The background of the slide is a dense, overlapping field of three-dimensional blue numbers. The numbers, including 0, 1, 2, 3, 4, 5, 6, 7, 8, and 9, are rendered in a light blue color with a subtle gradient and soft shadows, giving them a tangible, blocky appearance. They are scattered across the entire frame, creating a sense of depth and complexity.

# Singularity and Docker

An introduction to  
containerizing a  
researcher's workflow

# Table of Contents

What are Singularity and Docker?

Pros and Cons to using one over the other

Interactive Example

Where should you go from here?

# What is Singularity?



The gold-standard for containerization on HPC clusters



Preferred choice for mission-critical workflows

Used in aerospace, oil and gas, and biotechnology industries



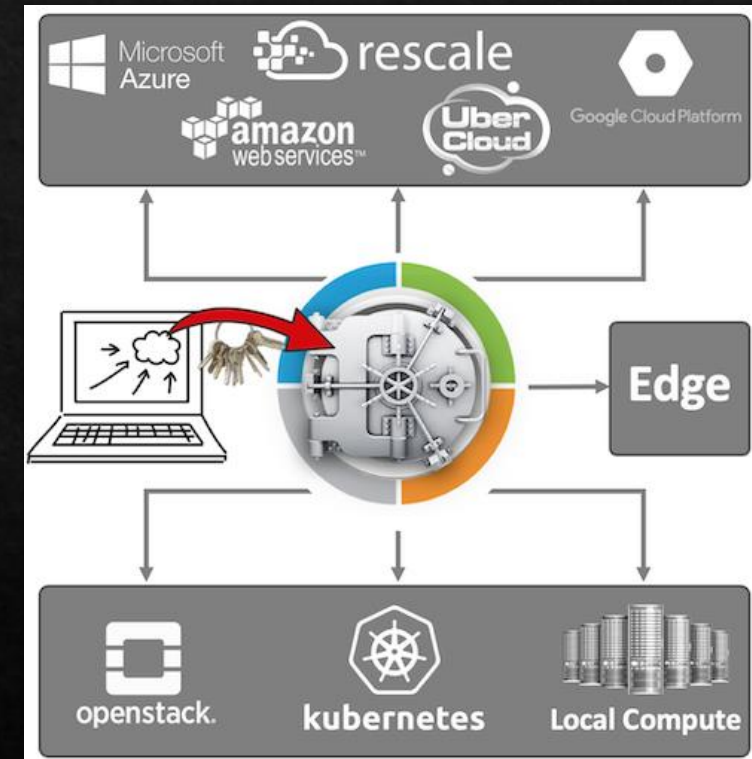
Security first mindset

No one is hacking you!



Extremely portable

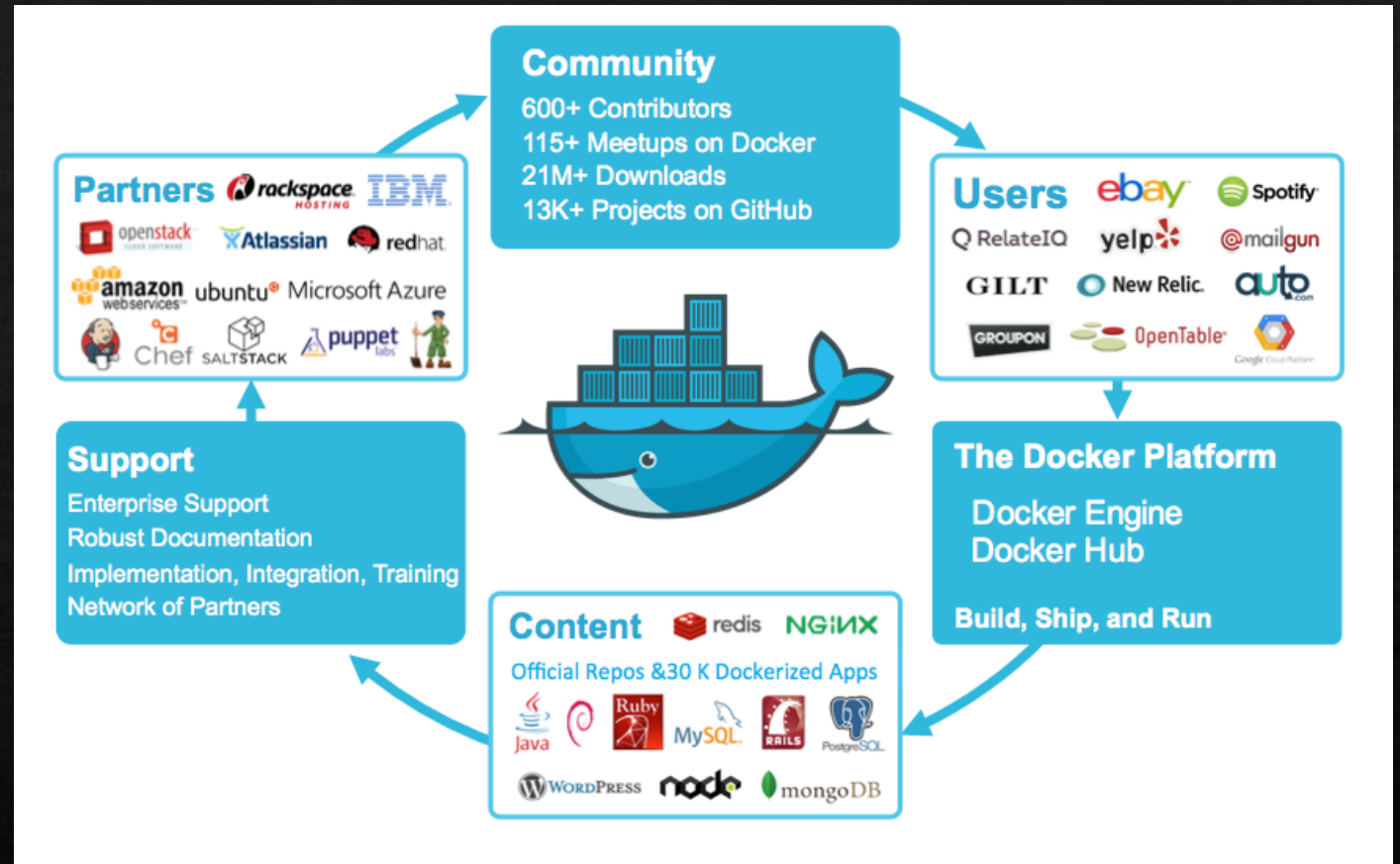
Can run in any environment that has singularity RE installed





