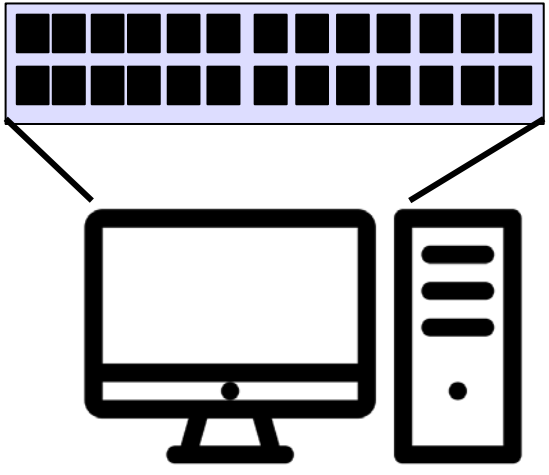
Containers and GPUs

Mats Rynge (rynge@isi.edu)
Christina Koch (ckoch5@wisc.edu)

GPUS

What is a GPU?

- GPU = Graphical Processing Unit
- Has hundreds to thousands of “cores” that can be used to parallelize work.



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GPU Use Cases

- Programs that map well to GPUs include:
  - Deep learning
  - Molecular dynamics
  - Anything with lots of number crunching (like matrix operations) and low(er) data load.

GPUs on the OSG

- Scale: 100s (vs 10,000s of CPUs)
- Variety of available GPU cards

- Same restrictions as always: not sure what you'll get, jobs can be interrupted

- May take longer to start

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Making robust GPU jobs

- Use a software strategy that can run on different GPU types:
  - Container
  - Install inside the job
- OR use job requirements to request certain kind of GPU (more limiting)

Submit File options

- Request GPUs with “request_gpus”
- Can use custom requirements

```
request_gpus = 1

requirements = (CUDACapability >= 6.0)
```

CONTAINERS

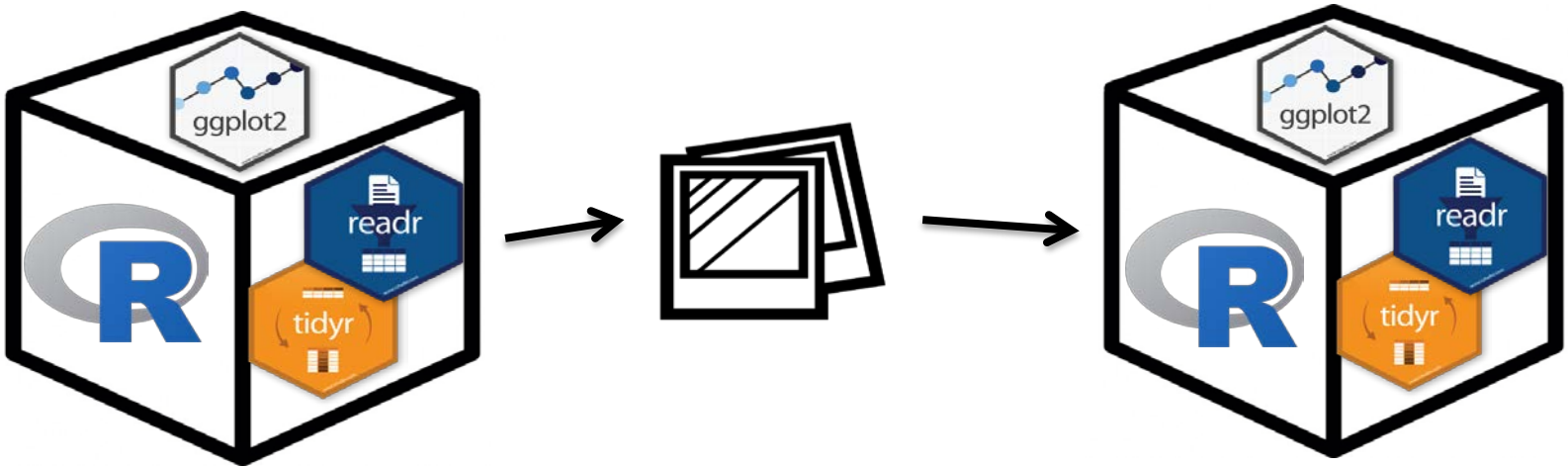
Returning to Our Analogy…

- Using a container is kind of like bringing along a whole kitchen…

Photo by PunkToad on Flickr, CC-BY

Containers

- Containers are a tool for capturing an entire job “environment” (software, libraries, operating system) into an “image” that can be used again.



