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Application Portability through Singularity

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Application Portability through Singularity

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Agenda

- Goals
- Virtualization
- Docker vs. Singularity at 10,000 ft.
- Creating Image
- Running Container
- Physical Size of Image File
- Memory Usage at Runtime
- Data Access Issues

with some live demo

Goals

- "Workflow/Pipeline Portability"

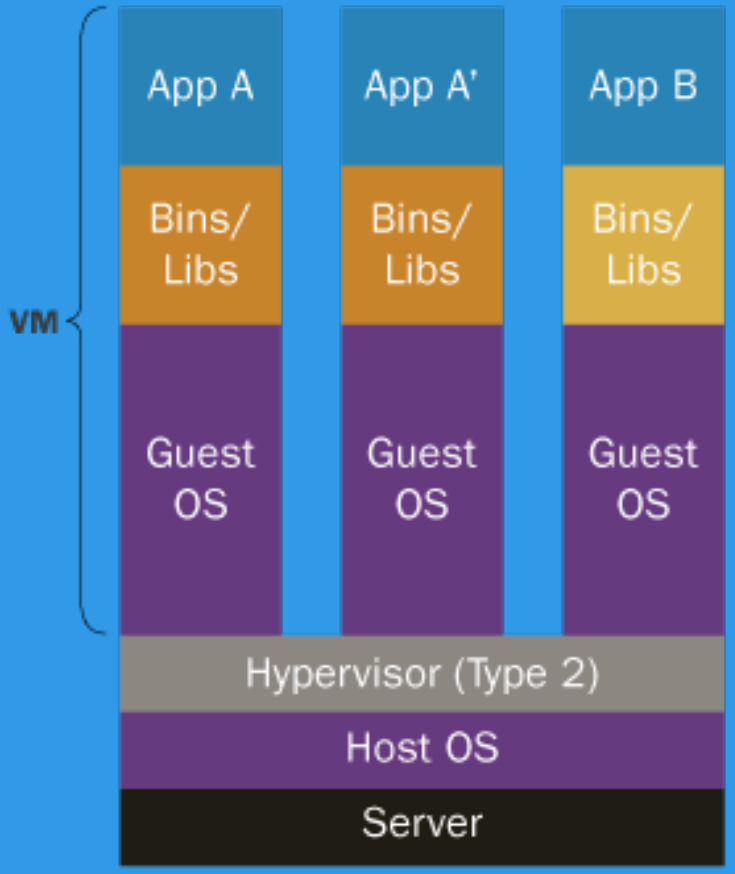
    1. Being able to run pipeline in various computing environments (Luna Cluster, NYGC, Amazon Cloud, Google Compute Cloud, …)

    2. Being able to easily manage and support different versions of software (bwa, gatk, R, python, Java, …) and avoid dependency conflicts.

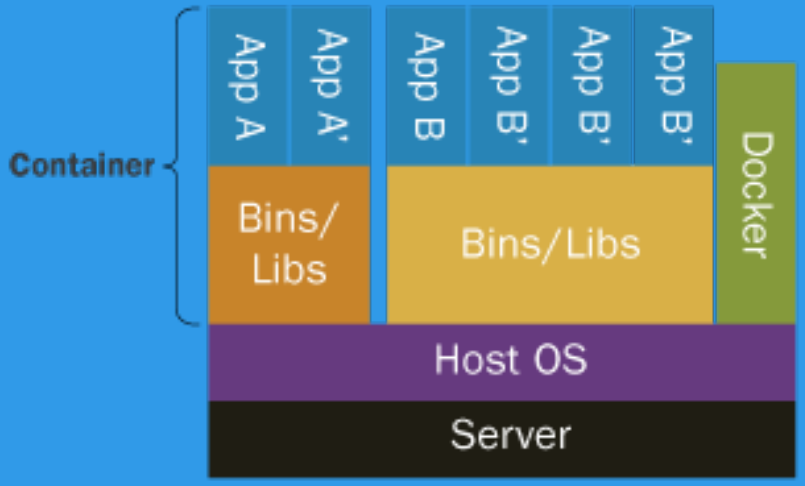
    3. Being able to cite the pipeline used in research, allowing others to run the exact same pipeline from their own computing environments which are most times different from the original one.

