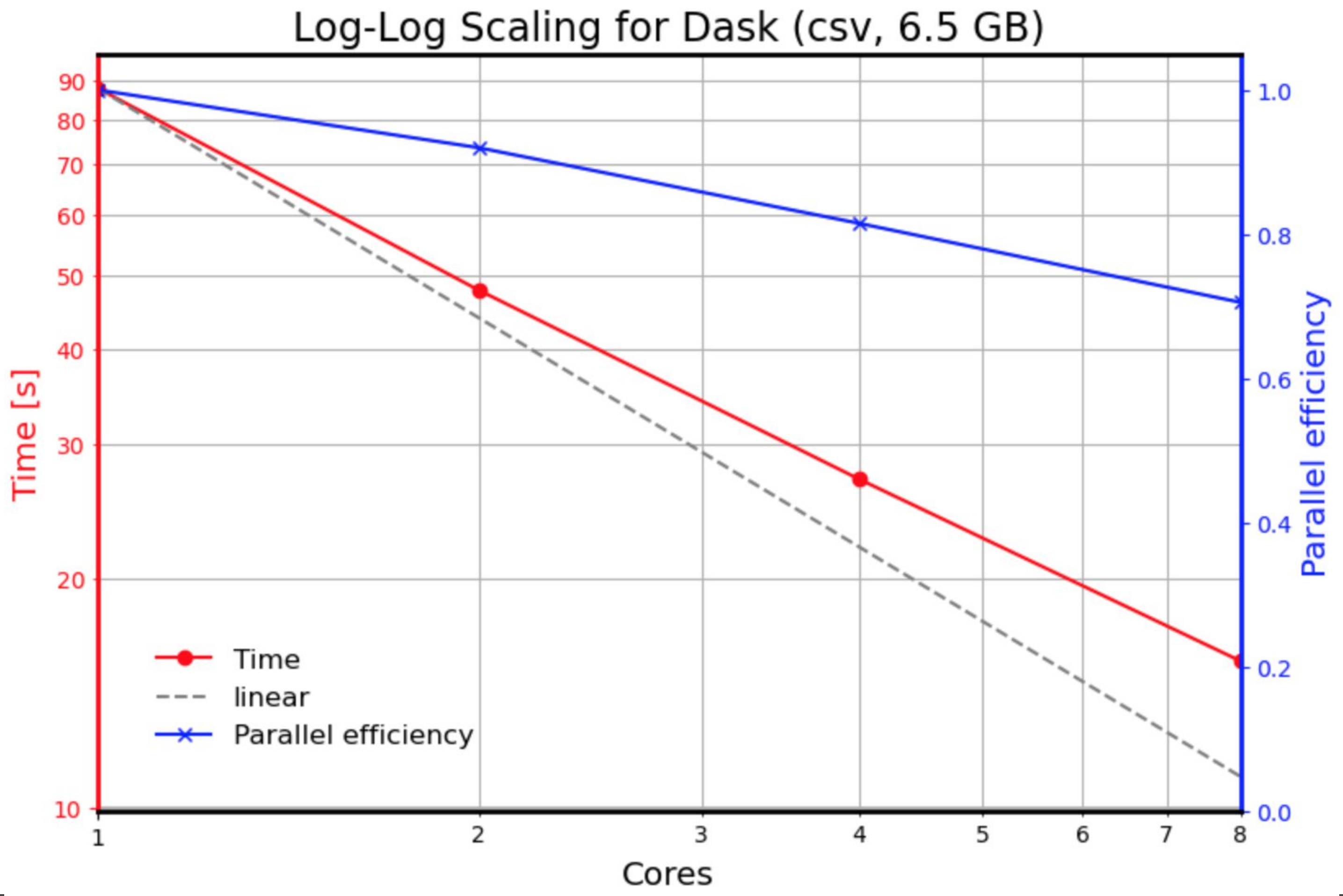
Results for running on SDSC Expanse GPU node with 10 CPU cores (Intel Xeon Gold 6248 2.5 GHz), 1 GPU (NVIDIA V100 SMX2), and 92 GB of memory (DDR4 DRAM), local storage (1.6 TB Samsung PM1745b NVMe PCIe SSD).