polaroid photos by Nick Bluth from the Noun Project

Container Motivations

Consistent environment (default images) - If a user does not specify a specific image, a default one is used by the job. The image contains a decent base line of software, and because the same image is used across all the sites, the user sees a more consistent environment than if the job landed in the environments provided by the individual sites.

Custom software environment (user defined images) - Users can create and use their custom images, which is useful when having very specific software requirements or software stacks which can be tricky to bring with a job. For example: Python or R modules with dependencies, TensorFlow

Enables special environment such as GPUs - Special software environments to go hand in hand with the special hardware.

Process isolation - Sandboxes the job environment so that a job can not peek at other jobs.

File isolation - Sandboxes the job file system, so that a job can not peek at other jobs' data.

Container Types

- Two common container systems:

Docker	Singularity
https://www.docker.com/	https://sylabs.io/

The container itself will always be some version of Linux - but can be run on Linux / Mac / Windows if Docker or Singularity is installed

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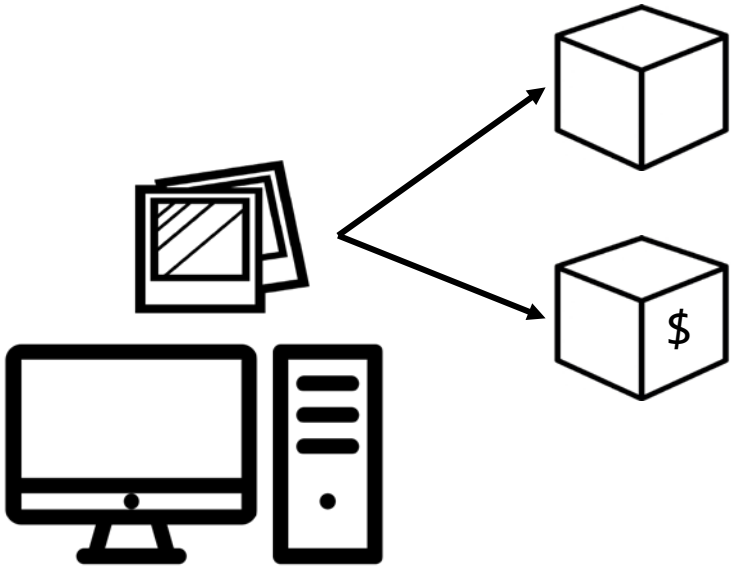
Focus on Docker

- Docker has well-established and well-documented ways to build container images. It has huge library of images!

- If you have a Docker image:
  - Can run with Docker
  - Can run with Singularity – Remember this
  - Can convert to a Singularity image

Running Containers




```
docker run <container> <command>
```

```
docker run –it <container> /bin/sh
```

