Migrating a Simple Data Analysis Program to the Cloud

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Science Technical Application and Research
for the Cloud
(STAR Cloud)

Agenda

- Background
- Project Goals
- The Cloud
- Area-Averaged Time Series
- Setting-Up the Cloud
- Conclusion

Background

Paul Lin
University of Pennsylvania , 2021
Intended Major: **Earth Science**

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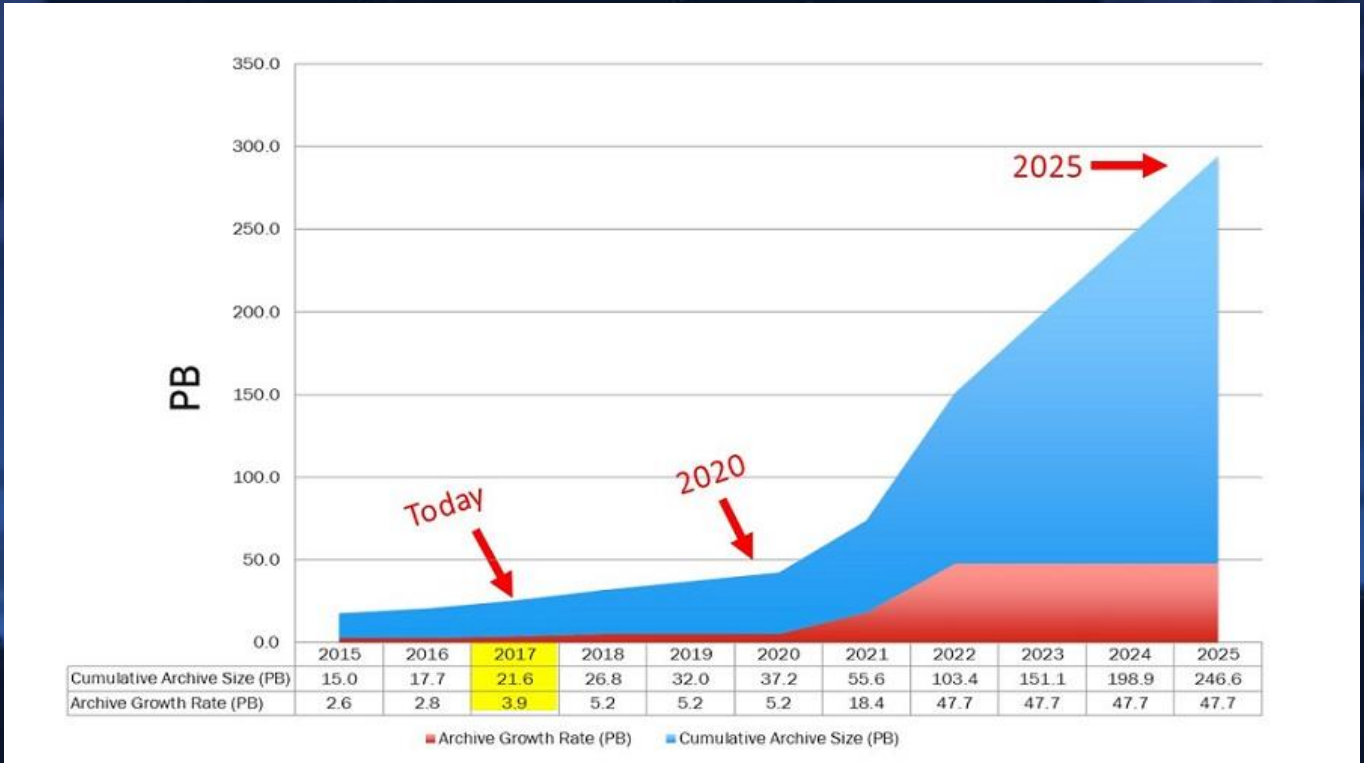
Major: **Environmental Science**

Project Goals

- Consider and test the advantages of the cloud while documenting and overcoming the pitfalls (so you won’t have to!)

