CONTAINERS AT TACC

October 11, 2017
(Since I’m the 4th or 5th speaker, not going to try and explain what containers are or why we use them.  TACC local details only!)
OUR GENERAL CONTAINERS PHILOSOPHY

- Develop with Docker
- Run locally with Docker
- Run your image at scale with us in Singularity!!!
CONTAINERS ARE SUPPORTED ON EVERY TACC PRODUCTION PLATFORM

Stampede
Stampede-2
• #12 HPC system in the world for computation 350k CPU core 18 PF
Lonestar 5 Cray XC40 30,000 Intel Haswell cores 1.25 PF
Wrangler Data Analytics 0.6 PB usable DSSD flash storage w 1 TB/s read rate + 10 PB Lustre
Maverick Interactive and GPU computing NVIDIA Kepler K40 GPGPU
Jetstream Production Cloud
Chameleon Cloud Testbed
Hikari Secure Computing
HOW DO I DO THIS?

- `module load tacc-singularity/2.3.1`
- In job script (usually Slurm):
  - `singularity exec <Image name> <command> <parameters>`
  - Or, pull from a repo:
    - `singularity exec docker://<registryname>/<imagename> <command> <params>`
- That’s it, you are running!

- If you use one of our supported repository, we have hacked in a few extra bells and whistles that will automatically be supported in your image.
A BIT OF HISTORY, AND SOME UPGRADES WE’VE MADE

- We started public support in October of 2016 on Stampede
  - But only in some one off cases for particular users (originally FMRI processing).
- We now support more than 3,500 containerized apps!

- We are committed to continuing to support containers, from Day 1, on every production platform, now and future.
- Images pulled from BioContainers (3,500+) are automatically modded to have $HOME, $SCRATCH, and $WORK defined and mounted, with the same filesystems you see native on TACC Systems.
- Making future changes to our Modules systems, so cloud/container friendly things like “Module load Python latest” will work.
CROWDSOURCING RESEARCH SOFTWARE

- **Conda**
  - Package, dependency and environment management for any language

- **BioConda**
  - Conda “channel” specializing in Bioinformatics. 2000+ Github recipes + build system that turns them into Conda packages. 135 contributors!

- **BioContainers**
  - Community framework that maintains BioConda packages as Docker containers
All of these available on Stampede 2!
OUTCOMES

- Use nearly any public Docker image
  - Bioinformatics & computational biology
  - Machine & deep learning
  - Data analytics applications
  - New user-developed codes
- Develop locally. Package with Docker. Share & use nearly anywhere (Stampede, Comet, AWS, Azure, Jetstream, localhost, etc.)
  - Increase collaborativity
  - Increase velocity of exploration
THANKS!
DISCUSSION...