Virtualization

Containers vs. VMs



Containers are isolated, but share OS and, where appropriate, bins/libraries



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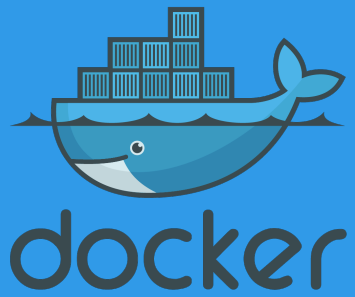
Virtualization

- Virtual Machine
  - VirtualBox (samtools in BioLinux)
- Container
  - Docker (samtools)
  - Singularity (samtools)



LIVE DEMO

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Docker vs. Singularity at 10,000 ft.

	Docker	Singularity
Goal	DevOps, Microservices	Application Portability
Application Level Virtualization	Good	Good
HPC Friendly	Not Really	Yes
Security 	Root Privilege Required for Running Containers	No Change in Security Paradigm
Adopters	Many Internet Companies	UC Berkeley, Stanford, NIH, …
Image Repository 	Good Docker Hub	Premature Singularity Hub (can use Docker Hub)

Docker vs. Singularity at 10,000 ft.

	Docker	Singularity
GPU	Via 3rd Party	Native Access Native Support
MPI	No	Yes (built-in support)
Daemon	Required	Not Required
Unix Pipes 	Not Quite As Expected	No Surprise
Version	1.13	2.2

Creating Image

- Many Options, but Here Are Some:

1. Import from Repository and Use As Is
   - Singularity Hub
   - Docker Hub
   - Other Docker private registries (e.g. BioShadock)

2. Build Your Own
   a. Start from Docker image first
      and then convert to Singularity image.
   b. Create Singularity image from scratch.

Creating Image

- Import from Repository and Use As Is

1. Go to Docker or Singularity Hub or other image repository.
2. Search and get image name.
3. Use "singularity create" command.
4. User "singularity import" command.

LIVE DEMO

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Creating Image

- Build Your Own

1. Make a text document describing how image should be constructed:
   - *Dockerfile*
   - *Singularity*

2. Start from a base image (CentOS, Ubuntu, Alpine, …)

3. Install software into the image
   - Compile source code
   - Use package manager such as yum, apt-get, or conda

4. Use "singularity create" command.

5. User "singularity bootstrap" command.

Depending on what base image you use and how to install software into the image, the final image size can vary.

LIVE DEMO

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Running Container

- No user contextual changes
- No change in security paradigm
  - The same file permission on host is respected inside the container.
- Bring Your Own Environment (BYOE)
  - e.g. whoami, pwd, env, home directory

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Physical Size of Image File

Container	Author	samtools	bwa
Docker	BioContainers	1.24 GB	1.23 GB
Docker	BioShadock	247 MB	321 MB
Docker	Jaeyoung @ MSKCC	15 MB	9 MB
Singularity	Jaeyoung @ MSKCC	21 MB	21 MB

- Depending on what base image you use and how to install software into the image (e.g. source compile vs. conda), the final image size can vary even for the same software.
- BioContainers uses conda to install tools inside a container, which seems to be one of the reason the image is so big (i.e. image must include conda).
- Docker utilizes cache so it doesn't need to download 1.2GB image every time.