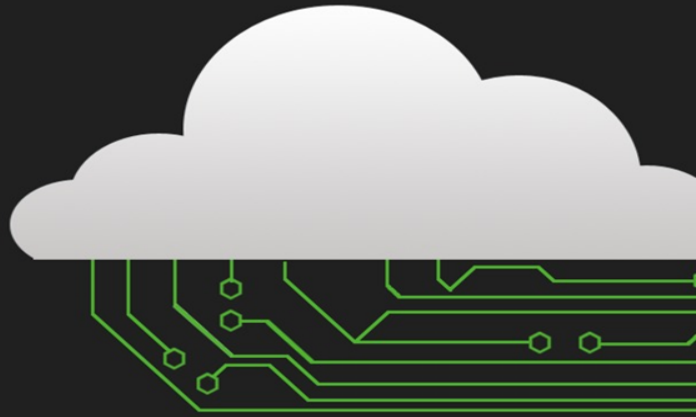
- Investigate the cloud’s ability to outperform local machines for running Earth science code

Big Data is Getting Bigger



	2015	2016	2017	2018	2019	2020	2021	2022	2023	2024	2025
Cumulative Archive Size (PB)	15.0	17.7	21.6	26.8	32.0	37.2	55.6	103.4	151.1	198.9	246.6
Archive Growth Rate (PB)	2.6	2.8	3.9	5.2	5.2	5.2	18.4	47.7	47.7	47.7	47.7

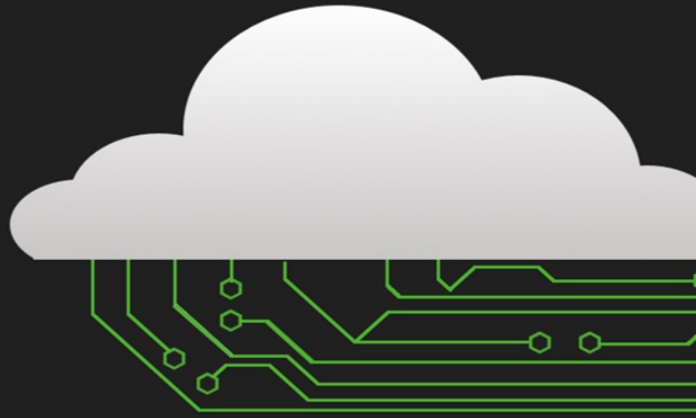
The Cloud



What is the Cloud?

“Cloud computing is the on-demand delivery of compute power, database storage, applications, and other IT resources through a cloud services platform via the internet with pay-as-you-go pricing.”

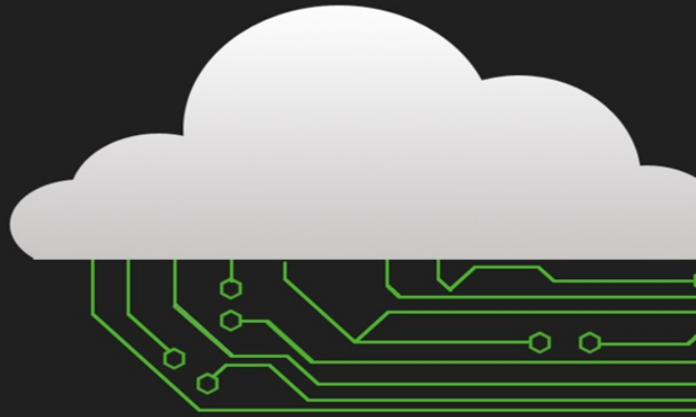
- Amazon Web Services



Why Cloud?

