CONDA Environments and Jupyter Notebook on Expanse: Scalable & Reproducible Data Exploration and ML

CIML Summer Institute 2023

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COMPUTING WITHOUT BOUNDARIES

EXPANSE

SAN DIEGO SUPERCOMPUTER CENTER

UNIVERSITY OF CALIFORNIA SAN DIEGO

Outline

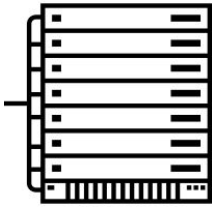
- When to run on Expanse
- Setup a portable and reproducible software environment
- Use the Expanse Portal
- Run Jupyter Lab on Expanse
- Scale up calculations on CPU/GPU
- Parameterize a Jupyter Notebook
- Run Jupyter Lab in batch
- Get ready to use Expanse: accounts, allocations
- Best Practices for Authoring Jupyter Notebooks

When to run on Expanse

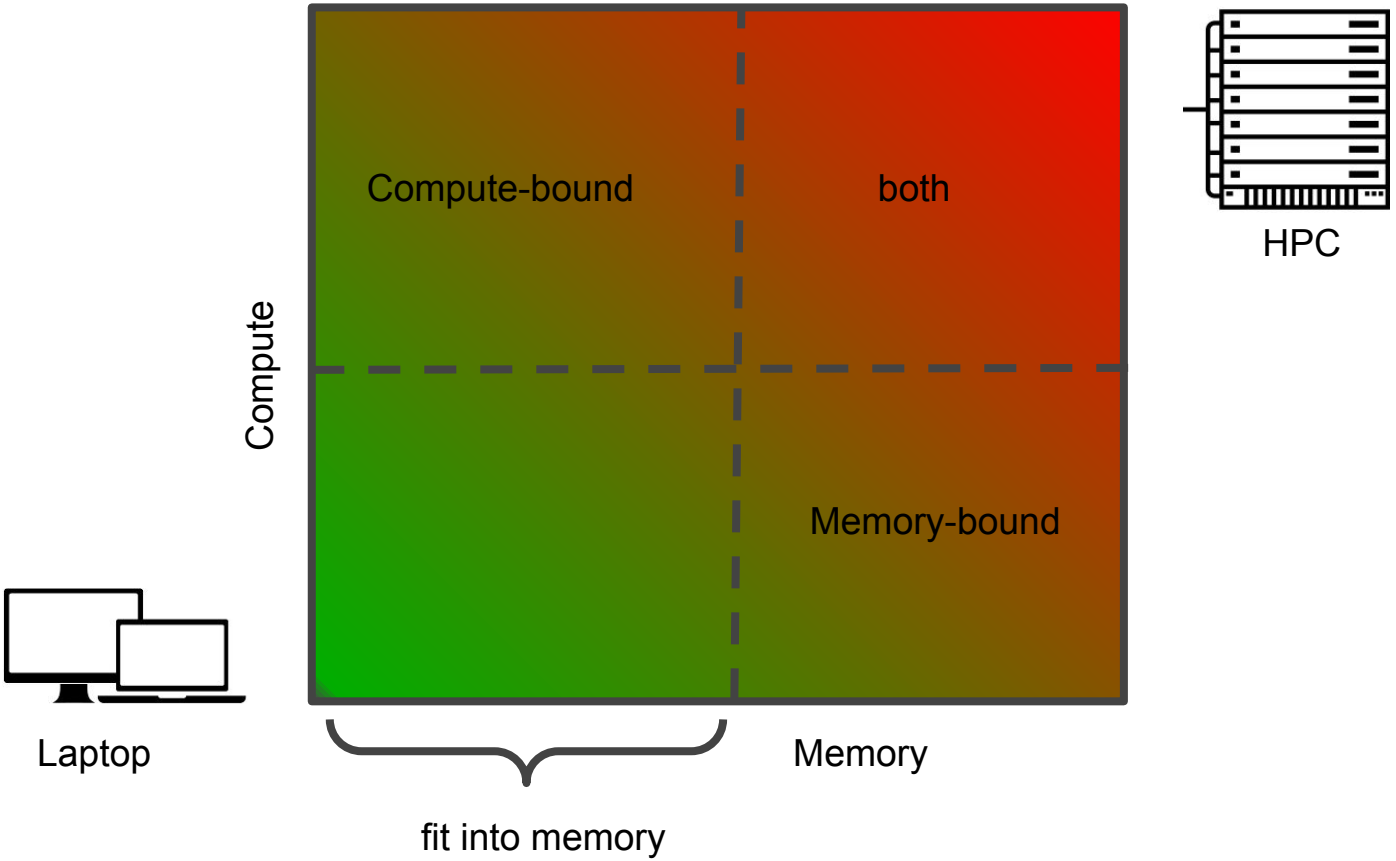
Laptop/Desktop

- 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
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

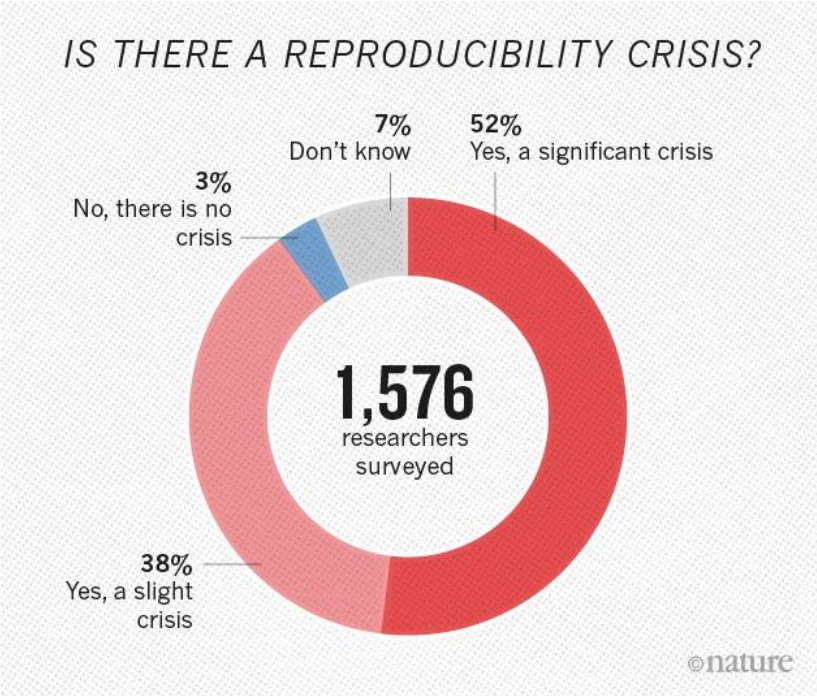
Reproducibility Crisis?

"More than 70% of researchers have tried and failed to reproduce another scientist's experiments, and more than half have failed to reproduce their own experiments."

Nature, 2016, M. Baker, 1,500 scientists lift the lid on reproducibility

"Nature journal editors … will, on a case-by-case basis, ask reviewers to check how well the code works."

Nature, 2018, Does your code stand up to scrutiny?



