Migrating a Simple Data Analysis Program to the Cloud

By: Diane Portillo and Paul Lin

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**

Diane Portillo
DePaul University, 2018
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

![Graph showing the growth of big data from 2015 to 2025 in petabytes (PB)].

**Cumulative Archive Size (PB):**
- 2015: 15.0
- 2016: 17.7
- 2017: 21.6
- 2018: 26.8
- 2019: 32.0
- 2020: 37.2
- 2021: 55.6
- 2022: 103.4
- 2023: 151.1
- 2024: 196.9
- 2025: 246.6

**Archive Growth Rate (PB):**
- 2015: 2.6
- 2016: 2.8
- 2017: 3.9
- 2018: 5.2
- 2019: 5.2
- 2020: 5.2
- 2021: 18.4
- 2022: 47.7
- 2023: 47.7
- 2024: 47.7
- 2025: 47.7

**Note:** The graph indicates a significant increase in the cumulative archive size and archive growth rate from 2015 to 2025.
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

File A: January 1, 2018
Global Mean: 293.572

File B: January 2, 2018
Global Mean: 293.579

File C-J: Jan 3-10, 2018
Global Mean: 293.608

Daily Mean of Global SST

Degrees (Kelvin)

Day (January 2018)
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.

- **GHRSSST Level 4 MUR Global Foundation Sea Surface Temperature Analysis (v4.1)**
Area-Averaged Time Series Steps

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”

Read File A, File B...
Load and Process File A Data
Calculate File A Mean
Load and Process File B Data

Calculate File B Mean
Load and Process Files...
Calculate Files...
Use Means to Produce Graphs
Execution Path 2: Parallel via “Dask”

1. Read File A, File B...
2. Load and Process File A Data
3. Load and Process File B Data
4. Load and Process Files...
5. Calculate File A Mean
6. Calculate File B Mean
7. Calculate File Means...
8. Produce Line Graphs Using the Means

Legend:
- Process 1
- Process 2
- Process 3
- Process 4
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
<table>
<thead>
<tr>
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<th>16GB Mac</th>
<th>32.8GB Cloud</th>
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</thead>
<tbody>
<tr>
<td><strong>Serial</strong></td>
<td>213 sec</td>
<td>82 sec</td>
</tr>
<tr>
<td><strong>Dask</strong></td>
<td>627 sec</td>
<td>52 sec</td>
</tr>
</tbody>
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Execution Runtimes

- Serial: 213 sec on 16GB Mac vs. 82 sec on 32.8GB Cloud, 2.6x faster
- Dask: 627 sec on 16GB Mac vs. 52 sec on 32.8GB Cloud, 4.1x faster
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

Step 1: Choose an Amazon Machine Image (AMI)
An AMI is a template that contains the software configuration (operating system, application server, and applications) required to launch your instance. You can select an AMI provided by AWS, our user community, or the AWS Marketplace, or you can select one of your own AMIs.

Quick Start
- Amazon Linux 2 AMI (HVM), SSD Volume Type - ami-b70554c8
  - Amazon Linux 2 comes with five years support. It provides Linux kernel 4.14 tuned for optimal performance on Amazon EC2, systemd 219, GCC 7.3, Glibc 2.29, Binutils 2.29.1, and the latest software packages through extras.
  - Root device type: ebs
  - Virtualization type: hvm
  - ENA Enabled: Yes
  - 64-bit

- Amazon Linux AMI 2018.03.0 (HVM), SSD Volume Type - ami-cfe4b2b0
  - The Amazon Linux AMI is an EBS-backed, AWS-supported image. The default image includes AWS command line tools, Python, Ruby, Perl, and Java. The repositories include Docker, PHP, MySQL, PostgreSQL, and other packages.
  - Root device type: ebs
  - Virtualization type: hvm
  - ENA Enabled: Yes
  - 64-bit

- Red Hat Enterprise Linux 7.5 (HVM), SSD Volume Type - ami-6871a115
  - Red Hat Enterprise Linux version 7.5 (HVM), EBS General Purpose (SSD) Volume Type
  - Root device type: ebs
  - Virtualization type: hvm
  - ENA Enabled: Yes
  - 64-bit

- SUSE Linux Enterprise Server 12 SP3 (HVM), SSD Volume Type - ami-3c062943
  - SUSE Linux Enterprise Server 12 Service Pack 3 (HVM), EBS General Purpose (SSD) Volume Type, Public Cloud, Advanced Systems Management, Web and Scripting, and Legacy modules enabled.
  - Root device type: ebs
  - Virtualization type: hvm
  - ENA Enabled: Yes
  - 64-bit
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 (e.g., 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.