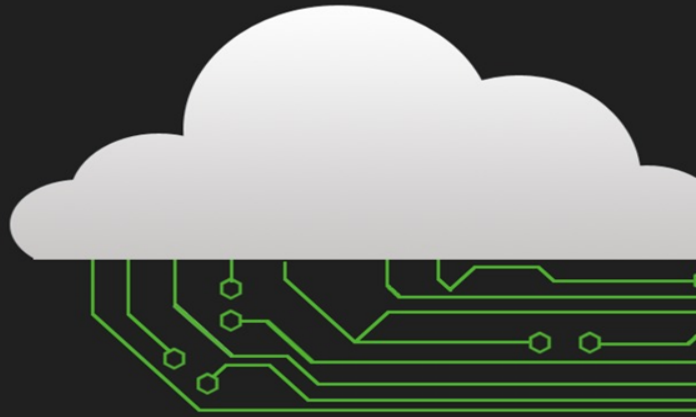
Advantages

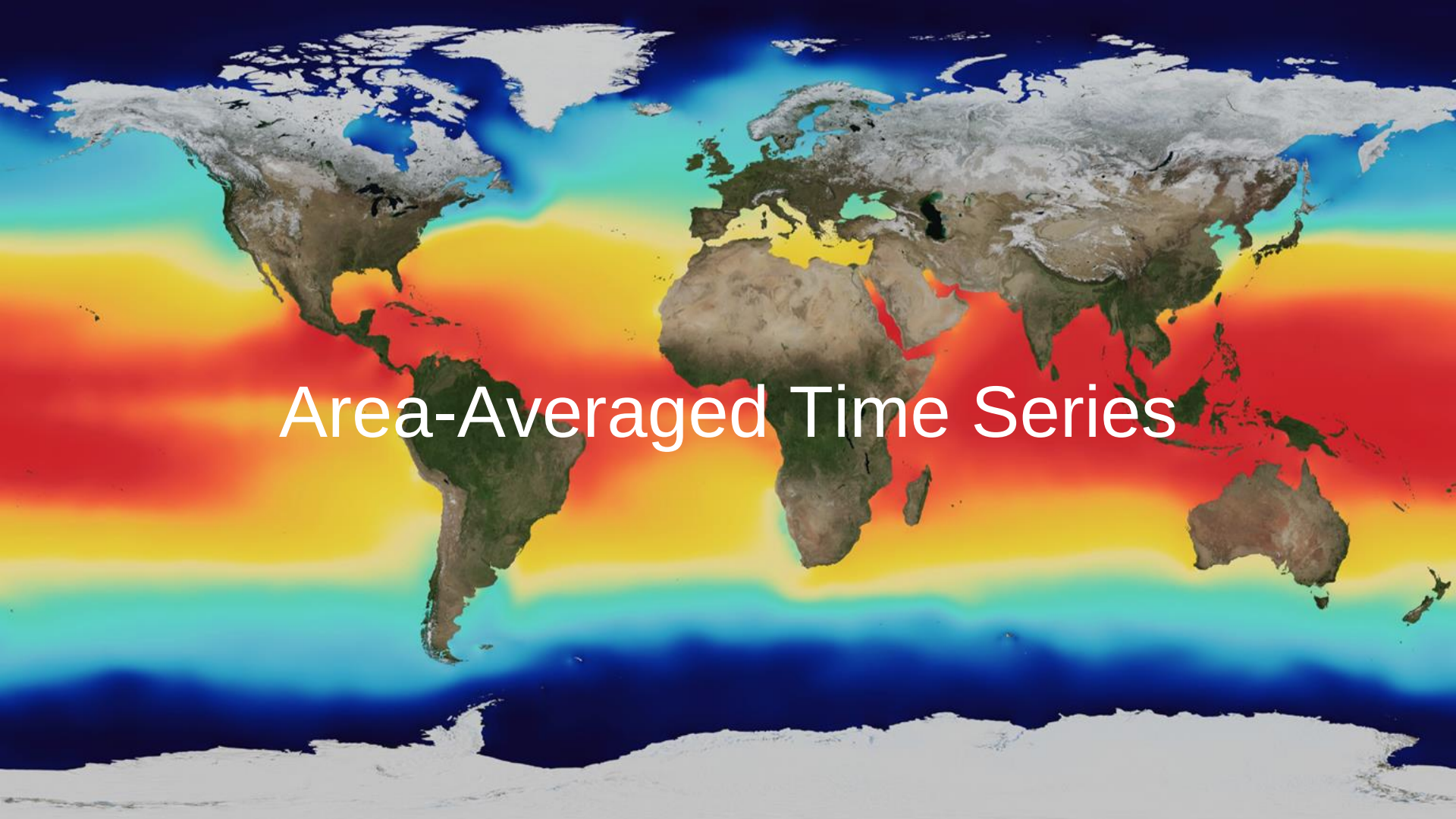
- *Performance*:
  accelerated & pooled computing
- *Ease-of-Use*:
  shared resources for networks, storages, servers, and applications
- *Portability*:
  movable datasets
- *Cost-Effectiveness*:
  pay-as-you-go costs to bypass excessive upfront costs
- *Elasticity On-Demand*:
  ability to instantaneously scale-up or down resources



For an Earth Scientist?

