

GCSC

11/17/2021

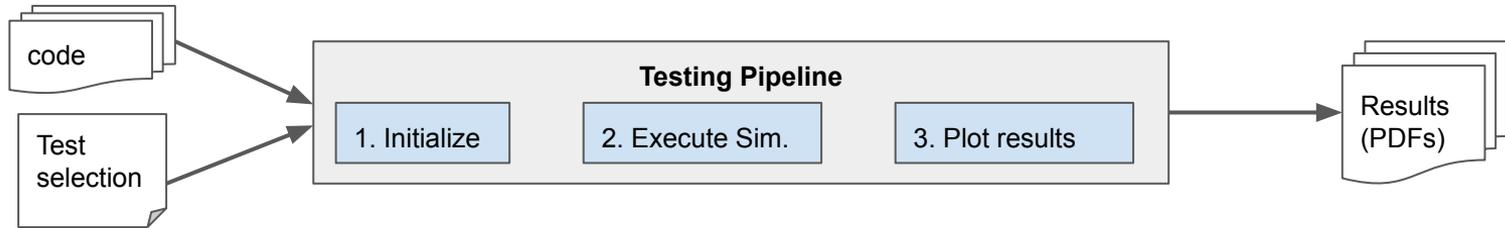
# Tooling for the cloud

## Objective

Streamline testing GEOS-Chem pull-requests and structural updates

## Solution

Use automated pipelines on AWS to initiate, execute, and plot the results of test simulations.



## What we need

1. Premade environments to execute the tests in (i.e., container images)
2. A means of synchronizing GEOS-Chem input data (i.e., keeping the data repository up-to-date)
3. The actual “pipeline infrastructure”

# Pre-built test environments: EC2 Image Builder

## What we need

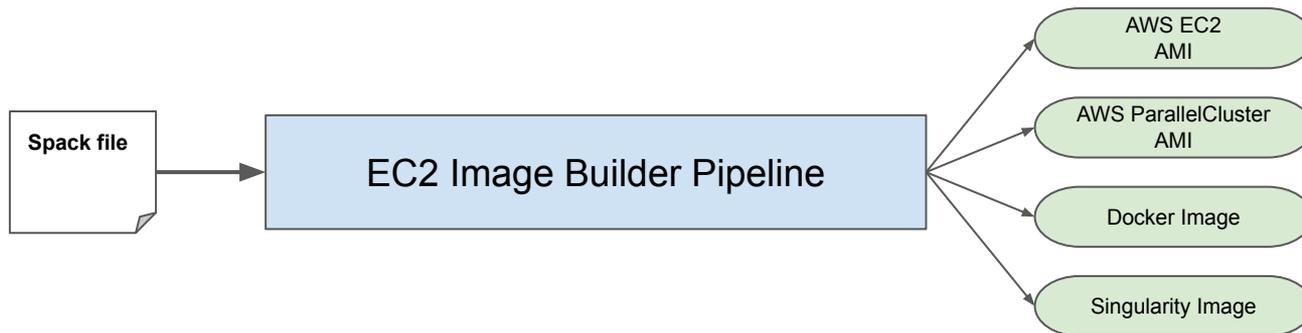
A set of container images for testing GEOS-Chem with different compilers and MPI.

## Challenge

Maintaining more than a few images is a burden.

## The Solution

We can use EC2 Image Builder to build images from a spack configuration file.