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

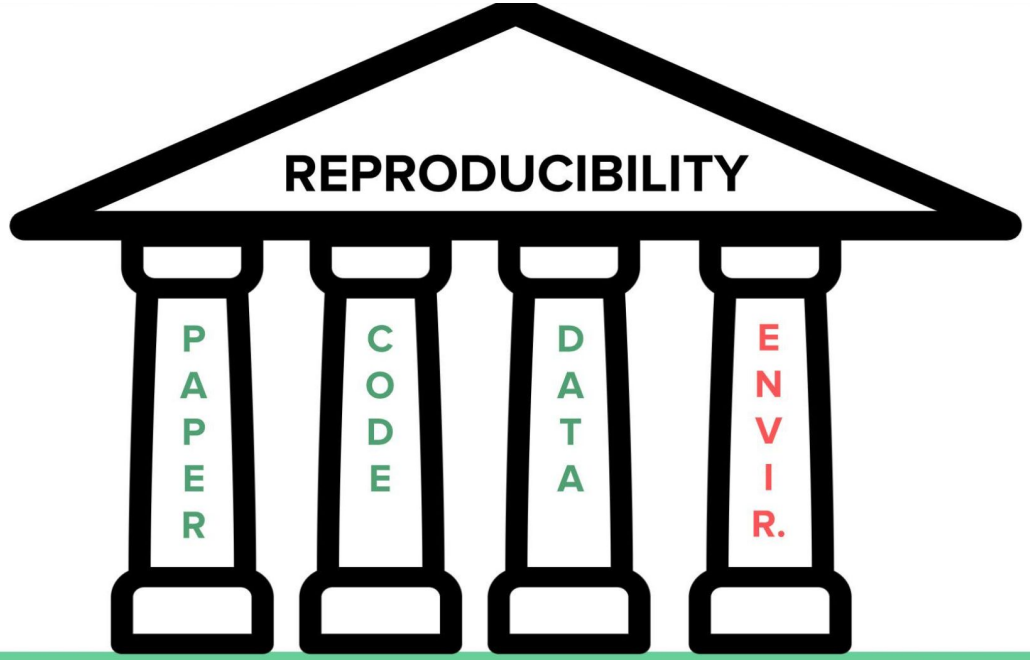
large input data or parameter sets

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

Four Pillars of Reproducible Research



Open Science

- Open access publications
- Open source code
- Open data
- Open execution environment

http://theoryandpractice.org/2016/05/Reproducibility-Symposium/

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

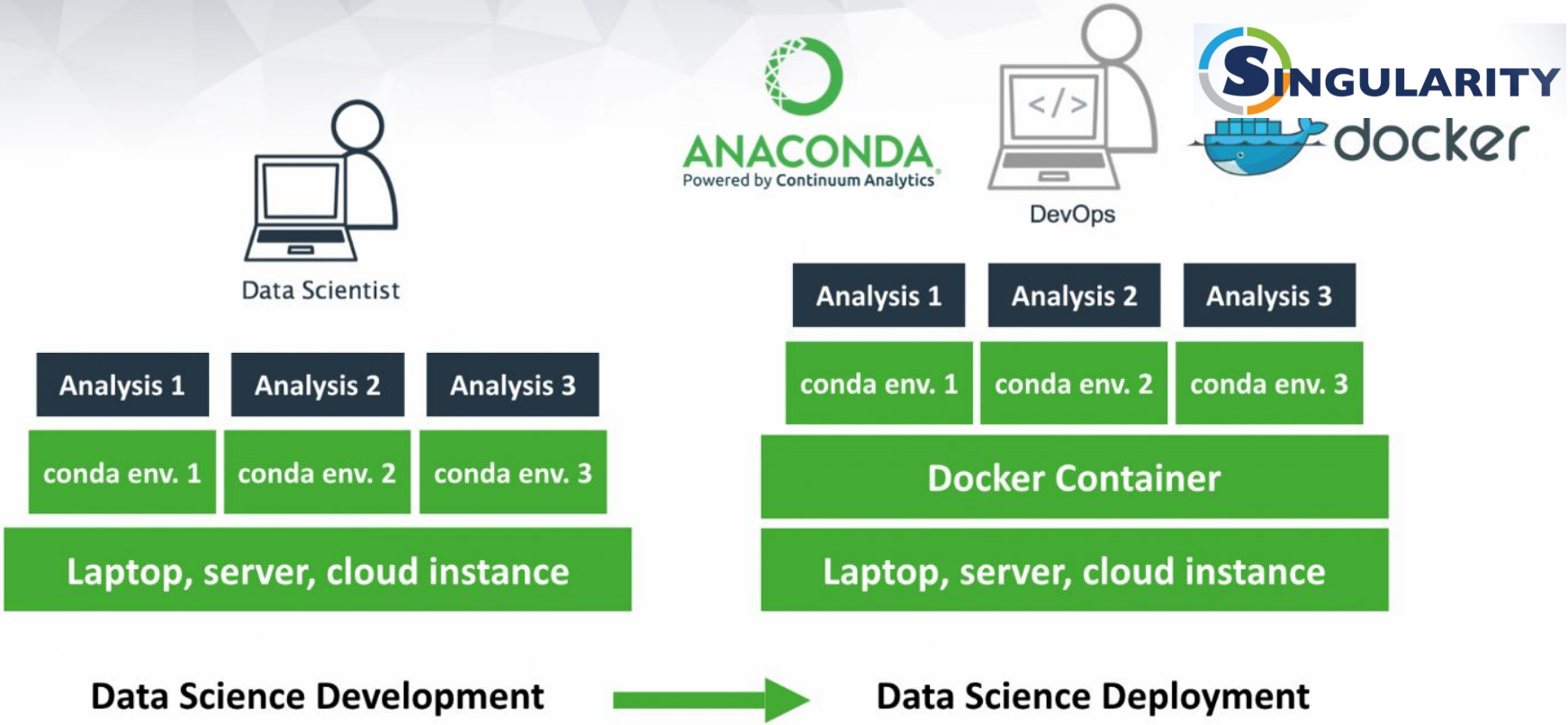
Scalable compute infrastructure

Reproducible Environments

CONDA

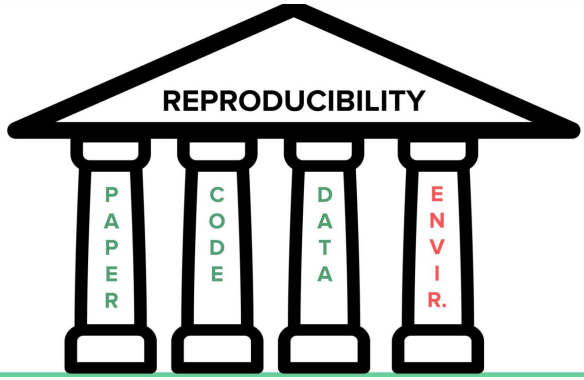
- Beginner
- Experience with Conda
- Exploratory development
- Frequently changing dependencies
- Easy to compose an environment with many dependencies
- Run on single node on Expanse
- Supported on Linux, Mac, Windows
- Run on native OS

- 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



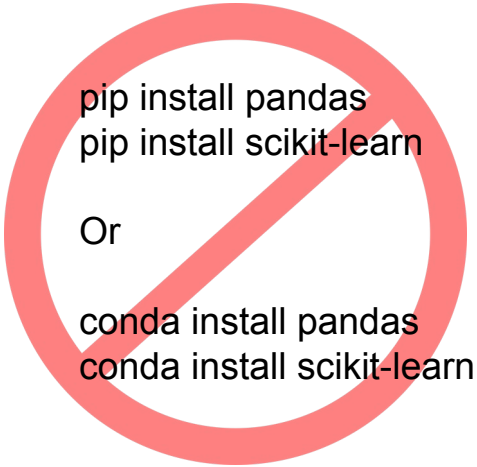
Source: https://medium.com/@patrickmichelberger/getting-started-with-anaconda-docker-b50a2c482139

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?