- Faster
  - Commercial cloud CPUs are usually faster than ours...
- Bigger
  - Many levels of storage
- Cheaper
  - Pay only for what you use
    - CPU
    - Storage



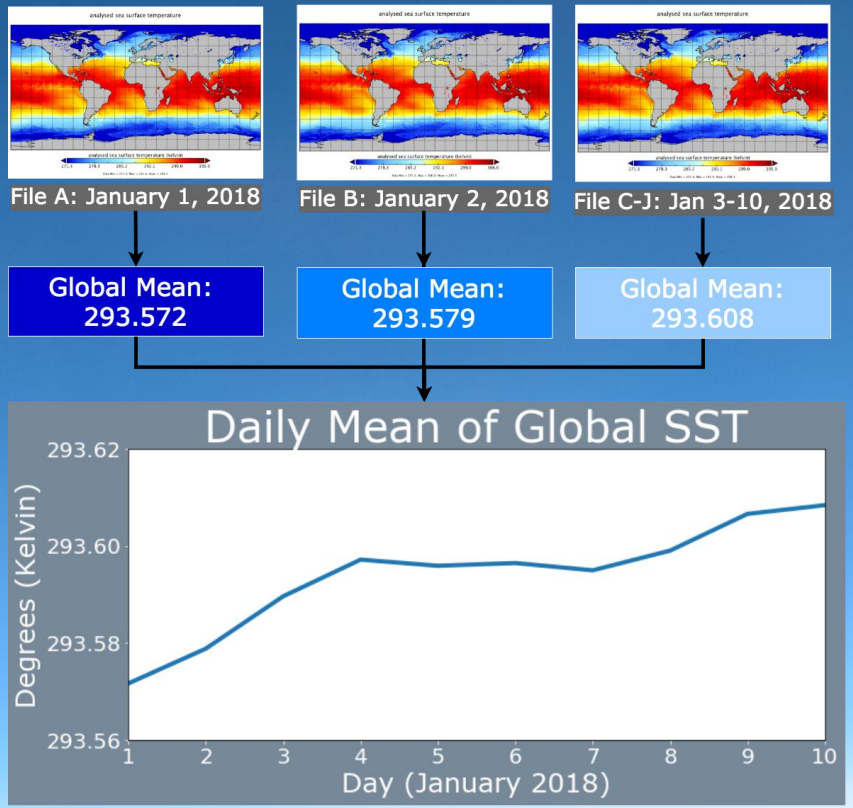

Area-Averaged Time Series

Area-Averaged Time Series

- Used daily average Sea Surface Temperature (SST) data of 10 days to create a graph

- Parallelize executions

Area-Averaged Time Series



Area-Averaged Time Series Data

- Data was collected from *PODAAC*, captured by multiple satellite instruments
  - NASA's AMSRE, MODIS on the NASA Aqua and Terra platforms, the US Navy microwave WindSat radiometer, AVHRR on several NOAA satellites, and in situ SST observations from the NOAA iQuam project.
- GHRSST Level 4 MUR Global Foundation Sea Surface Temperature Analysis (v4.1)