Memory Usage at Runtime

Docker on Ubuntu VM

```
top - 11:22:43 up  9:11,  1 user,  load average: 4.70, 2.63, 1.36
Tasks: 201 total,   2 running, 199 sleeping,   0 stopped,   0 zombie
%Cpu(s): 50.2 us, 43.3 sy,  0.0 ni,  6.1 id,  0.0 wa,  0.0 hi,  0.4 si,  0.0 st
KiB Mem :  1016272 total,    67364 free,   410520 used,   538388 buff/cache
KiB Swap:  1045500 total,   702172 free,   343328 used.   431428 avail Mem

  PID USER      PR  NI    VIRT    RES    SHR S %CPU %MEM     TIME+ COMMAND
 3433 chunj     20   0  676584  30564  10864 R 33.0  3.0   0:36.23 gnome-termi+
 8719 root      20   0    6348    888    704 S 19.0  0.1   0:18.29 samtools
```

Singularity on CentOS VM

```
top - 11:27:44 up  9:38,  3 users,  load average: 0.37, 0.08, 0.03
Tasks: 157 total,   3 running, 154 sleeping,   0 stopped,   0 zombie
Cpu(s): 42.5%us, 56.9%sy,  0.0%ni,  0.6%id,  0.0%wa,  0.0%hi,  0.0%si,  0.0%st
Mem:   1020072k total,   908664k used,   111408k free,    54960k buffers
Swap:  2064380k total,     2800k used,  2061580k free,   330116k cached

  PID USER      PR  NI  VIRT  RES  SHR S %CPU %MEM    TIME+  COMMAND
 2762 chunj     20   0  462m  18m  10m R 84.8  1.8   1:58.28 gnome-terminal
10543 chunj     20   0  6288  712  524 S  9.0  0.1   0:01.46 samtools
```

samtools view sample.bam / 92 MB bam / measured with the top program

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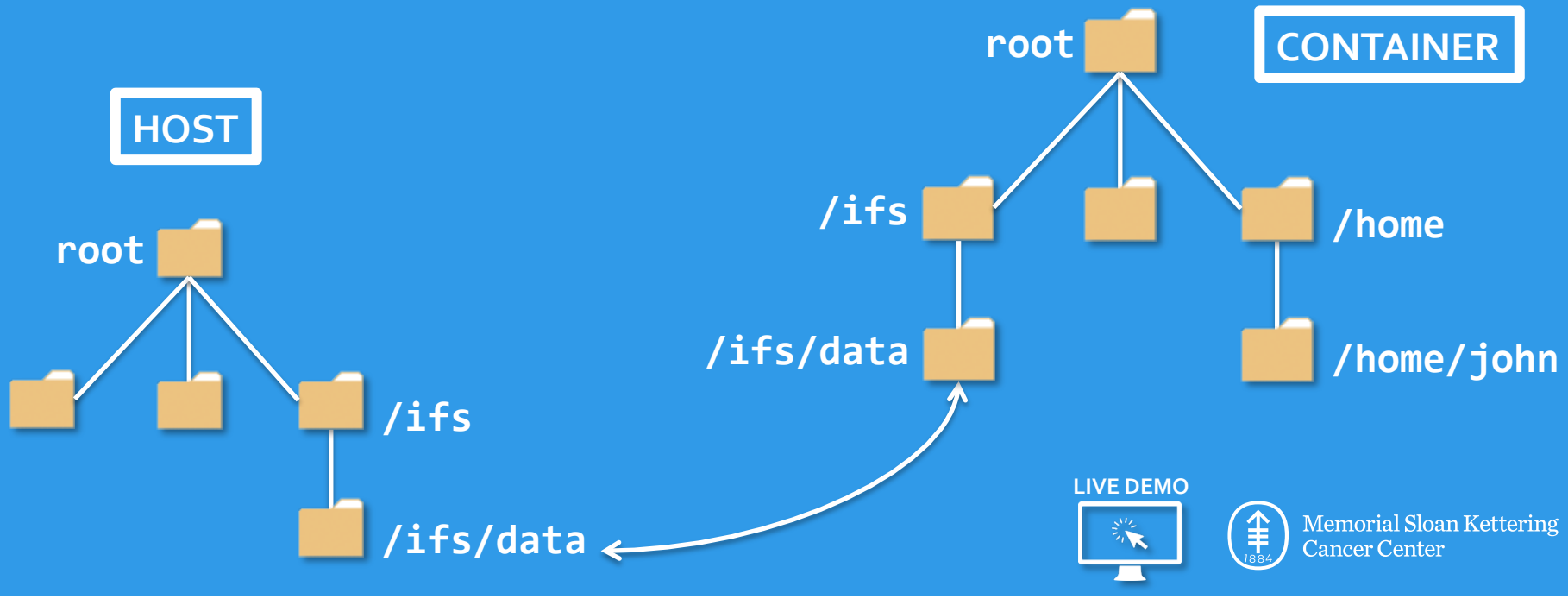
Data Access Issues