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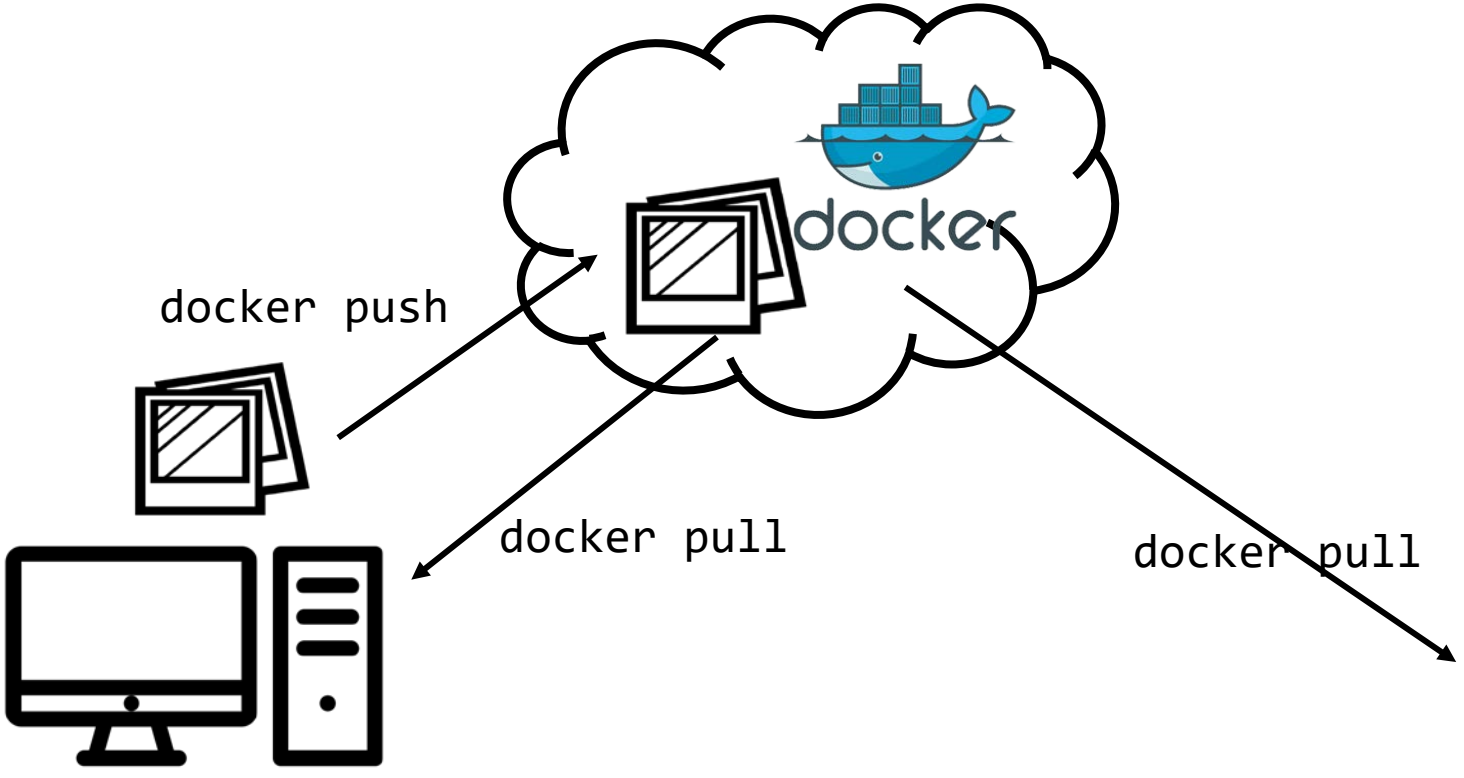
Docker Hub