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 environment 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
```

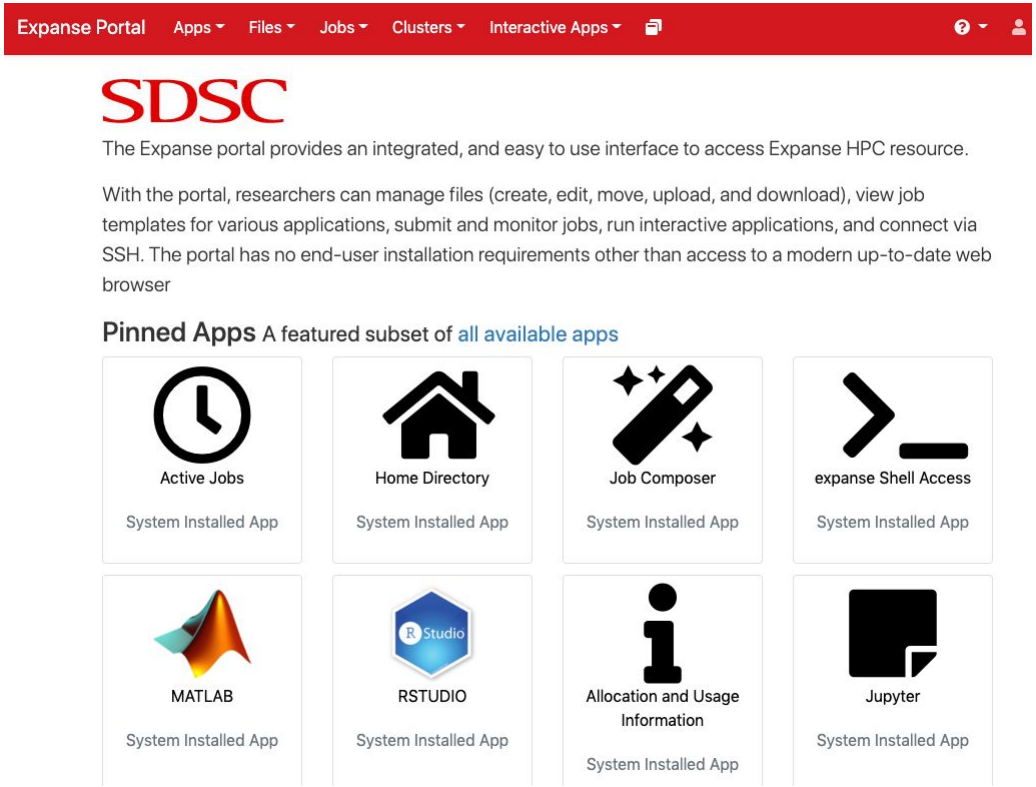
Expanse: **Do not** create a Conda environment in your home directory (network file system)
-> Use the **galyleo** script!

Deactivate conda environment

```
conda deactivate
```

Use the Expanse Portal to check allocations, job status, manage files, open a terminal window

Expanse Portal



Login with your ACCESS credentials:
https://portal.expanse.sdsc.edu/

Note, for this workshop use your trainxx credentials and sign in on the training page:
https://portal.expanse.sdsc.edu/training

Expanse Allocations CPU/GPU

Open OnDemand / Allocation and Usage Information

Resource: Expanse

Project ID:

submit

Allocation and Usage Information

Name	Project	Used	Available	Used By Project
pwrose	sds184	117	5000	165

Open OnDemand / Allocation and Usage Information

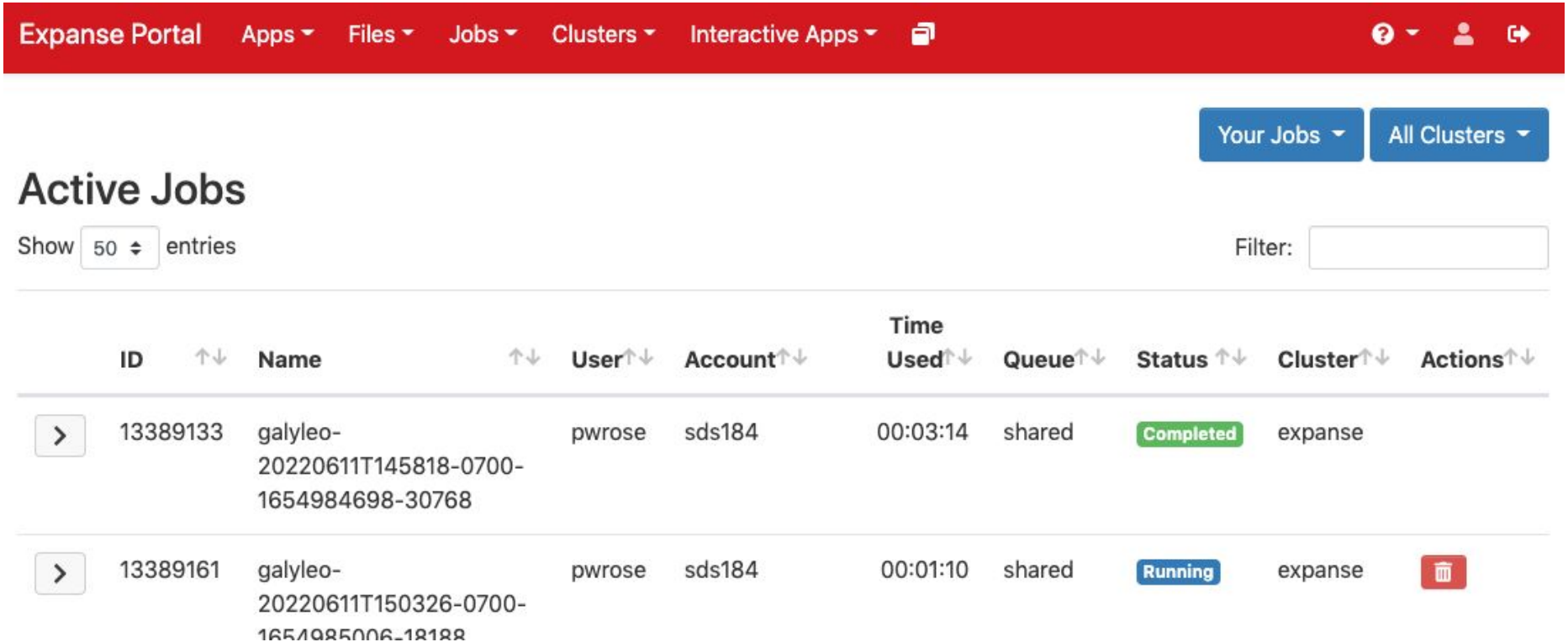
Resource: Expanse GPU

Project ID:

submit

Allocation and Usage Information

Name	Project	Used	Available	Used By Project
pwrose	sds184	20	250	244


Expanse Portal
Apps
Files
Jobs
Clusters
Interactive Apps
Your Jobs
All Clusters
Active Jobs
Show 50 entries
Filter:
ID
Name
User
Account
Time Used
Queue
Status
Cluster
Actions
13389133
galyleo-20220611T145818-0700-1654984698-30768
pwrose
sds184
00:03:14
shared
Completed
expanse
13389161
galyleo-20220611T150326-0700-
pwrose
sds184
00:01:10
shared
Running
expanse

Run Jupyter Lab on Expanse

Galyleo Script

Launches Jupyter Lab/Notebook on high-performance computing (HPC) systems.

Establishes an HTTPS-secured connection between the notebook server and your web browser.

Documentation: https://github.com/mkandes/galyleo

See also: Marty Kandes' webinar: https://education.sdsc.edu/training/interactive/202112_running_jupyter_notebooks_on_expanse/index.html

Using Galyleo

1. Prepend path to galyleo to your path (e.g., add to `.bash_profile` file)