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)

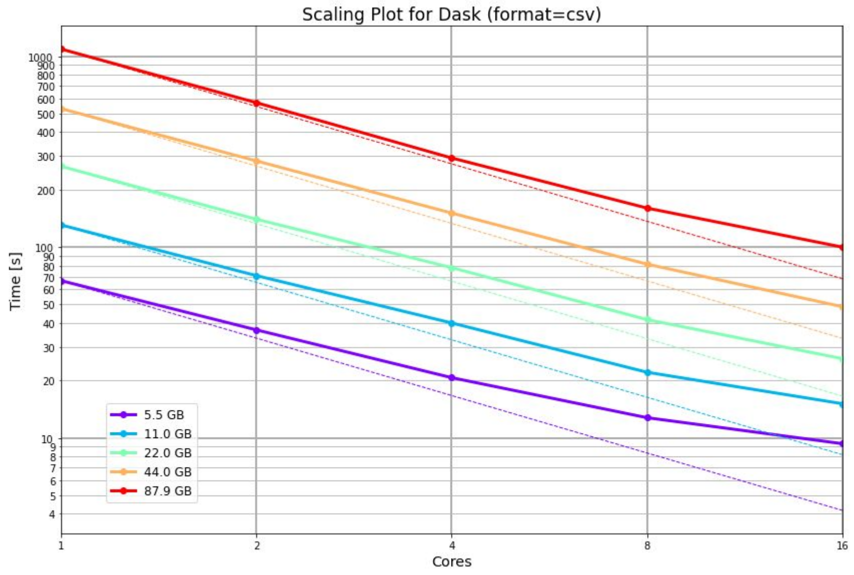
Dataframe Library	time(5.4 GB) (s)	time(21.4 GB) (s)	time(43.7 GB) (s)	Parallel	Out-of-core	CPU/GPU
Pandas	56.3	222.4	-- [2]	no	no	CPU
Dask	15.7	42.1	121.8	yes	yes	CPU
Spark	14.2	31.2	56.5	yes	yes	CPU
cuDF	3.2	-- [2]	-- [2]	yes	no	GPU
Dask-cuDF	7.3	11.9	19.0	yes	yes	GPU