Area-Averaged Time Series Steps

Read Data Files

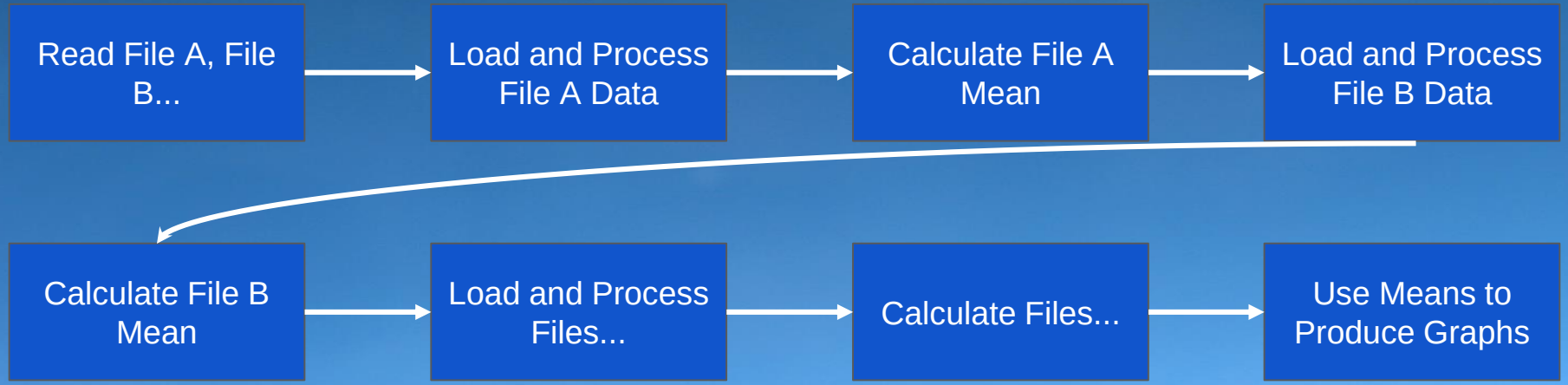
Process Data

Calculate Mean

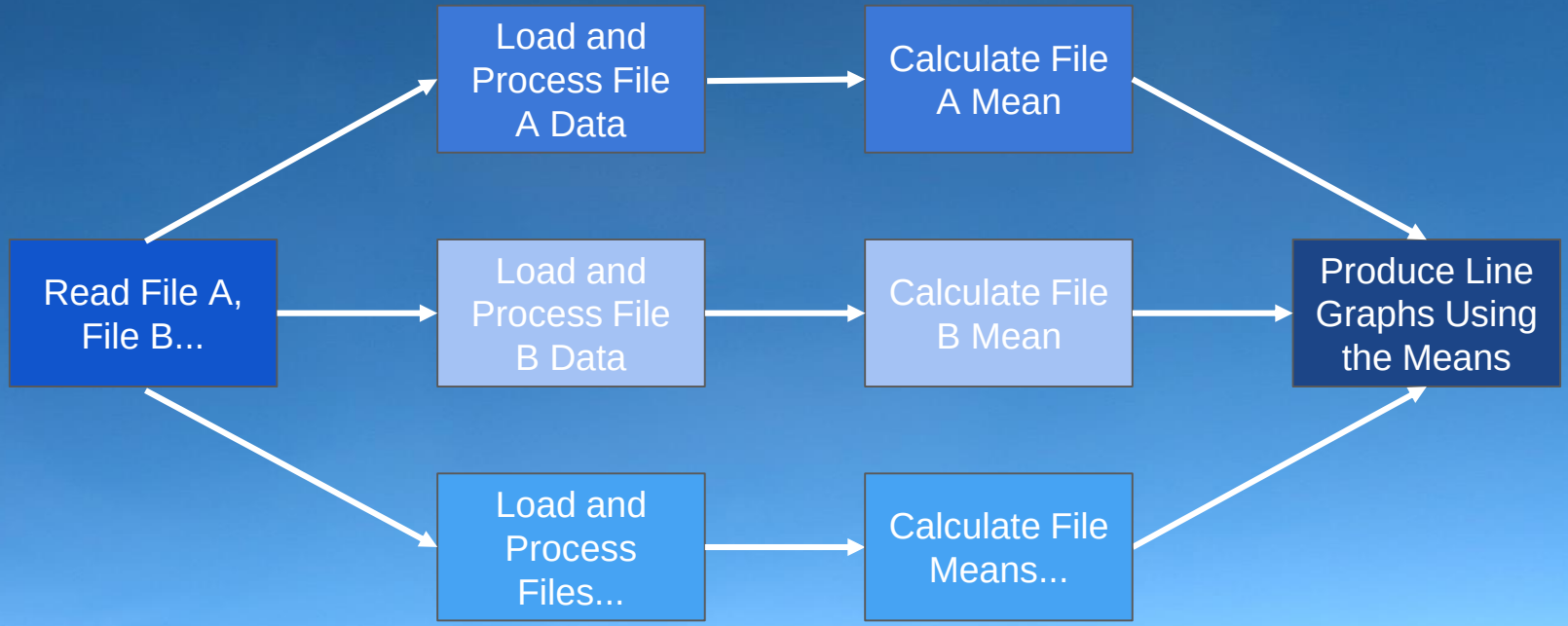
Generate Graph

1. Import python libraries
2. Read datasets (GHRSST: Group for High Resolution Sea Surface Temperature from MODIS)
3. Mask dataset array to account for null values
4. Weigh by latitude array