```
export PATH="/cm/shared/apps/sdsc/galyleo:${PATH}"
```

2. Launch your Jupyter Notebook session using a Conda environment.yml file

```
galyleo launch --account <account_number> --partition shared
--cpus 10 --memory 20 --time-limit 01:30:00 --conda-env
df-parallel --conda-yml "${HOME}/df-parallel/environment.yml"
--mamba
```

3. Copy and paste generated URL into your web browser

```
https://anchovy-passion-placidly.expanse-user-content.sdsc.edu?
token=48ee984b9ea07a96c17aaec000bc5fcf
```

Progress Bar and Jupyter Launch

Satellite Reverse Proxy Service

SDSC Expanse

Job State: Proxied

In Queue — Running — Mapped — Proxied

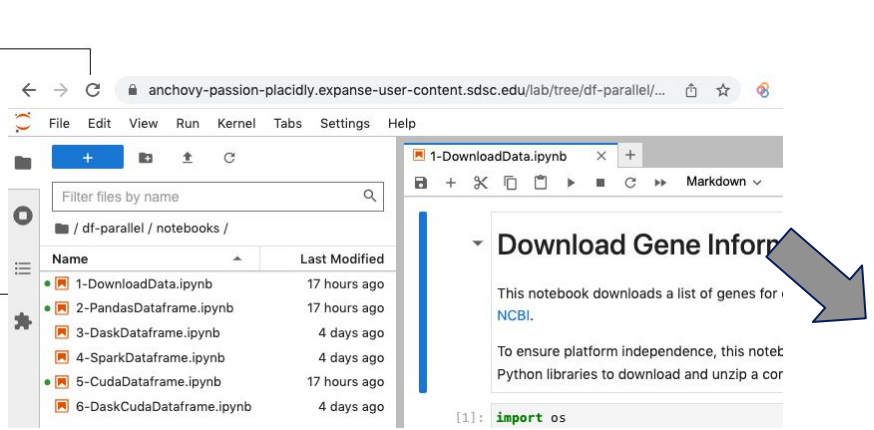
In Queue
Job has not yet started.

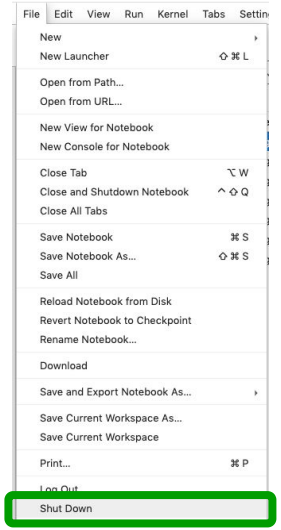
Running
Job has started, but has not redeemed Satellite Token.

Mapped
Job has redeemed Satellite Token, but no proxy entry exists yet.

Proxied
Proxy entry created, ready to go!

Dead
Job died or exited, no further progress will occur.





File-> Shut Down to terminate process!

Running the Dataframe Examples

Clone the Git repo

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

Run on CPU (Pandas, Dask, Spark dataframes)

