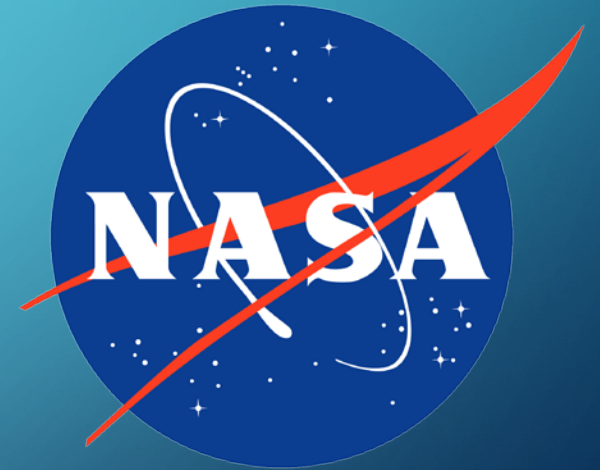# ANALYZING PERFORMANCE OF CONTAINERIZED CLIMATE MODELS IN SINGULARITY ON A SUPERCOMPUTER

COMPUTER SCIENCE / IT

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INTRODUCTION AND BACKGROUND

- Software is currently deployed in HPC via modules and package managers

- Containers provide easy software deployment and different environments

- Singularity vs Docker - Singularity is made for HPC and can make use of docker resources.

This is Discover, a supercomputing cluster with over 129,000 cores for NCCS!

QUESTION / INVESTIGATION

- Testing to see whether a containerized version of a part of GEOS (Goddard Earth Observing System) can compete with a non-containerized version

- Mainly looking at performance impact on containerized versions

- GEOSgcm and GEOSfvdycore were containerized

- GEOSfvdycore was containerized for testing

METHODS AND APPROACH

- Had to learn usage of Singularity & Slurm – Used Docker and PBS before NASA

- Created multiple containers for testing, including Debian 10, Fedora 33, and CentOS 7

- Before containerizing GEOSfvdycore, the base libraries had to be containerized first
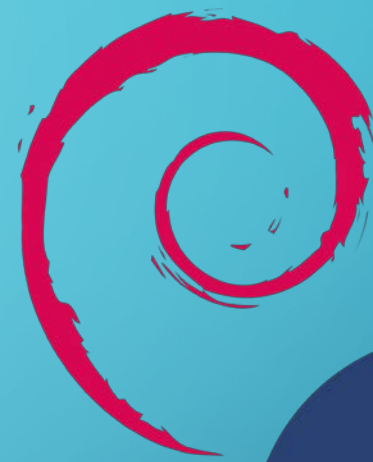
METHODS AND APPROACH

- Two parts to a run: Actually setting up the experiment and then running.

- Wanted to see longer and shorter compute times.

- Horizontal resolution of experiments was changed to get a better idea of efficiency

- Each container and the non-containerized version got 3 runs on a single node for longer and shorter compute times
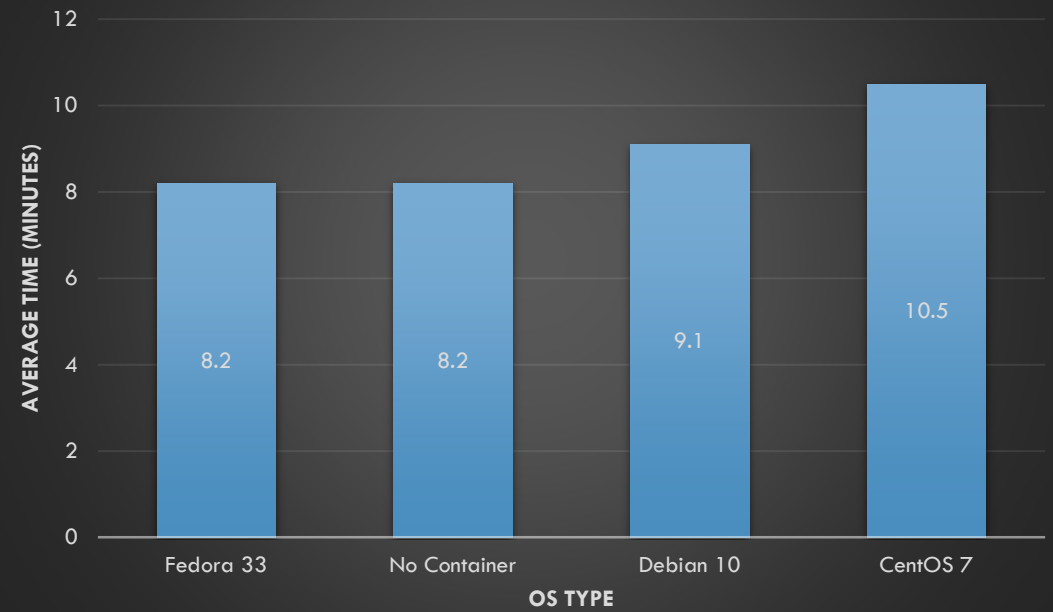
RESULTS AND GRAPHS