- "How can programs inside container access data files outside container?"
- We prefer data path */ifs/…* in the host machine to be mapped exactly as */ifs/…* inside the container.
- This way, we can reuse the existing code base without any further modification.
- However, we'd like to achieve portability outside MSKCC.

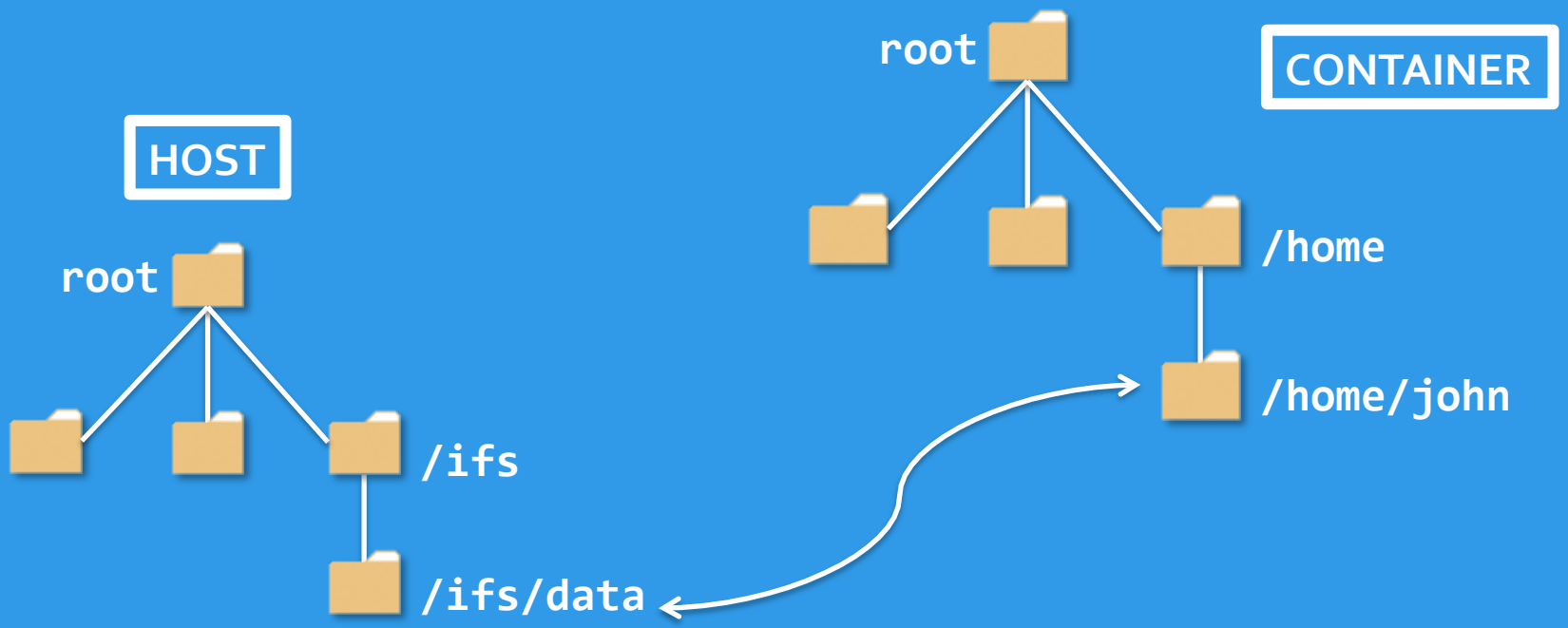
Data Access Issues

- Bind Paths / File Sharing via *--bind*
- Bind point must already exists within the container.
- If not, we can enable overlay:
  - *enable overlay = yes* in *etc/singularity.conf*
  - Some limitations still exists. Sometimes RHEL7 kernel crashes.
  - Overlay file system required.