```
galyleo launch --account <account_number> --partition shared --cpus 10
--memory 20 --time-limit 01:30:00 --conda-env df-parallel
--conda-yml "${HOME}/df-parallel/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 01:30:00 --conda-env df-parallel-gpu
--conda-yml "${HOME}/df-parallel/environment-gpu.yml" --mamba
```

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

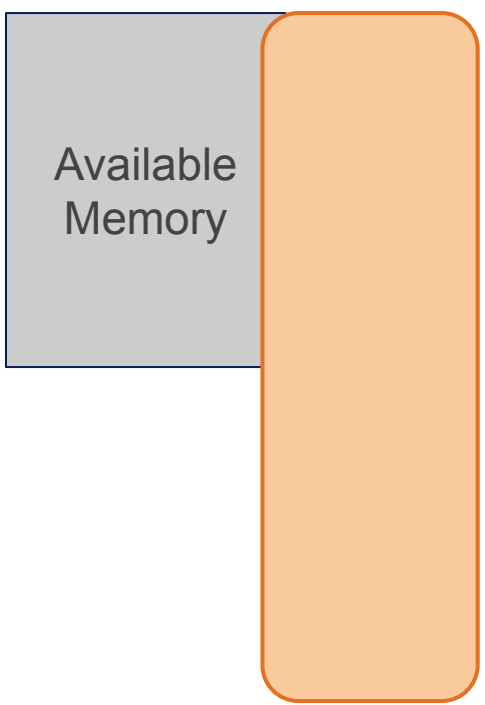
Task 1 - Launch Jupyter Lab on Expanse using a CONDA environment

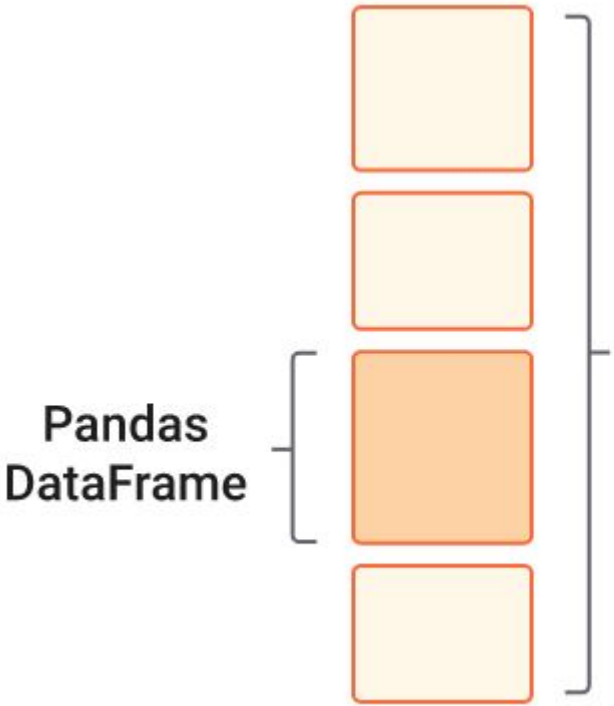
- Clone df-parallel Git repository
- Start galyleo on a GPU node
- Paste the URL for your Jupyter Lab session into your browser

- Follow the instructions in section 3.3:
  - https://github.com/ciml-org/ciml-summer-institute-2023

Scale up Calculations on CPU/GPU

Processing large Datasets on CPU





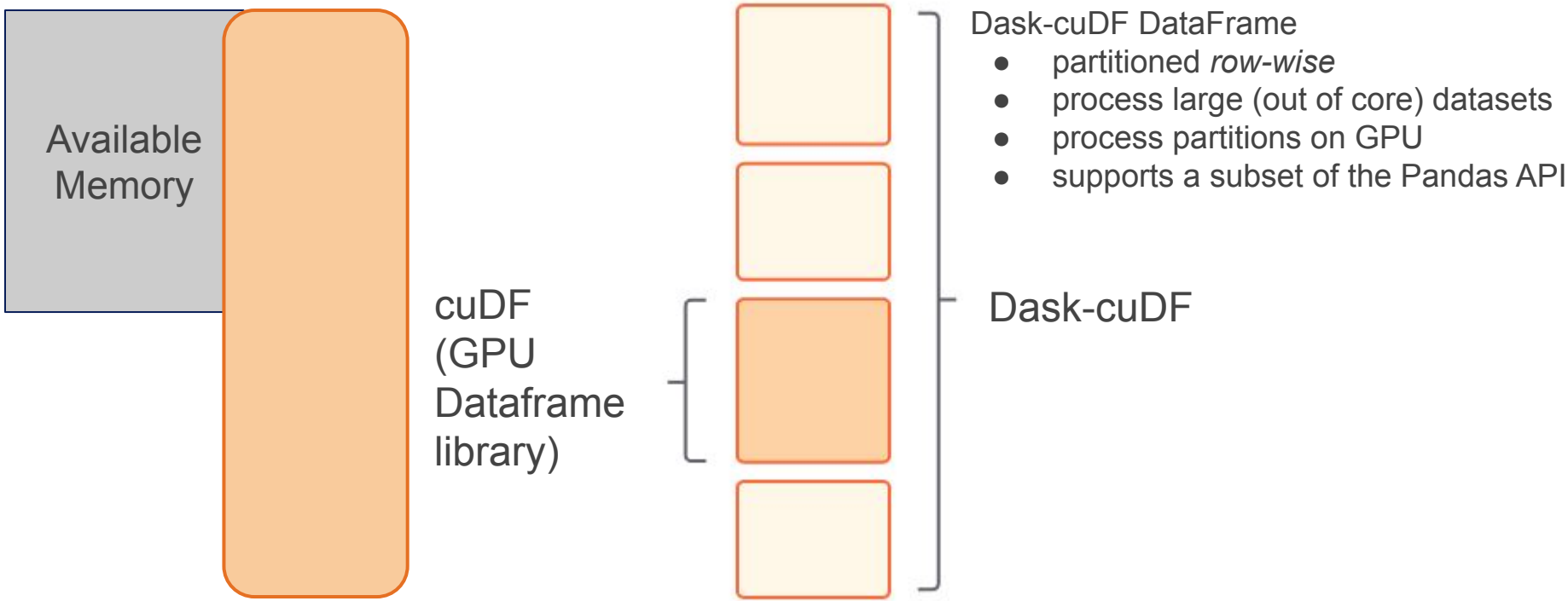
Dask DataFrame

- 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.

Task 2 - Run Jupyter Lab Interactively