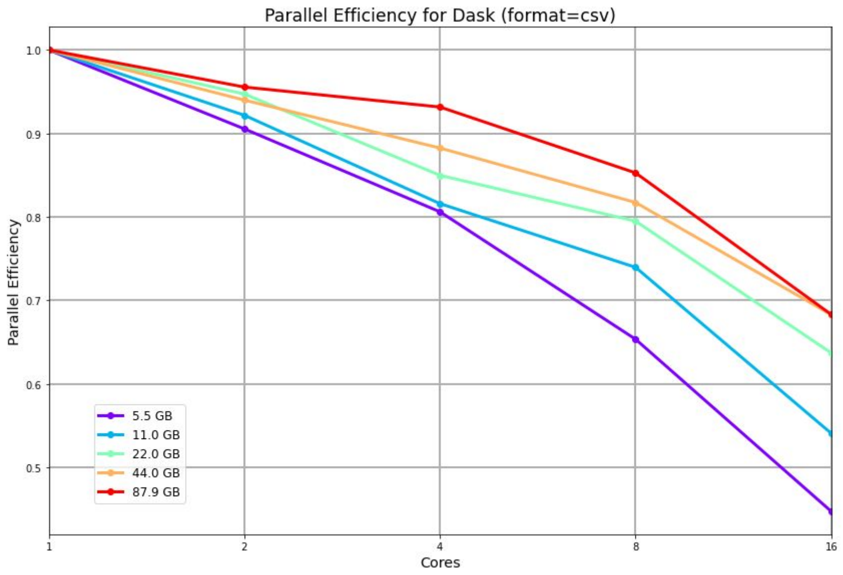
[2] out of memory


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

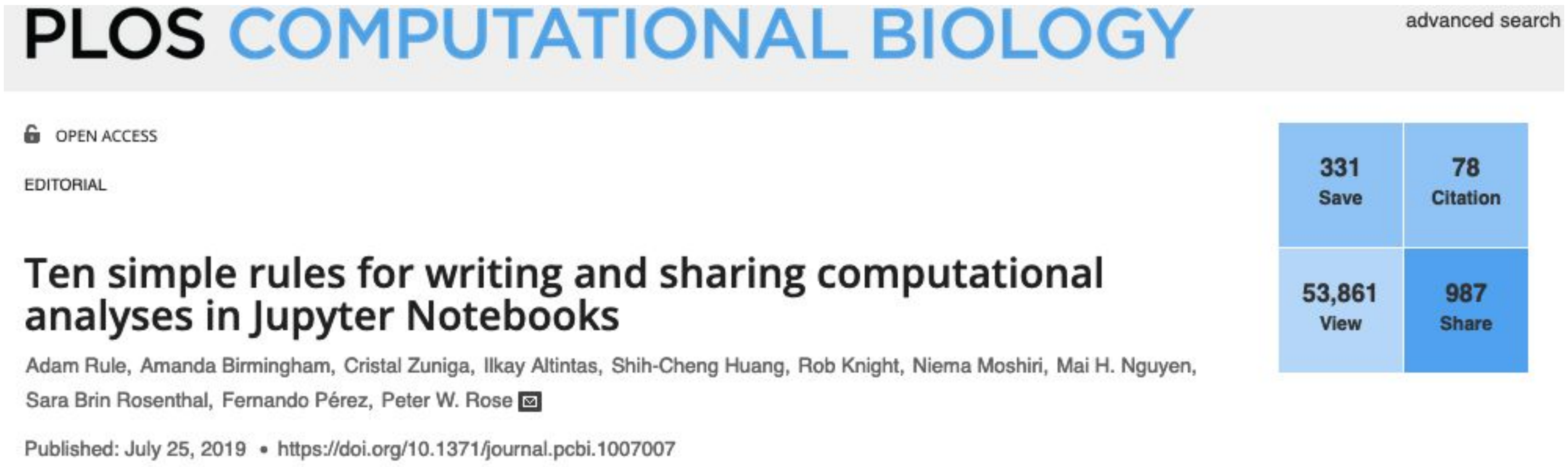
```
papermill input.ipynb output.ipynb -p variable1 value1 -p variable2 value2
```

Get ready to use Expanse: accounts, allocations

Expanse Allocation

- Trial allocation: 100 GPU and/or 1000 CPU hours
  consult@sdsc.edu
- Apply for allocations through ACCESS
  - **EXPLORE** (400K) Great for resource evaluation, graduate student projects, small classes and training events, benchmarking, code development and porting, and similar small-scale uses.
  - **DISCOVER** (1.5M) Designed for research grants with modest resource needs, Campus Champions, large classes and training events, NSF graduate fellowships, benchmarking and code testing at scale, and gateway development.
  - **ACCELERATE** (3M) Best for experienced users with mid-scale resource needs, consolidating multi-grant programs, collaborative projects, preparing for Maximize ACCESS requests, and gateways with growing communities.
  - **MAXIMIZE** (>3M) The choice for large-scale research activities that need more resources than the limit for Accelerate ACCESS projects.

Best Practices for Authoring Jupyter Notebooks


PLOS COMPUTATIONAL BIOLOGY

advanced search

OPEN ACCESS

EDITORIAL

Ten simple rules for writing and sharing computational analyses in Jupyter Notebooks

Adam Rule, Amanda Birmingham, Cristal Zuniga, Ilkay Altintas, Shih-Cheng Huang, Rob Knight, Niema Moshiri, Mai H. Nguyen, Sara Brin Rosenthal, Fernando Pérez, Peter W. Rose

