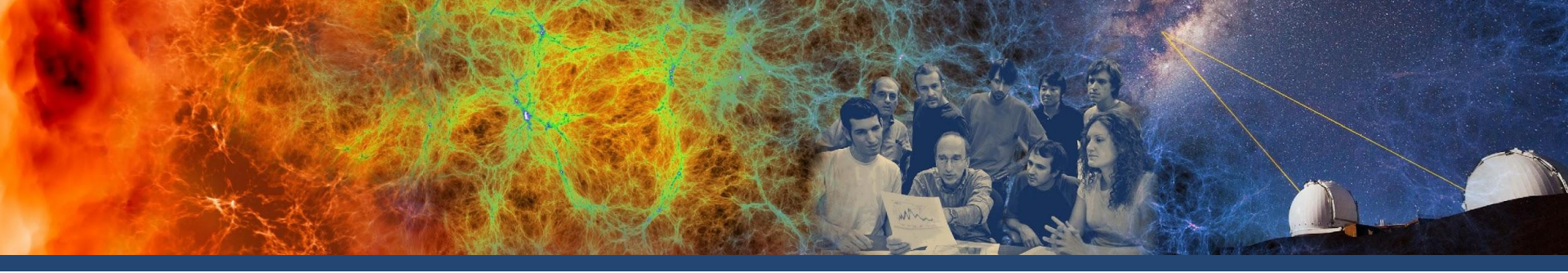
# Containers for HPC

## Session 3

Slides: https://bit.ly/20250313Container
Q&A Doc & Survey

NERSC Containers Training
13 March 2025

NERSC Staff



# Additional Building Tips

# Multi-Arch Containers

**Perlmutter is a linux/amd64 machine**

- If you build on Perlmutter with the default settings, your container will work on Perlmutter
- If you build using your own machine, you may need to change the container platform
  - Important if you are using Docker on an M-series Mac
  - Important if you want containers to be cross-platform

**Building Multi-Arch Containers**

- Add `--platform=linux/arm64,linux/amd64` for both ARM and x86 to your build line
- Native architectures will compile much faster
- Multi-arch builds will be larger than single-arch builds

# Iterate Version Numbers

Easy to increment a version number when building!

```
$ podman-hpc build -t hifrominside:1.2 .
```

- Use podman-hpc to build a container
- Tag this container with a name and **version**
- Build this container using a file called Containerfile found here

**Note:** Some people use *latest* to denote the most recent update. Use this based on your trust of the updaters!

**Why?**

- There is an issue with doubled up names/versions we can avoid
- It makes cleaning up easier

Help for when you forget is on the next slide!

# Whoops! Fixing Common Issues

**Note:** Colors indicate approximate work required to get back to where you were

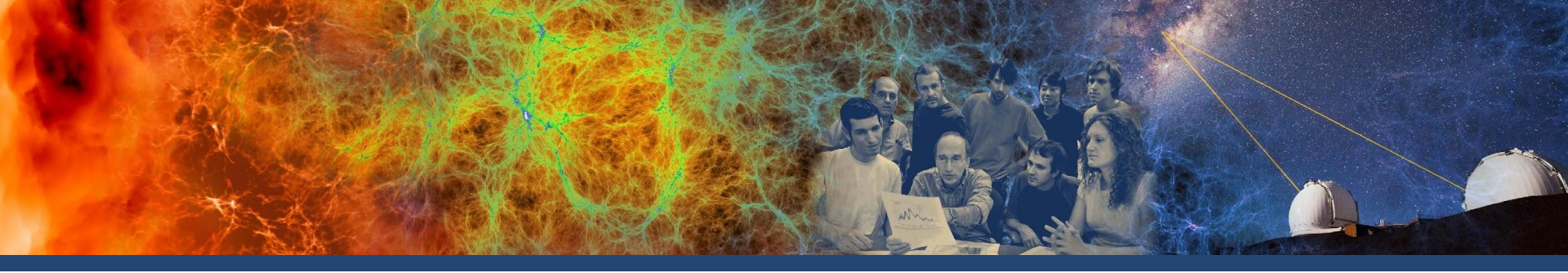
These can help podman-hpc versioning issues:

- Try `podman-hpc rmsqi image:tag` to remove the squash image
- Try deleting all of your migrated images in `$SCRATCH/storage`
- Clear out the local cache: `cd /images; podman-hpc unshare; rm -rf *; exit`

There are other ways podman-hpc can get in a bad state - try these:

- Try `podman-hpc prune; podman-hpc image rm --force $(podman-hpc image ls -aq)`
- Directories to delete: `~/.local/share/containers`, `~/.config/containers`, `/run/user/<userid>/overlay*`, `/tmp/<userid>_hpc`
- Also try: `podman-hpc system reset; podman-hpc system migrate`

**Tip:** Get your userid with the command `id`



# Advanced Topics

# SPIN

## SPIN is NERSC's method for running persistent containers

- Containers are often used outside of HPC for persistent compute
  - Things like databases, scientific gateways, or workflow managers are always running in the background
- NERSC users can create containers and run in this way using the SPIN service

## More information on the SPIN website

- More details on how SPIN is run
- Information on self-guided and interactive training
- Links to documentation

# Containers as Custom Jupyter Kernels

You can use a container of your choice as a Jupyter Kernel at NERSC

- Build your container
  - Include everything you want available
  - Include ipykernel
- Set up a kernelSpec. **Either**:
  - Copy one from us, modify for your needs and put it in `$HOME/.local/share/jupyter/kernels/<name>/kernel.json`
  - Set one up using `shifter --image=myimage:v1.2.3 </path/to/your/image/python> -m ipykernel install --prefix $HOME/.local --name env --display-name MyEnvironment`
    - Note: you also have to prepend some shifter things into the kernelspec. See here for details
- Start Jupyter as normal and select MyEnvironment from the available kernels

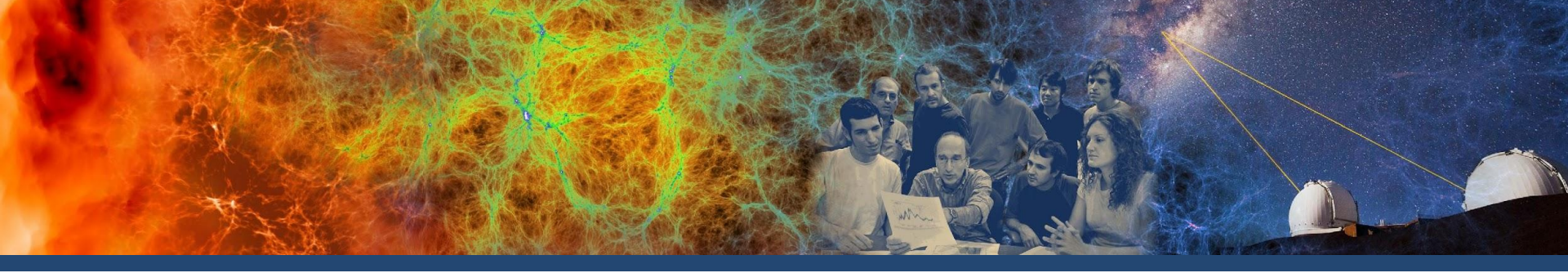
**Note:** Instructions and sample kernelspec files are here

**Note:** podman-hpc for Jupyter kernels is still experimental.

# Other Cool Container Things

- Run multiple containers in the same job for Shifter
- Do graphics forwarding with podman-hpc
- Use the CrayPE within a Shifter container
- Profile applications within podman-hpc
- Use VSCode within a Shifter container
- Run PyTorch using Shifter
- Use Spack within a Shifter container