# Synchronizing In

## What we need

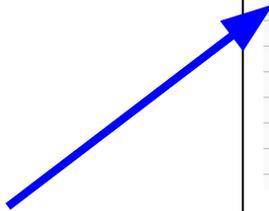
A way to automatically get new data

## Solution

Use the bashdatacatalog to facilitate

Example **catalog**: EmissionsInputs-13.2.1.csv

	A	B	C	D
1	<b>Path to collection</b>	<b>Collection URL</b>	<b>Enabled</b>	<b>Notes</b>
2	HEMCO/ACET/v2014-07	<a href="http://geoschemdata.wustl.edu/ExtData/HEMCO/ACET/v2014-07">http://geoschemdata.wustl.edu/ExtData/HEMCO/ACET/v2014-07</a>		1
3	HEMCO/AEIC/v2015-01	<a href="http://geoschemdata.wustl.edu/ExtData/HEMCO/AEIC/v2015-01">http://geoschemdata.wustl.edu/ExtData/HEMCO/AEIC/v2015-01</a>		1
4	HEMCO/AFCID/v2018-04	<a href="http://geoschemdata.wustl.edu/ExtData/HEMCO/AFCID/v2018-04">http://geoschemdata.wustl.edu/ExtData/HEMCO/AFCID/v2018-04</a>		1
5	HEMCO/ALD2/v2017-03	<a href="http://geoschemdata.wustl.edu/ExtData/HEMCO/ALD2/v2017-03">http://geoschemdata.wustl.edu/ExtData/HEMCO/ALD2/v2017-03</a>		1
6	HEMCO/AnnualScalar/v2014-07	<a href="http://geoschemdata.wustl.edu/ExtData/HEMCO/AnnualScalar/v2014-07">http://geoschemdata.wustl.edu/ExtData/HEMCO/AnnualScalar/v2014-07</a>		1
7	HEMCO/APEI/v2016-11	<a href="http://geoschemdata.wustl.edu/ExtData/HEMCO/APEI/v2016-11">http://geoschemdata.wustl.edu/ExtData/HEMCO/APEI/v2016-11</a>		1
8	HEMCO/BIOFUEL/v2019-08	<a href="http://geoschemdata.wustl.edu/ExtData/HEMCO/BIOFUEL/v2019-08">http://geoschemdata.wustl.edu/ExtData/HEMCO/BIOFUEL/v2019-08</a>		1
9	HEMCO/BROMINE/v2015-02	<a href="http://geoschemdata.wustl.edu/ExtData/HEMCO/BROMINE/v2015-02">http://geoschemdata.wustl.edu/ExtData/HEMCO/BROMINE/v2015-02</a>		1
10	HEMCO/C2H6_2010/v2019-06	<a href="http://geoschemdata.wustl.edu/ExtData/HEMCO/C2H6_2010/v2019-06">http://geoschemdata.wustl.edu/ExtData/HEMCO/C2H6_2010/v2019-06</a>		1
11	HEMCO/CEDS/v2021-06	<a href="http://geoschemdata.wustl.edu/ExtData/HEMCO/CEDS/v2021-06">http://geoschemdata.wustl.edu/ExtData/HEMCO/CEDS/v2021-06</a>		1
12	HEMCO/CH3I/v2014-07	<a href="http://geoschemdata.wustl.edu/ExtData/HEMCO/CH3I/v2014-07">http://geoschemdata.wustl.edu/ExtData/HEMCO/CH3I/v2014-07</a>		1
13	HEMCO/CMIP6/v2020-03	<a href="http://geoschemdata.wustl.edu/ExtData/HEMCO/CMIP6/v2020-03">http://geoschemdata.wustl.edu/ExtData/HEMCO/CMIP6/v2020-03</a>		1
14	HEMCO/DICE_Africa/v2016-10	<a href="http://geoschemdata.wustl.edu/ExtData/HEMCO/DICE_Africa/v2016-10">http://geoschemdata.wustl.edu/ExtData/HEMCO/DICE_Africa/v2016-10</a>		1
15	HEMCO/DMS/v2015-07	<a href="http://geoschemdata.wustl.edu/ExtData/HEMCO/DMS/v2015-07">http://geoschemdata.wustl.edu/ExtData/HEMCO/DMS/v2015-07</a>		1
16	HEMCO/DUST_DEAD/v2019-06	<a href="http://geoschemdata.wustl.edu/ExtData/HEMCO/DUST_DEAD/v2019-06">http://geoschemdata.wustl.edu/ExtData/HEMCO/DUST_DEAD/v2019-06</a>		1
17	HEMCO/EDGARv42/v2015-02	<a href="http://geoschemdata.wustl.edu/ExtData/HEMCO/EDGARv42/v2015-02">http://geoschemdata.wustl.edu/ExtData/HEMCO/EDGARv42/v2015-02</a>		1
18	HEMCO/EDGARv43/v2016-11	<a href="http://geoschemdata.wustl.edu/ExtData/HEMCO/EDGARv43/v2016-11">http://geoschemdata.wustl.edu/ExtData/HEMCO/EDGARv43/v2016-11</a>		1
19	HEMCO/GEIA/v2014-07	<a href="http://geoschemdata.wustl.edu/ExtData/HEMCO/GEIA/v2014-07">http://geoschemdata.wustl.edu/ExtData/HEMCO/GEIA/v2014-07</a>		1
20	HEMCO/GFED4/v2015-10	<a href="http://geoschemdata.wustl.edu/ExtData/HEMCO/GFED4/v2015-10">http://geoschemdata.wustl.edu/ExtData/HEMCO/GFED4/v2015-10</a>		1
21	HEMCO/GFED4/v2020-02	<a href="http://geoschemdata.wustl.edu/ExtData/HEMCO/GFED4/v2020-02">http://geoschemdata.wustl.edu/ExtData/HEMCO/GFED4/v2020-02</a>		1