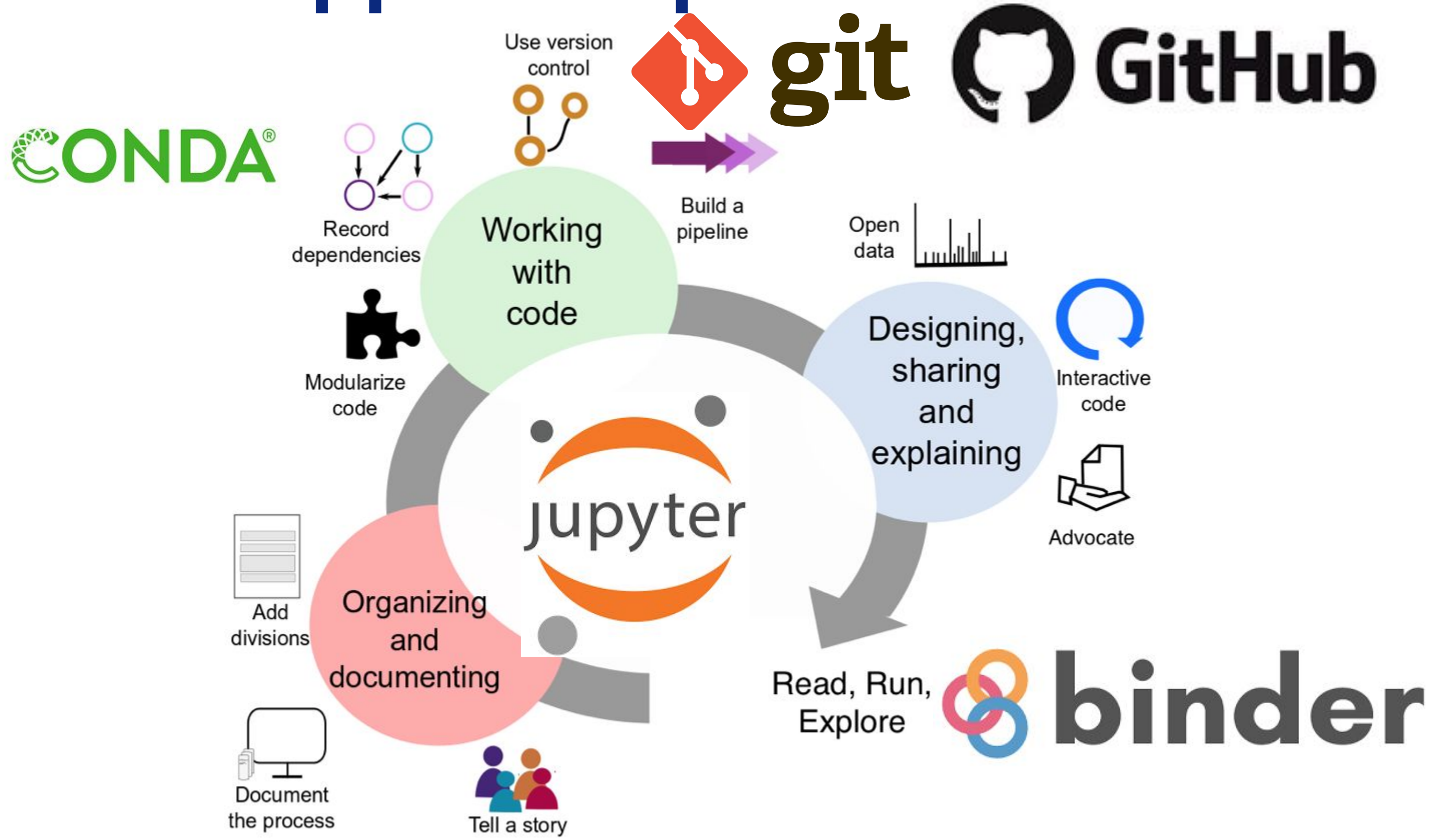
Published: July 25, 2019 • https://doi.org/10.1371/journal.pcbi.1007007

331 Save	78 Citation
53,861 View	987 Share

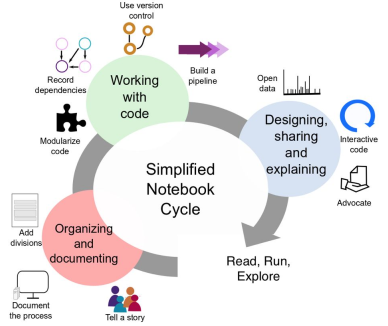
Paper: https://doi.org/10.1371/journal.pcbi.1007007

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

Tools to Support Reproducible Workflows

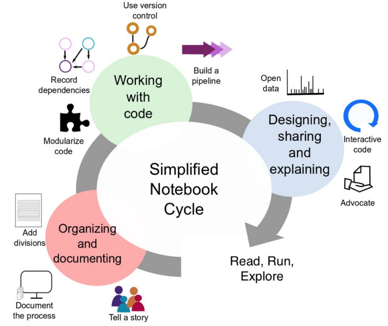


Organizing and Documenting



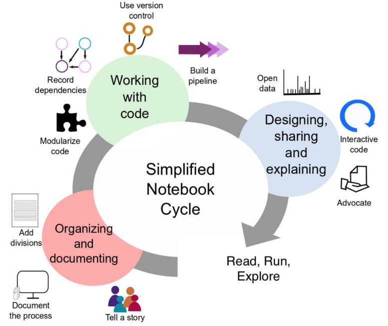
- **Rule 1: Tell a Story for an Audience**
  - Beginning - introduce topic
  - Middle - describe steps
  - End - interprets results
  - Describe not just what you did, by why you did it, how the steps are connected, and what it all means.
  - Adjust your description depending on the intended audience
- **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