Take a look through our Application list - many are containerized



# Wrap Up

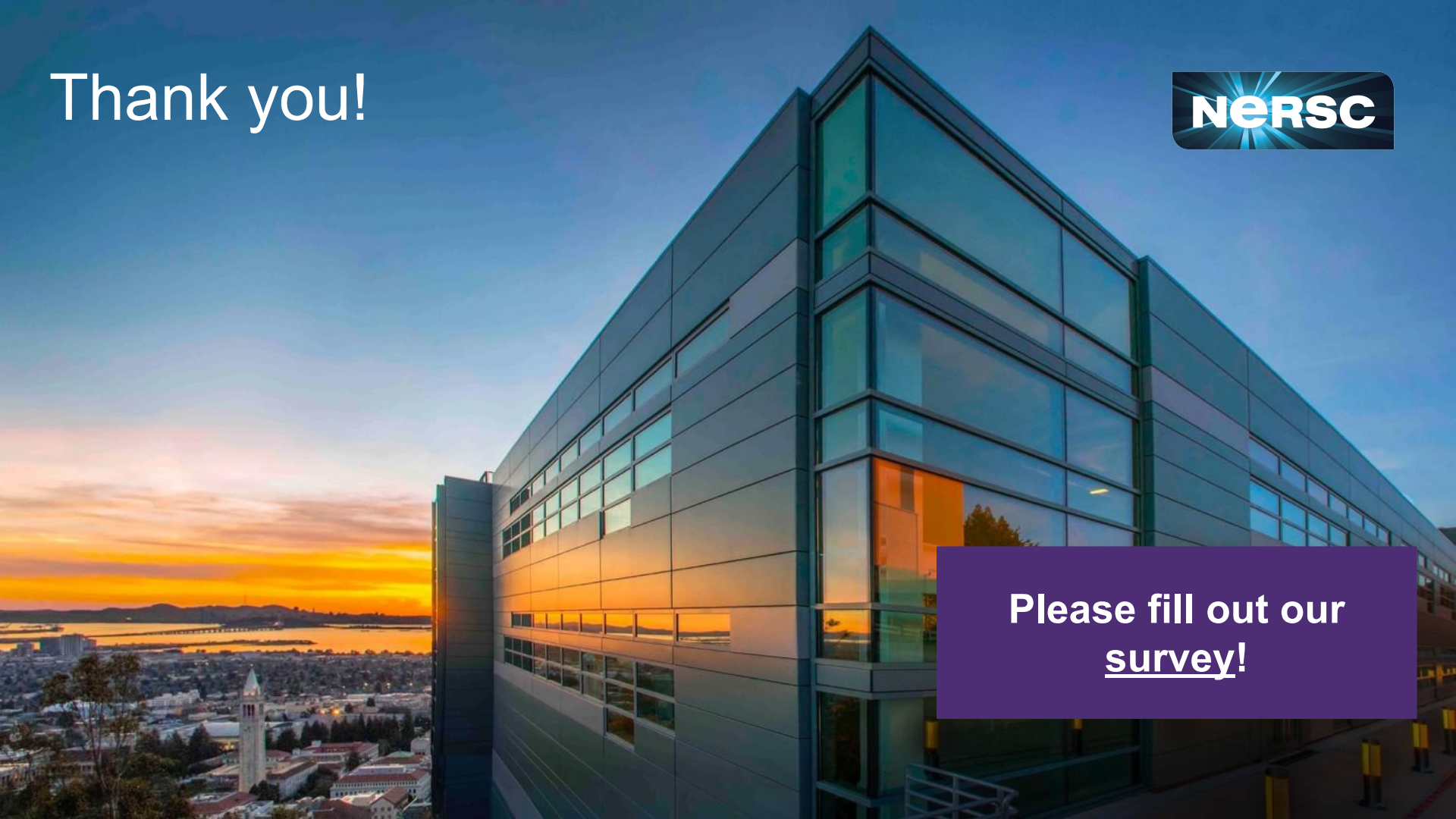
# Where to go from here?

- NERSC documentation and examples
  - Shifter and a Shifter training
  - podman-hpc
- Registries
  - NERSC registry (and docs page): private and free with NERSC account
  - DockerHub: free public or paid private
  - Quay.io: free public or paid private

- Submit NERSC Help tickets via the portal
- NERSC user appointment: nersc.as.me

**Please fill out our survey!**

# Thank you!



**Please fill out our survey!**