5. Calculate mean
6. Apply scale factors and additional offsets
7. Generate graph based with dates on x-axis and means on y-axis

Execution Path 1: Serial via “For Loop”

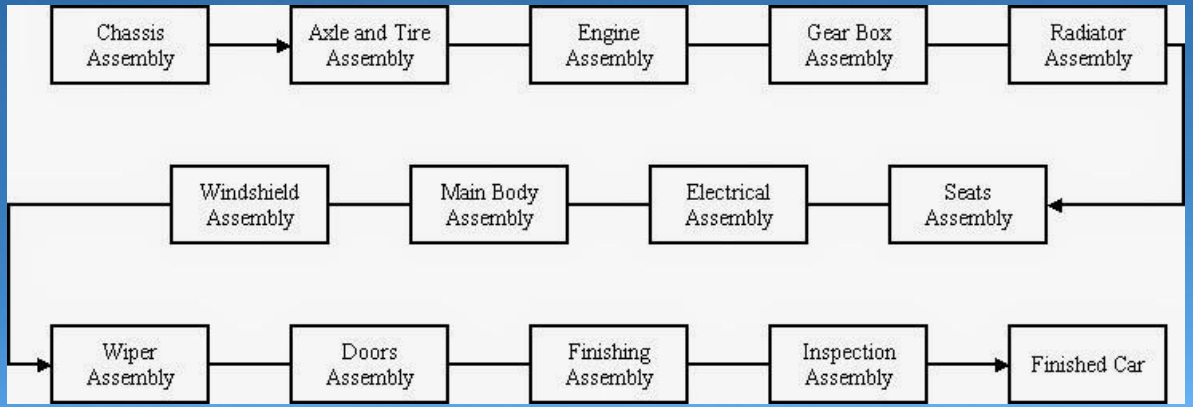


Execution Path 2: Parallel via “Dask”



What is Dask?

Imagine yourself as a car manufacturing manager…



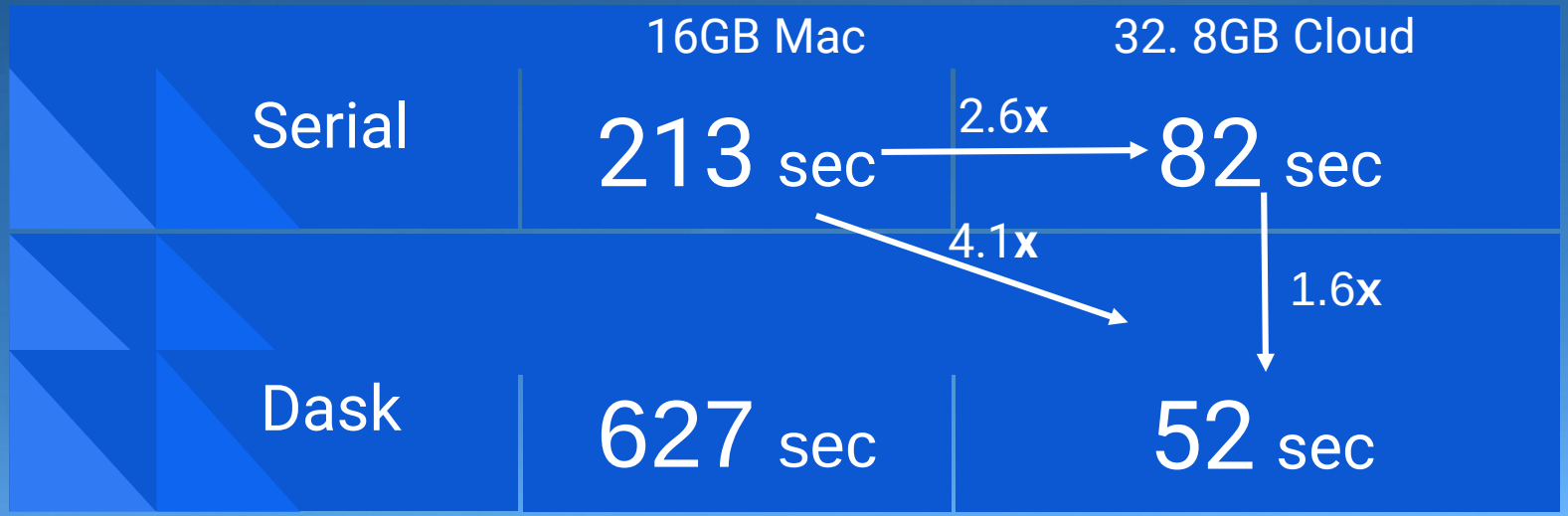
What is Dask?