- Compare the runtimes for 5 dataframe libraries
- Follow the instructions in section 3.3:
  https://github.com/ciml-org/ciml-summer-institute-2023

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

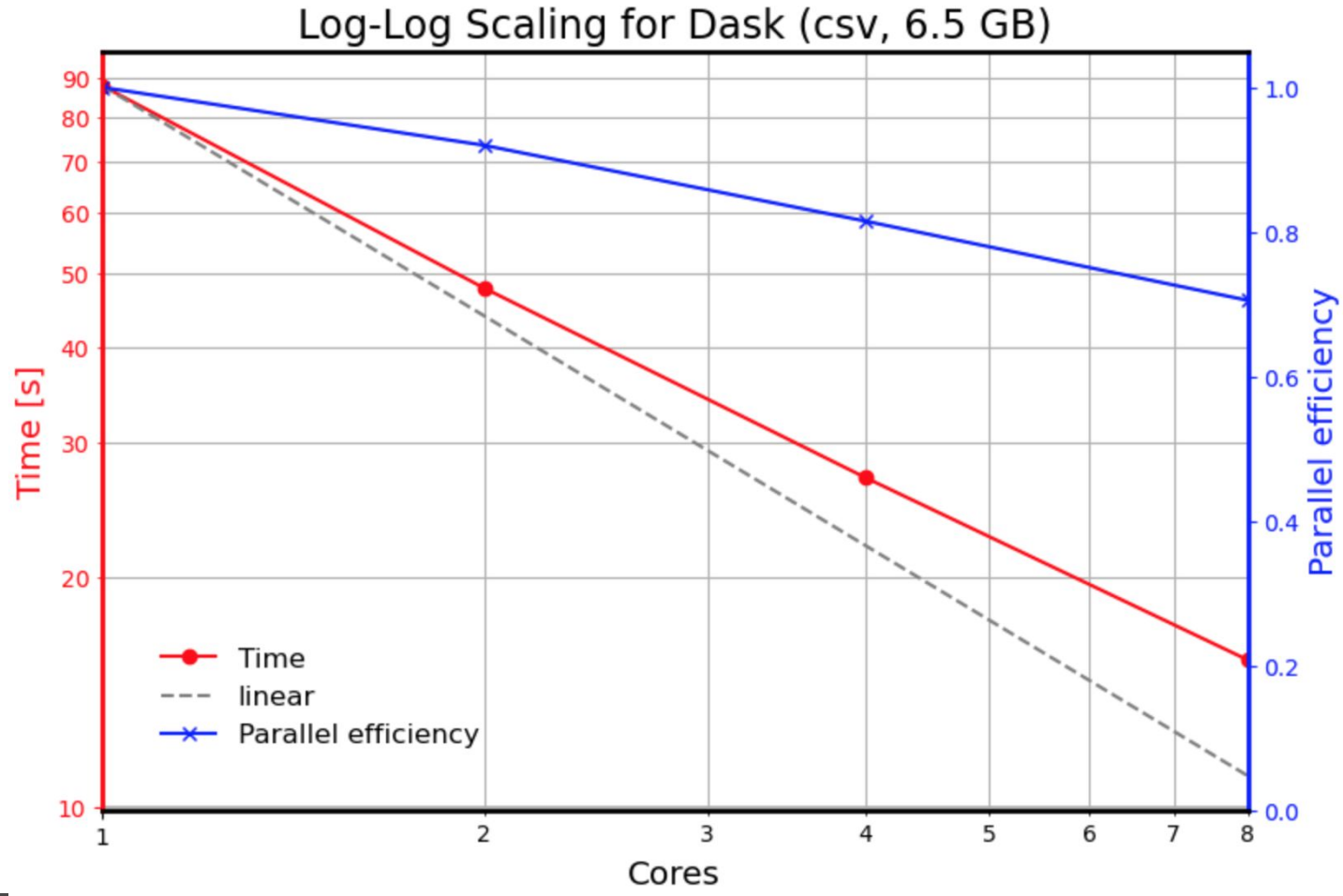
Parallel Efficiency

Task 3 - Assess Parallel Efficiency

- Evaluate the parallel efficiency for scaling up from 1 to 8 CPUs.

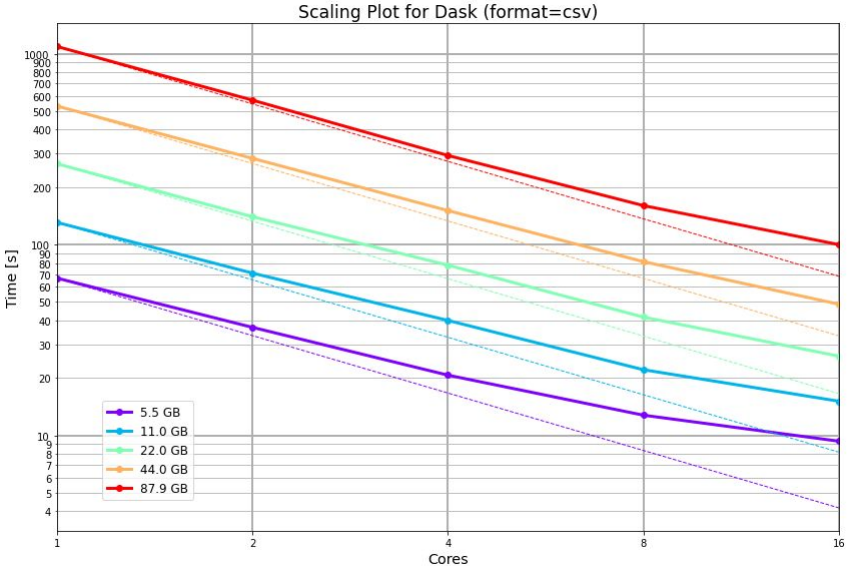
- Follow the instructions in section 3.3:

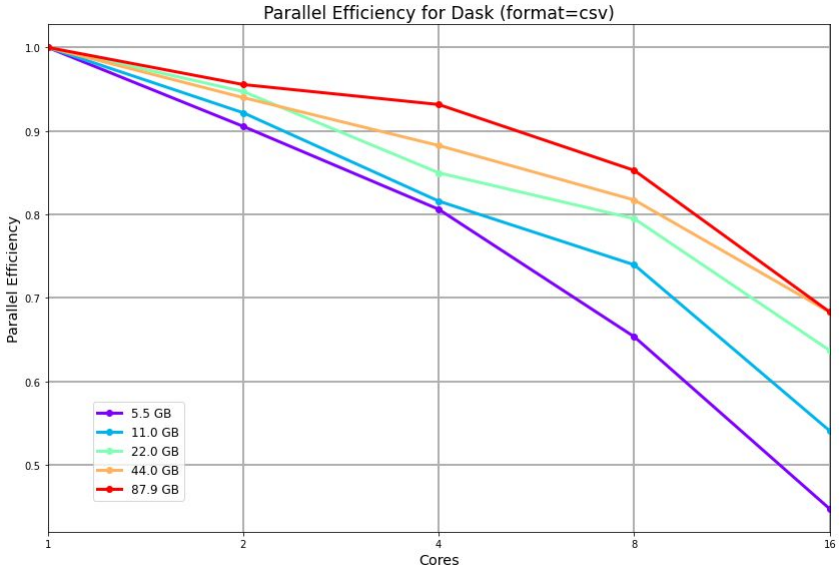
  https://github.com/ciml-org/ciml-summer-institute-2023


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

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

Vertical & Horizontal Partitioning

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

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.

- They can be partitioned for query efficiency

Run Jupyter Lab in Batch

Run Jupyter Lab in Batch

Example batch file

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

Submit job