Data Access Issues

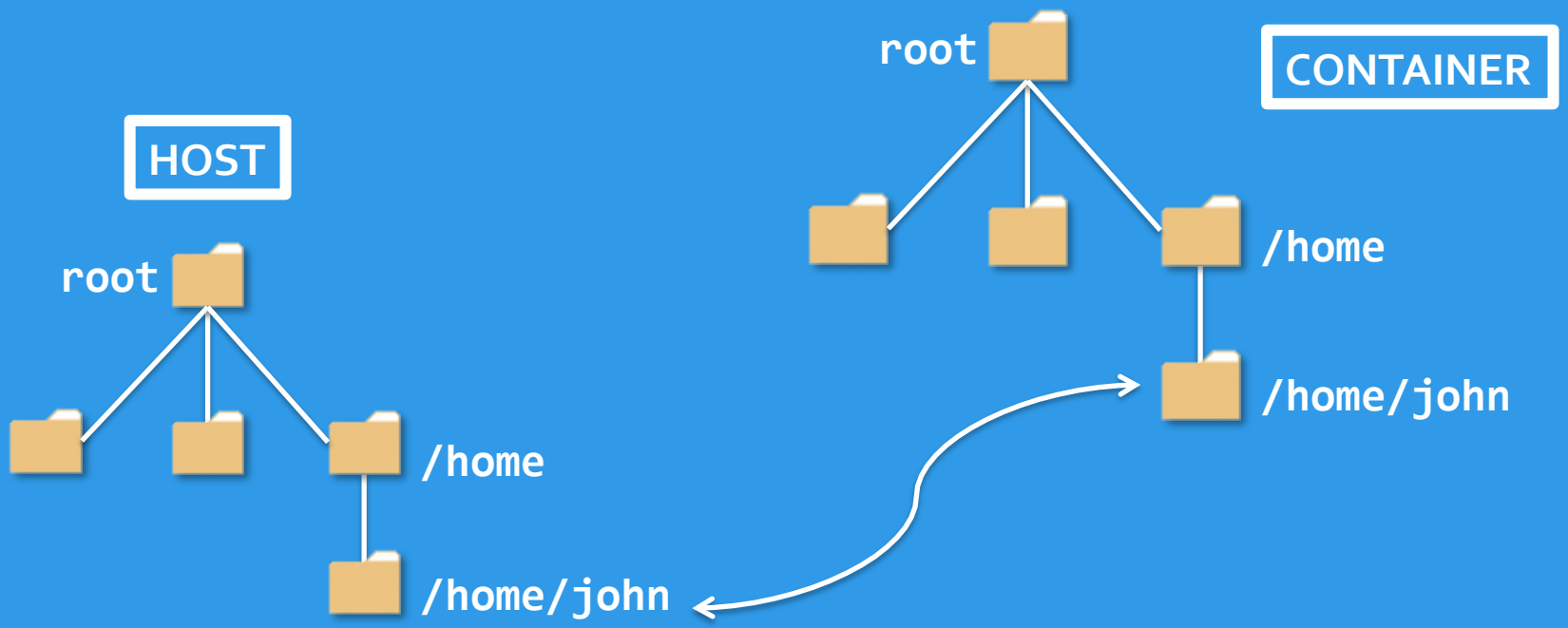
- Override User's Home Directory via *--home*
- The directory that will be configured to be user's new home directory must belong to that user.



LIVE DEMO

Data Access Issues

- Store Data Files in User's Home Directory
  - Everything user has in his/her directory will be fully accessible within the container.



LIVE DEMO

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Other Notes for Singularity

- Portable when binary compatibility is met.
- Singularity must be installed and accessible on the system (not daemon).
- Dramatic changes even from v2.0 to v2.2 such as image definition file format.
- Image creation requires sudo, but running does not.
- You have to create an empty image with some size.

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QUESTIONS