Created to scale computational libraries and the surrounding ecosystem of packages

- Parallelization
- Fast simultaneous processing
- Dask hides overhead

```
70  @dask.delayed
71  def mean(weighted_mask):
72      data_mean = weighted_mask.mean().compute(scheduler='threads')
73      return data_mean
```

Execution Runtimes



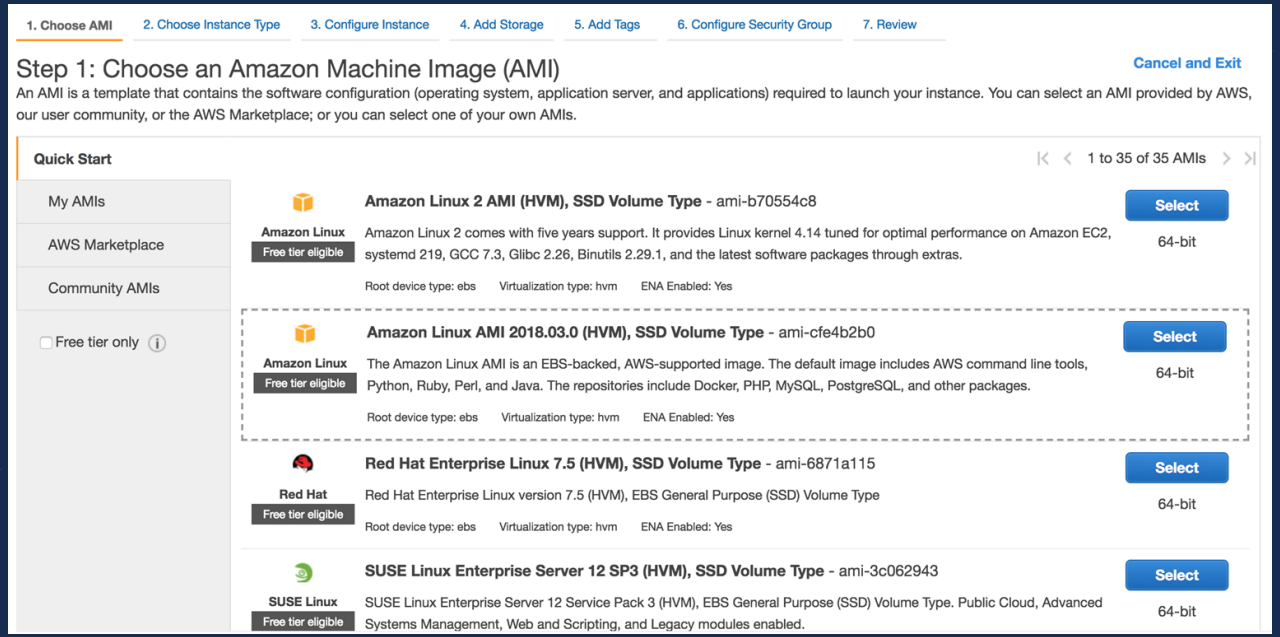
Setting-Up the Cloud

1. Create an AWS Account ☹️

- Unfortunately, we cannot currently provide guidance here… yet.