# Automating Simulations on AWS

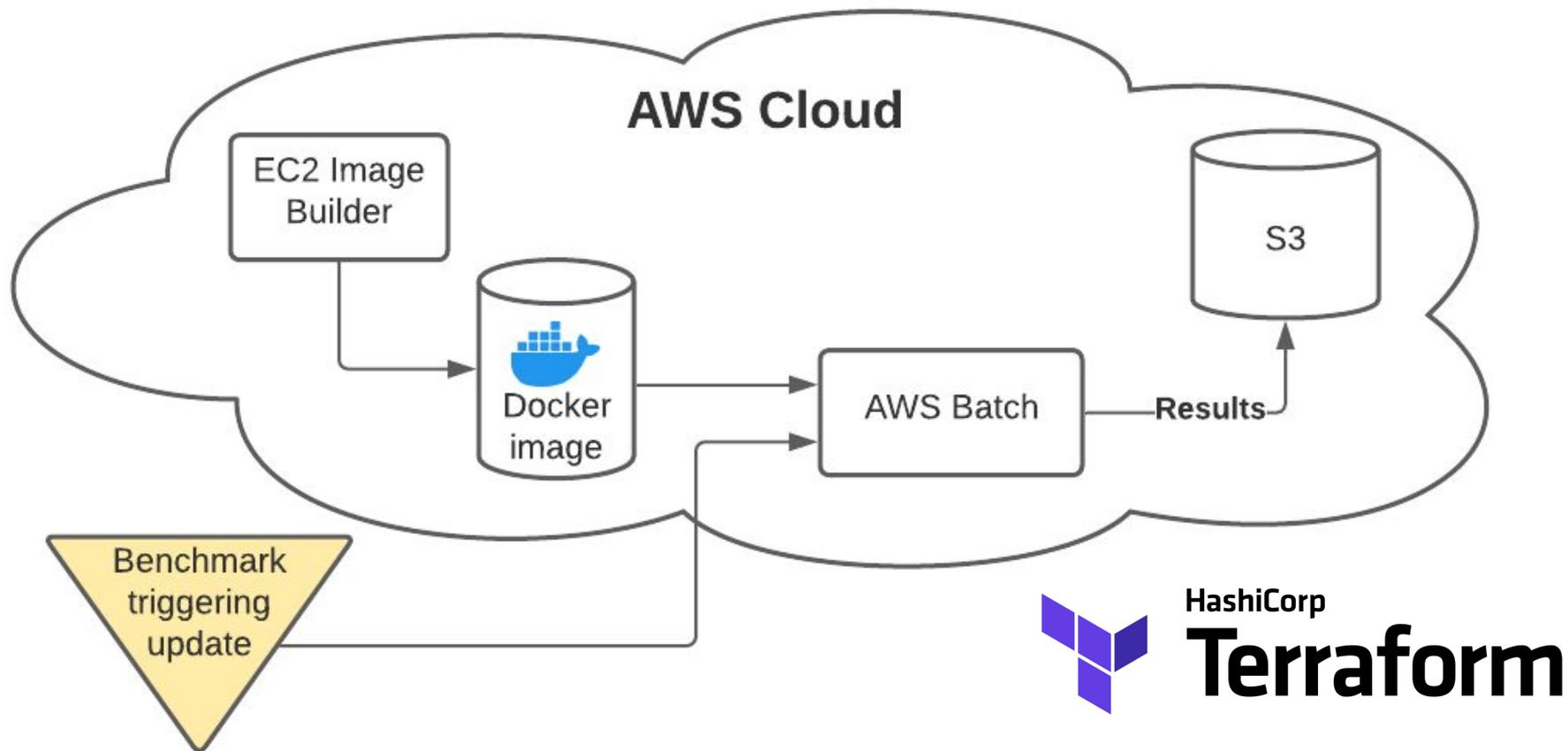
## Goal:

- Creation of automated pipelines to trigger benchmarks runs for GCClassic and GCHP

## Plan:

- Creation of runtime docker environment with EC2 image builder
- Management and deployment of EC2 instances with AWS Batch
- Plots automatically pushed to S3
- Management of AWS infrastructure with Terraform (IaC)

# Pipeline Infrastructure: Proposed Architecture



# GEOS-Chem Website

## **Updates that were applied:**

- People and Projects map is back!
- Removed the Harvard-specific branding
- Greater prominence of citation and new developments information
- Adjusted mobile display of meetings menu
- Small cosmetic updates (font and coloring)

Thanks for your feedback and feel free to send more thoughts!