```
sbatch problem.sh
```

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

- execute notebook on the command line

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

- execute notebook in Python

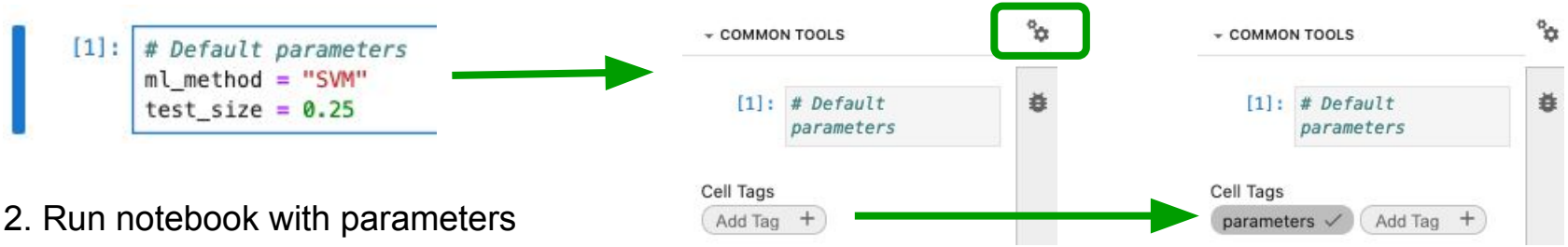
```
import papermill as pm
pm.execute_notebook("input.ipynb", "output.ipynb")
```

- parameterize notebook (pass arguments to Jupyter Notebooks)

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

Parameterize a Notebook

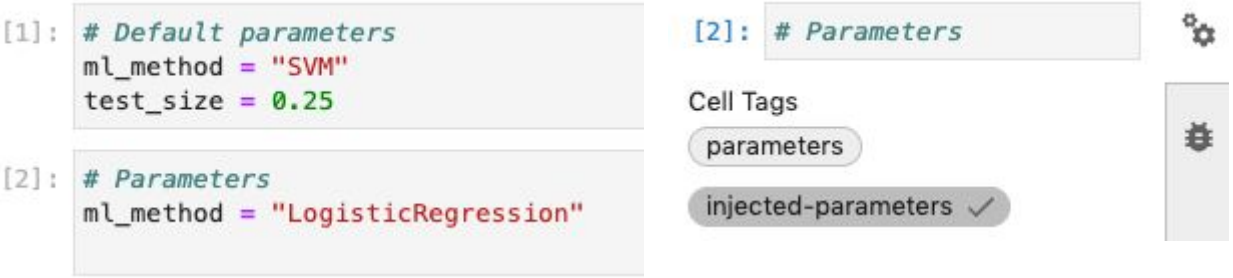
1. Select cell, add “parameters” tag and save notebook



2. Run notebook with parameters

```
papermill input.ipynb output.ipynb -p ml_method LogisticRegression
```

3. The output “executed” notebook has parameter injected



Task 4 - Run Jupyter Lab in Batch

- Parameterize dataframe notebooks
- Edit problem.sh batch file
- Submit the batch job
- Examine the “executed” output notebooks

- Follow the instructions in section 3.3:
  - https://github.com/ciml-org/ciml-summer-institute-2023

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
  https://allocations.access-ci.org/prepare-requests-overview

Allocation	Credit Threshold
Explore ACCESS	400,000
Discover ACCESS	1,500,000
Accelerate ACCESS	3,000,000
Maximize ACCESS	Not awarded in credits.

Allocation Levels

Explore	Discover	Accelerate	Maximize
Resource evaluation, grad student projects, small classes and training events, benchmarking, code development and porting, similar small-scale uses.	Grants with modest resource needs, Campus Champions, large classes and training events, NSF graduate fellowships, benchmarking and code testing at scale, gateway development.	Mid-scale resource needs, consolidating multi-grant programs, collaborative projects, preparation for Maximize ACCESS requests, gateways with growing communities.	Large-scale research projects.

Expanse Allocation

- Expanse is an XSEDE computing resource
- Apply for an Expanse trial account
  - https://portal.xsede.org/allocations/startup#rapidaccess-trial
- Submit a submit a proposal through the XSEDE Allocation Request System
  - https://portal.xsede.org/allocations/announcements

How much does it cost to run the jobs?

Run on CPU (Pandas, Dask, Spark dataframes)