OS Type vs. Average Time for Longer Computations
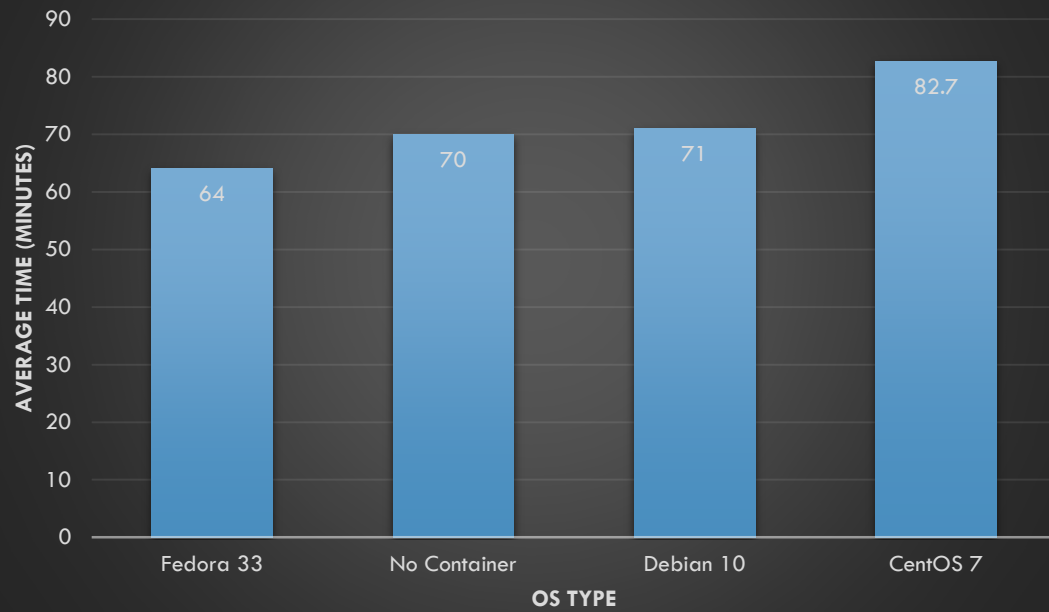
OS Type vs. Average Time for Shorter Computations

DISCUSSIONS AND CONCLUSIONS

- Tests definitely indicate that containers can compete with non-containerized versions

- Containers could have done well from having up-to-date software libraries that GEOSfvdycore depends upon compared to Discover

- Topics to move forward on this project would include minimizing the container size and improving how models can be executed

REFERENCES AND ACKNOWLEDGEMENTS

- Singularity documentation https://sylabs.io/docs/

- Slurm documentation https://slurm.schedmd.com/documentation.html

- MPI Tutorial https://mpitutorial.com/

- GEOS-5 wiki https://geos5.org/wiki/index.php?title=GEOS-5_Earth_System_Modeling_and_Data_Assimilation

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