Applying Container Technology to the NOAA-GFDL MSD FRE Workflow

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Outline

- NOAA-GFDL MSD
- Post-processing
- The problem
- The solution
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- Dockerfile
- How it runs
- Runscript
- Challenges
- Timeline + The Future

NOAA-GFDL MSD

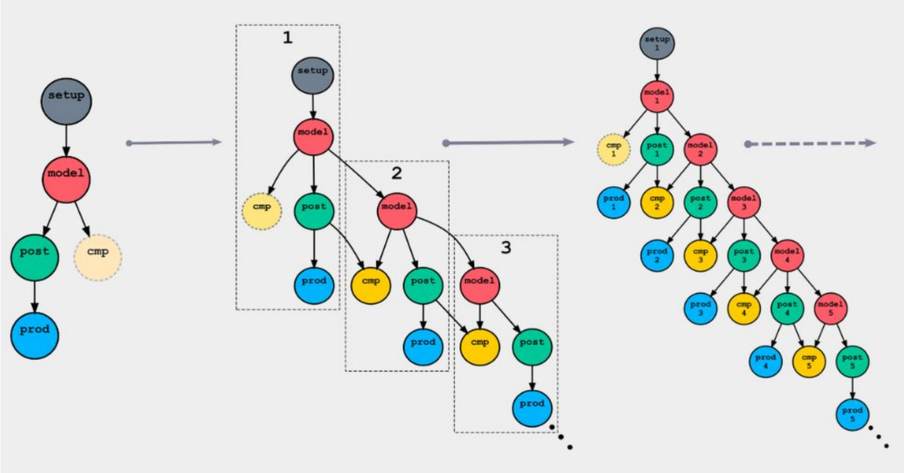
NOAA-GFDL is NOAA's Geophysical Fluid Dynamics Laboratory located in Princeton, New Jersey

- Established in 1955
- One of ten NOAA research laboratories

Modeling Systems Division (MSD) is responsible for the development and maintenance of the Flexible Modeling System (FMS) Runtime Environment (FRE)

Post-processing Overview

- Post-processing is necessary to convert raw model output to useful scientific data
- Workflow is managed via the cylc workflow engine
- Made up of (mostly) interdependent tasks but some are allowed to fail



The problem

The current method of post-processing is set up best for GFDL systems and requires a certain level of understanding to get started. This creates a few problems:

- Lack of portability
- Limited usefulness for the greater scientific community
- Reduced collaborative efforts
- Difficulty for new users

The solution

- Increase usability of GFDL post-processing workflow
  - Less steps to configure experiment
  - Software already installed in container
  - Simple instruction set

- Increase availability of GFDL post-processing workflow
  - Portability through cloud testing
  - Public release

Building the container

- Container image is built from a condaforge/mambaforge parent image (Ubuntu)
  - Installs needed packages
    - Python, csh, netcdf, etc.
  - Installs GFDL post-processing workflow
  - Creates conda environment
- GFDL GitLab container registry
  - Builds using on-prem gitlab self-hosted runner
  - Several applications are built including models and base containers
  - The post processing container image is built and maintained each release

Running the container

- When a user launches the post-processing container:
  - Use a SIF file
    - singularity exec
    - apptainer exec
  - Run script executes a series of configuration and workflow commands:
    - Environment setup
    - Post processing configuration
    - Starts workflow via cylc
- The container allows for simplistic post-processing by automating environment variable setup, directory creation, and directory clean up
- Run in different environments (GAEA, PPAN, Cloud)

Dockerfile/Runscript Highlights

Dockerfile installs the packages we need

```
# apt installs to /usr/bin/
RUN apt update \
  && apt -y install uuid-runtime time csh python bc

RUN conda env create --file
/opt/conda/cylc-flow-tools/cylc-flow-tools.yaml -p
/opt/conda/cylc-flow-tools \
  && git config --global --add safe.directory /mnt2 \
  && conda config --add pkgs_dirs
/opt/conda/cylc-flow-tools/lib/python3.11/site-packages
RUN conda install urwid==2.*
```

Runscript sets up environment and starts workflow

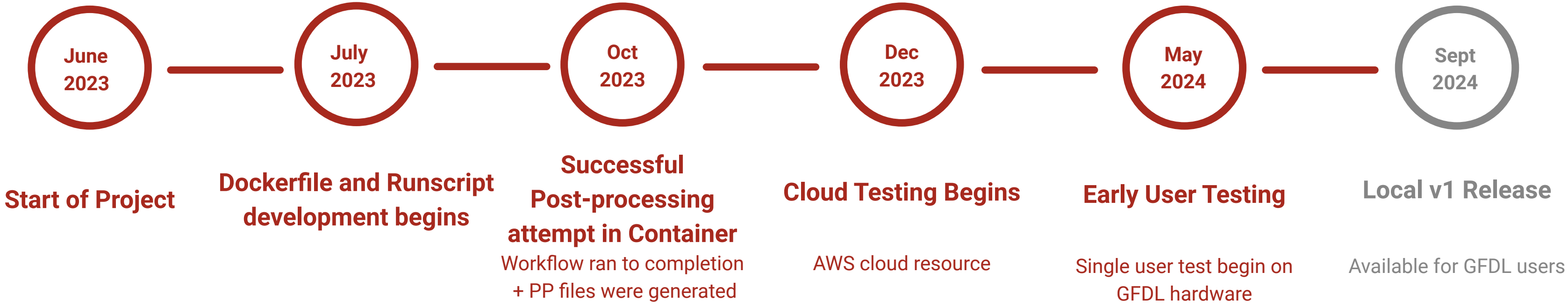
```
conda config --add envs_dirs /opt/conda
conda init --all
source /opt/conda/etc/profile.d/conda.sh
source ~/.bashrc
conda deactivate
conda activate /opt/conda/cylc-flow-tools

cylc stop --now $expname/run*
cylc clean $expname
rose macro --validate
bin/install-exp $expname
cylc play -v --no-detach $expname
```

Challenges

- Hard coded behavior within workflow scripts
- Updates to scripts
- Large file transfer to and storage on cloud resources
- Different behavior between on-prem and cloud running
- Troubleshooting task failure is more difficult in container

Timeline



June 2023

Start of Project

July 2023

Dockerfile and Runscript development begins

Oct 2023

Successful Post-processing attempt in Container

Workflow ran to completion + PP files were generated

Dec 2023

Cloud Testing Begins

AWS cloud resource

May 2024

Early User Testing

Single user test begin on GFDL hardware

Sept 2024

Local v1 Release

Available for GFDL users

The Future

- Continue user testing
- Test and compare performance to bare metal
- Be as efficient as possible
- Explore more ways to use container technology in our workflow
- New release available for all users

Summary

- Demonstrated ability to post-process in container environment
- Increased portability in post-processing
- Early release available locally at GFDL
- User testing underway
- Public release soon

Acknowledgments

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