- Efforts are underway to provide access to cloud computing to scientists

2. Choose, Instantiate, & Configure Virtual Machine (VM) Type



2. Choose, Instantiate, & Configure Virtual Machine (VM) Type

- VM - template containing software configuration (i.e. operating system, application server, and applications) required to launch your instance
- Consider the VM size to optimize the necessary storage and memory space
- *Caveat*: tradeoff exists between size/speed of machine and cost

2. Our VM Specs

- *Family*: Storage Optimized
- *Type*: ***d2.xlarge***
  - (14 ECUs, 4 vCPUs, 2.4 GHz, Intel Xeon E52676v3, 30.5 GiB memory, 3 x 2048 GiB Storage Capacity)

3. Install Python and other necessary python libraries in virtual machine

- Anaconda
  - Contains popular python packages (numPy, Pandas, etc.)
  - Useful for data science
  - Makes for easy deployment for a virtual environment
  - **`https://anaconda.org/`**

- Other python libraries
  - Dask: enables efficient parallel computations
  - NCO: a command line tool for processing netCDF data

4. Getting Datafiles into the Instance

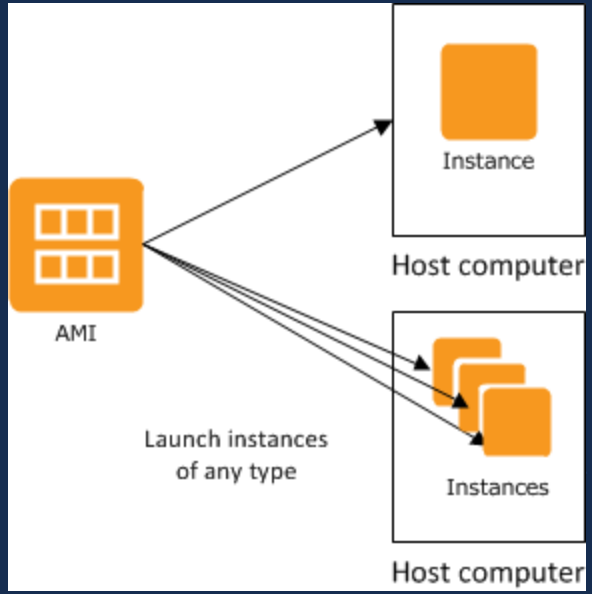
- Use SCP (secure copy protocol)
  - Make sure to be outside of virtual machine
  - `$ scp /local/directory/file.txt username@VM_host:destdir`

OR...

- Use wget
  - Downloads files from a network
  - `wget http://website.com/files/file.zip`

5. Saving an AMI (Amazon Machine Image)

- A template containing a software configuration (eg. operating system or applications)
- You launch an *instance* (VM), which is a copy of the AMI running as a virtual server in the cloud
- Can launch multiple instances of the same AMI
- Provided by AWS, the community, or create your own
- Can change configurations



Further Cloud Steps

1. Run programs in virtual machine!

(Optional): Sharing Virtual Machines
(Optional): Mounting Elastic Block Storage (EBS) Volume

- *Caveat:* EBS must be in same region as VM, EBS must be dismounted to avoid complications, EBS costs a lot of money!

Findings

- Setting up cloud VM’s can be done by people without programming experience
- Running identical programs yields much faster runtimes in the cloud than in local machines
- Cloud machines required more memory to run programs than local computers, but memory size is elastic
- Increasing the data volume better demonstrates Dask’s parallelization advantages

Possible Future Work

- Experiment with further parallelization methods beyond time (i.e.: geographical areas)
- Incorporate Dask Distributed code to spread computational load across multiple VMs
- Refactor more advanced science algorithms

Final Words...

You don’t need to be a comp. sci person to run analysis faster on cloud because:

- Access to big machines
- Access to packages like dask that parallelize with not a lot of effort

Further Details

4. Access Bastion Host

- SSH into the bastion host
  - Why?
    - Set-up a security group that's configured to listen only on the SSH port (TCP/22)
- Configure (Linux) instances in your VPC to accept SSH connections only from bastion instances.