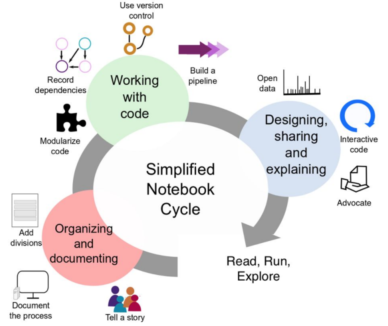
- **Rule 4: Modularize Code**
  - Use functions instead of duplicating code cells
- **Rule 5: Record Dependencies**
  - Manage your dependencies explicitly from the start using a tool such as
    - Conda’s environment.yml
    - pip’s requirements.txt
- **Rule 6: Use Version Control**
  - Consider using 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
    - 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

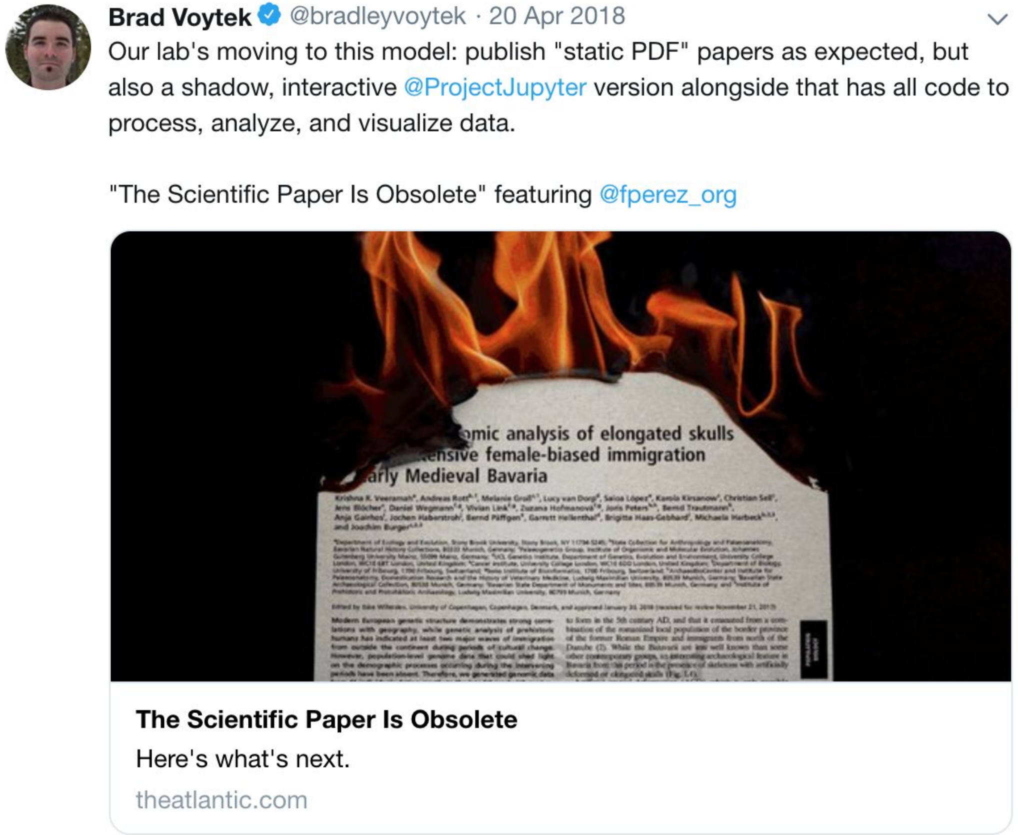
Sharing, explaining cont



- **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

omic analysis of elongated skulls
ensive female-biased immigration
arly Medieval Bavaria

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
- Get ready to use Expanse: accounts, allocations
- Best Practices for Authoring Jupyter Notebooks

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CyberTraining: Implementation: Small: Developing a Best Practices Training Program in Cyberinfrastructure-Enabled Machine Learning Research