# What is Docker?

- ◇ Another popular, ubiquitous containerization software
- ◇ Heavily used in the tech industry
  - ◇ Kubernetes anyone?
- ◇ Extremely adaptable to any kind of workflow
- ◇ Cross-Platform
  - ◇ Works on Linux, MacOS, and Windows



# The Pros and Cons of Singularity

## The Pros 😊

- ◆ Uber secure
  - ◆ Singularity containers are read-only
- ◆ Space efficient
  - ◆ Containers are compressed to conserve available storage space
- ◆ Installed on Roar
- ◆ Can easily manage system-level dependencies
- ◆ Interoperable with Docker

## The Cons ☹️

- ◆ Only supports static environments
- ◆ Only available for use on Linux
  - ◆ Need to use a work-around to build containers on Windows and Mac
- ◆ User community isn't as large as compared to Docker
  - ◆ Finding support can be a little difficult

# The Pros and Cons of Docker

## The Pros 😊

- ◆ Ubiquitous, virtually used everywhere
- ◆ Cached builds
  - ◆ Start from where you left off if build fails
- ◆ Support dynamic environments
- ◆ Can modify containers after being built from images
- ◆ Multithread container downloads and uploads

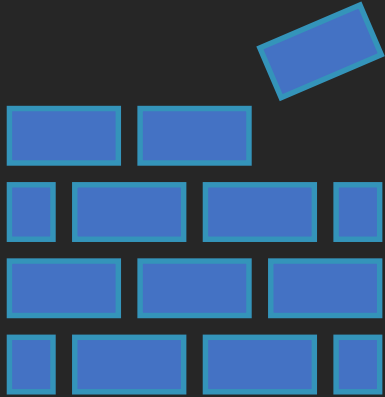
## The Cons 😞

- ◆ Not installed on the cluster
- ◆ Security is managed by user, not built-in
  - ◆ Container security has become an entire industry because of Docker
- ◆ Not resource conscious
  - ◆ Bloated containers



Interactive Example Time

# Set up your build environment!



- ◇ Open the terminal on your computer
- ◇ Create directory titled **VMs**
- ◇ Change into **VMs** directory and create **SINGULARITY** directory
- ◇ In **SINGULARITY** directory, enter the following commands:
  - ◇ `vagrant init sylabs/singularity-3.5-centos-7-64 --box-version 20191206.0.0`
  - ◇ `vagrant up`



# Time to build your container!

- ◆ Use the following commands:

- ◆ `vagrant ssh`

- ◆ `git clone https://github.com/NucciTheBoss/iask\_onboarding\_spring\_2021.git`

- ◆ `cd iask_onboarding_spring_2021/day_2`

- ◆ `sudo singularity build image.sif R-4.0.3-rstudio.def`

- ◆ sudo password is “**vagrant**”

- ◆ Now we wait!

A laboratory setting with a graduated cylinder in the foreground, partially filled with a blue liquid. The cylinder has a scale from 0 to 90. In the background, there are several other pieces of glassware, including a round-bottom flask with green liquid, a beaker with yellow liquid, and other flasks and beakers, some containing green or yellow liquids. The scene is dimly lit, with a dark, reflective surface in the foreground.

Demonstration!

# Where should you go from here?

- ◇ Feel free to play around with my repository:
  - ◇ [https://github.com/NucciTheBoss/iask\\_onboarding\\_spring\\_2021](https://github.com/NucciTheBoss/iask_onboarding_spring_2021)
- ◇ Experience is the greatest teacher!
  - ◇ Create your own containers
  - ◇ Play around with containers we already created
- ◇ Ask for help!
  - ◇ Will, Justin Petucci, and I use Singularity all the time
  - ◇ Add me as a collaborator on a git repository!
    - ◇ I can provide input if you need help!





*"That's all Folks!"*