docker
docker push
docker pull
docker pull
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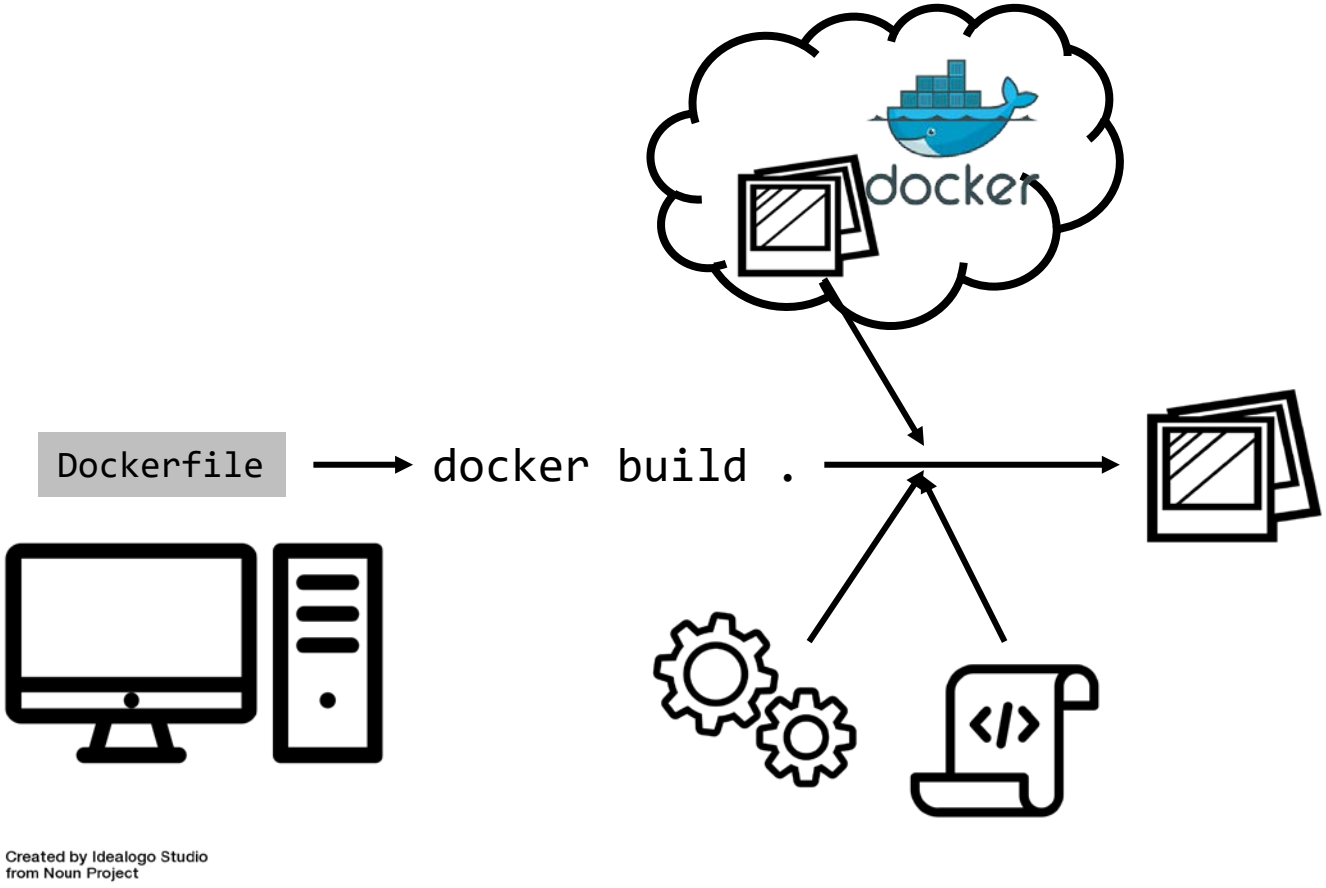
Building Containers



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Sample Dockerfile

```
# Start with this image as a "base".
# It's as if all the commands that created that image were inserted here.
FROM continuumio/miniconda:4.7.12

# Use RUN to execute commands inside the image as it is being built up.
RUN conda install --yes numpy

# Try to always "clean up" after yourself to reduce the final size of your image.
RUN apt-get update \
&& apt-get --yes install --no-install-recommends graphviz\
&& apt-get --yes clean \
&& rm -rf /var/lib/apt/lists/*
```