```
galyleo launch --account <account_number> --partition shared --cpus 10
--memory 20 --time-limit 00:30:00 --conda-env df-parallel
--conda-yml "${HOME}/df-parallel/environment.yml" --mamba
```

1 CPU or 2GB of memory are charged 1 CPU Service Unit (SU)/hour.
This job will be charged 10 SU/hour or 5 SUs for 30 minutes.

Run on GPU (Pandas, Dask, Spark, cuDF, Dask-cuDF dataframes)

```
galyleo launch --account <account_number> --partition gpu-shared --cpus 10
--memory 92 --gpus 1 --time-limit 00:30:00 --conda-env df-parallel-gpu
--conda-yml "${HOME}/df-parallel/environment_gpu.yml" --mamba
```

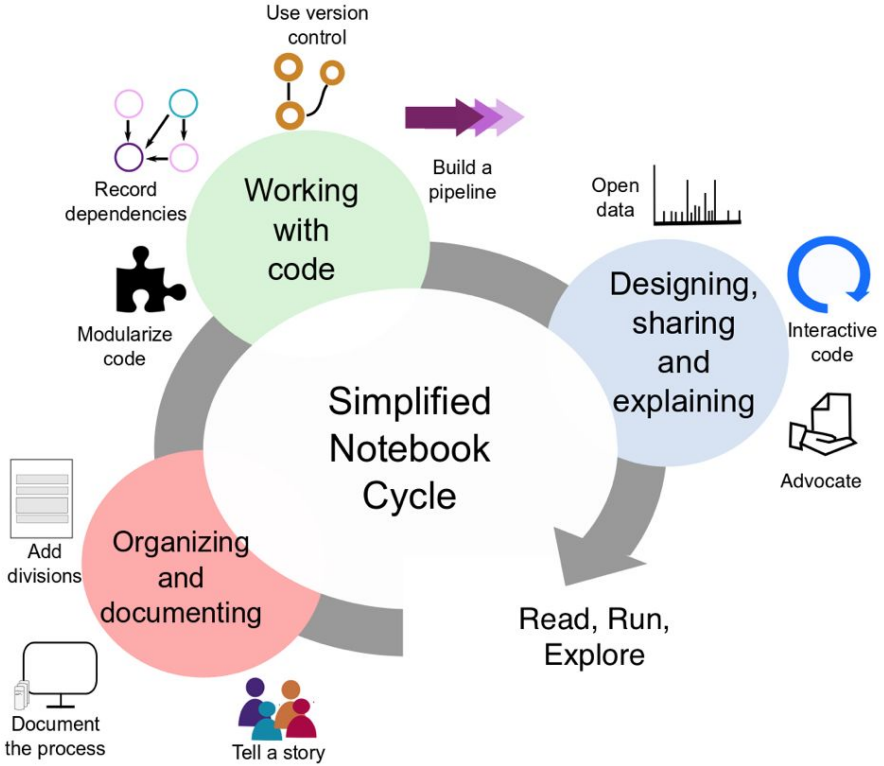
1 GPU or 10 CPUs or 92 GB of memory are charged 1 GPU Service Unit (SU)/hour.
This job will be charged 1 GPU SU/hour. The minimum charge for any job is 1 GPU SU.
So this job will use 1 GPU SU even though it's just run for 30 minutes.

Best Practices for Authoring Jupyter Notebooks

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

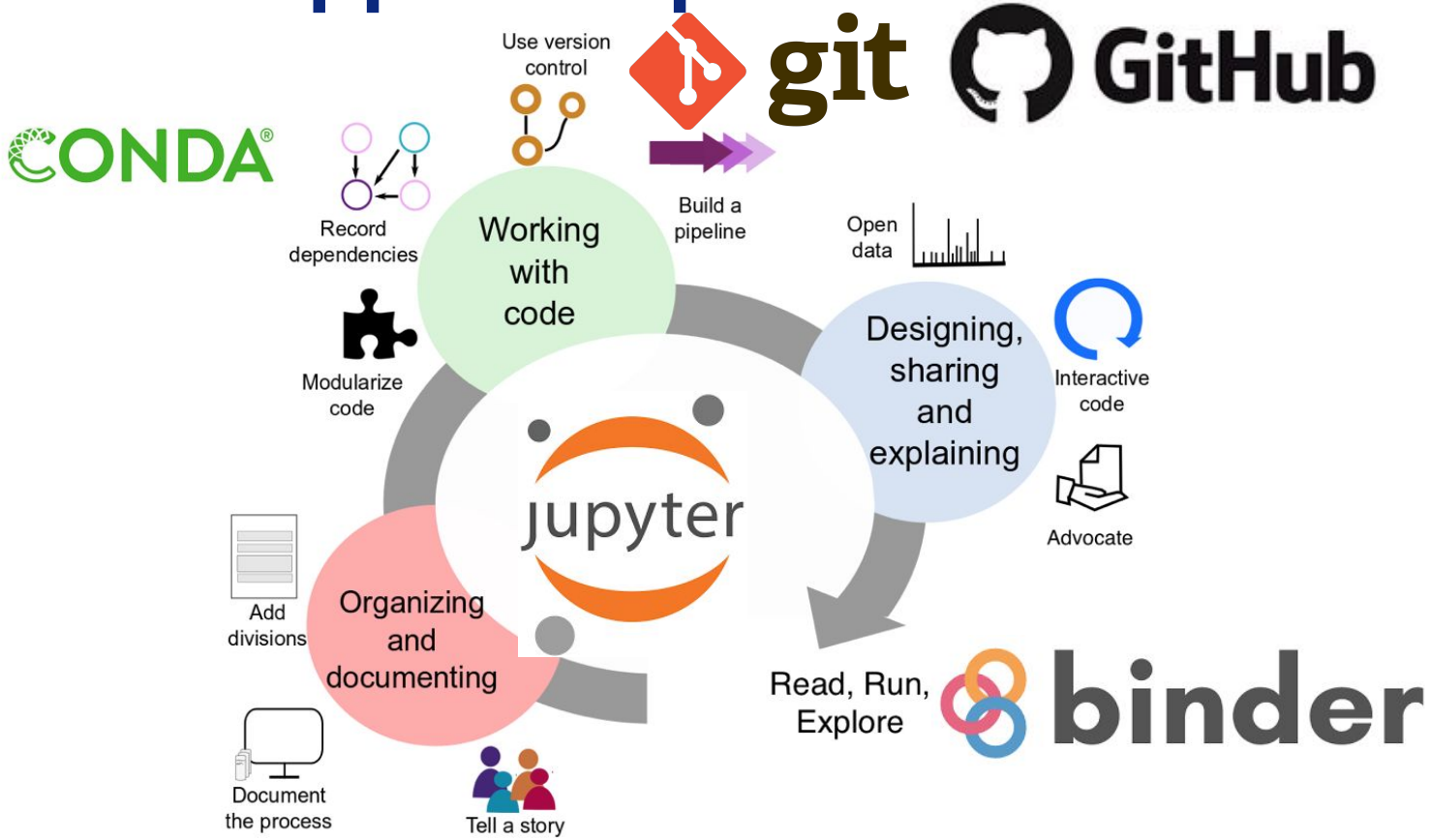
Git repo: https://github.com/jupyter-guide/ten-rules-jupyter

Ten Simple Rules

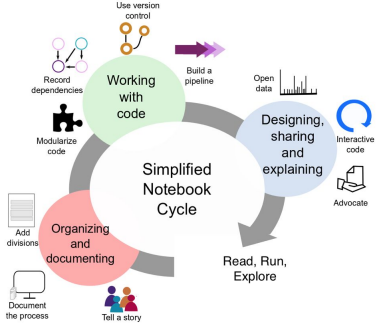


Ten Simple Rules for Writing and Sharing Computational Analyses in Jupyter Notebooks, PLOS Comp. Biol. 2019, https://doi.org/10.1371/journal.pcbi.1007007

Tools to Support Reproducible Workflows

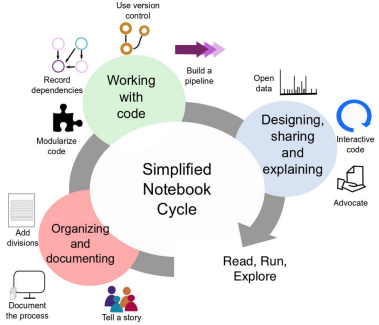


Organizing and Documenting



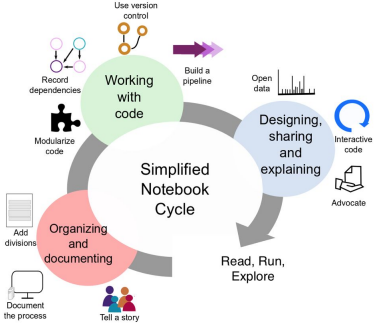
- **Rule 1: Tell a Story for an Audience**
  - Beginning - introduce topic
  - Middle - describe steps
  - End - interprets results
  - Describe not just what you did, by why you did it, how the steps are connected, and what it all means.
  - Adjust your description depending on the intended audience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



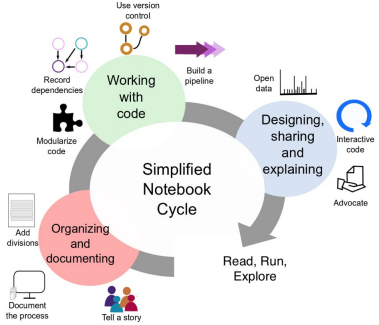
- **Rule 4: Modularize Code**
  - Use functions instead of duplicating code cells
- **Rule 5: Record Dependencies**
  - Manage your dependencies explicitly from the start using a tool such as
    - Conda's environment.yml
    - pip's requirements.txt
- **Rule 6: Use Version Control**
  - Consider using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

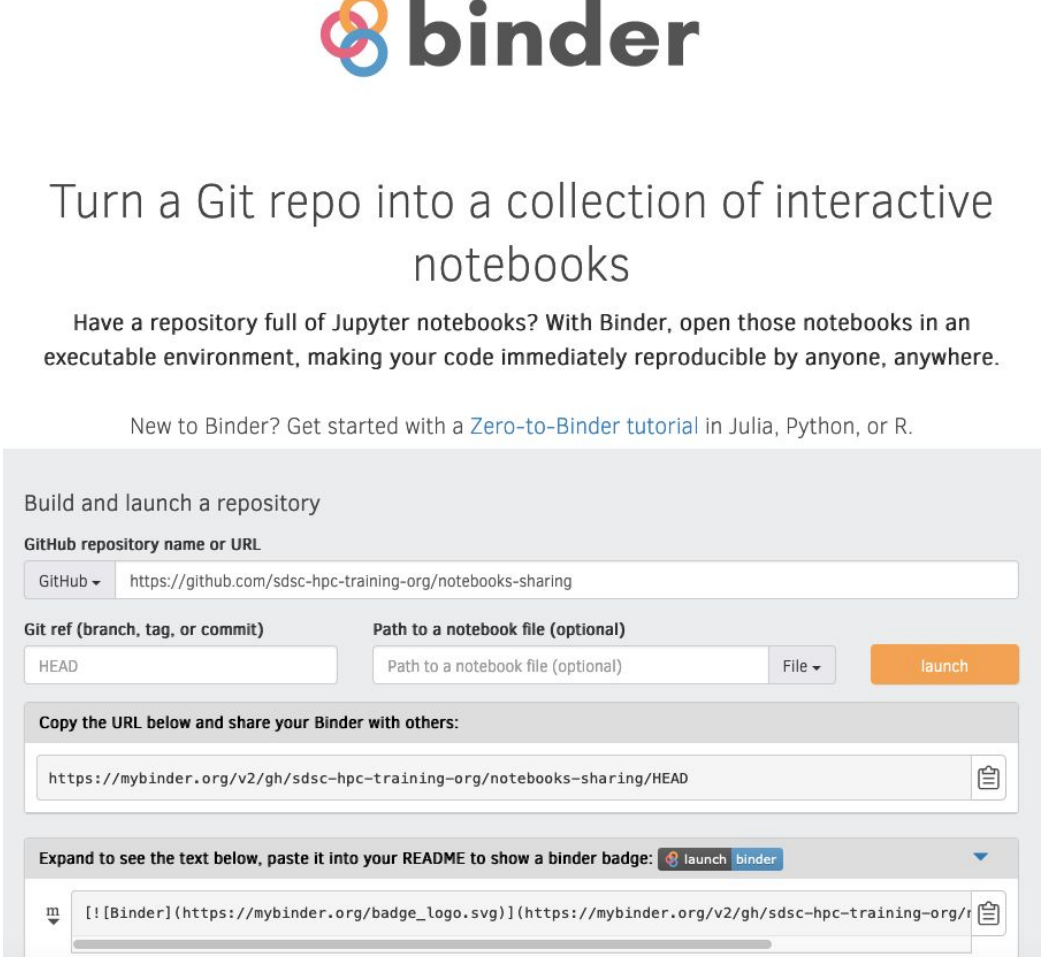
theatlantic.com

The  binder Project

https://mybinder.org/

A community that builds free and open-source tools for reproducible, sharable scientific environments that are workflow- and platform-agnostic.

Source: Chris Holdgraf, bit.ly/2019-elife-cc-holdgraf



Binder Limitations:

Provides a maximum of 2GB of memory

Only suitable for small projects

- few dependencies
- small data files

Launch can be slow or fail

Colab

- Works on a single notebook, not a whole Git repo
- Push changes directly to GitHub
- Cannot (easily) create a Conda environment
- Use pip install commands in notebook
- Supports GPUs
- Install rapidsai (includes cuDF)
  - see section “Cloud Instance GPUs”: Google CoLab w/ pip” **(**https://docs.rapids.ai/install**)**

Summary

- When to run on Expanse
- Setup a portable and reproducible software environment
- Use the Expanse Portal
- Run Jupyter Lab on Expanse
- Scale up calculations on CPU/GPU
- Parameterize a Jupyter Notebook
- 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