cvmfs-singularity-sync

Containers are defined using Docker

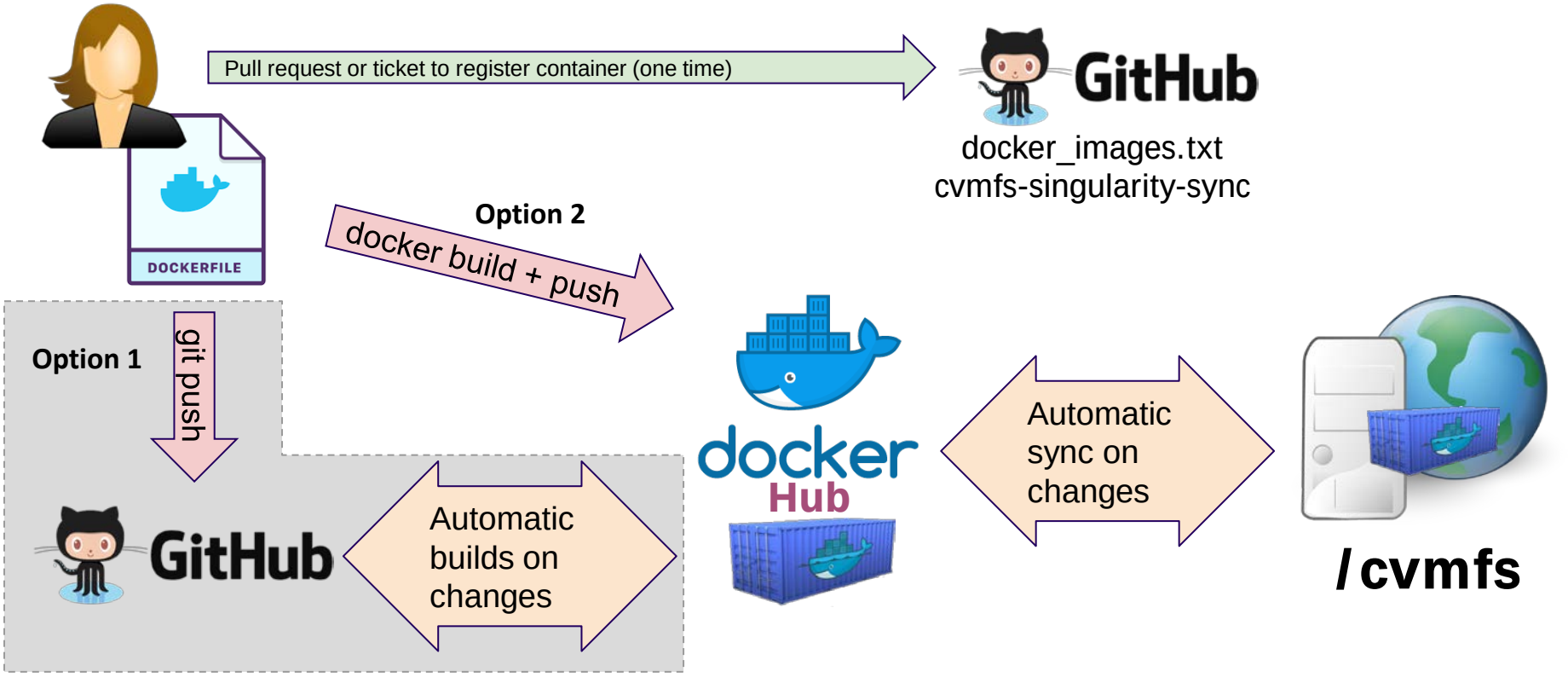
- Public Docker Hub

… and executed with Singularity

- No direct access to the Singularity command line - that is controlled by the infrastructure

https://github.com/opensciencegrid/cvmfs-singularity-sync
(next slide)

User-defined Container Publishing



CVMFS Repositories

```
/cvmfs/
      ams.cern.ch
      atlas.cern.ch
      cms.cern.ch
      connect.opensciencegrid.org
      gwosc.osgstorage.org
      icecube.opensciencegrid.org
      ligo-containers.opensciencegrid.org          <- large project with their own containers
      nexo.opensciencegrid.org
      oasis.opensciencegrid.org                    <- “modules” software
      singularity.opensciencegrid.org              <- general containers (next few slide)
      snoplus.egi.eu
      spt.opensciencegrid.org
      stash.osgstorage.org                         <- ~1PB of user published data
      veritas.opensciencegrid.org
      xenon.opensciencegrid.org
```

Extracted Images

OSG stores container images on CVMFS in extracted form. That is, we take the Docker image layers or the Singularity sif files and export them onto CVMFS. For example, ls on one of the containers looks similar to ls / on any Linux machine:

```
$ ls /cvmfs/singularity.opensciencegrid.org/opensciencegrid/osgvo-el7:latest/
cvmfs  host-libs  proc  sys  anaconda-post.log     lib64
dev    media      root  tmp  bin                  sbin
etc    mnt        run   usr  image-build-info.txt  singularity
home   opt        srv   var  lib
```

Result: Most container instances only use **a small part** of the container image **(50-150 MB)** and that part is **cached** in CVMFS!