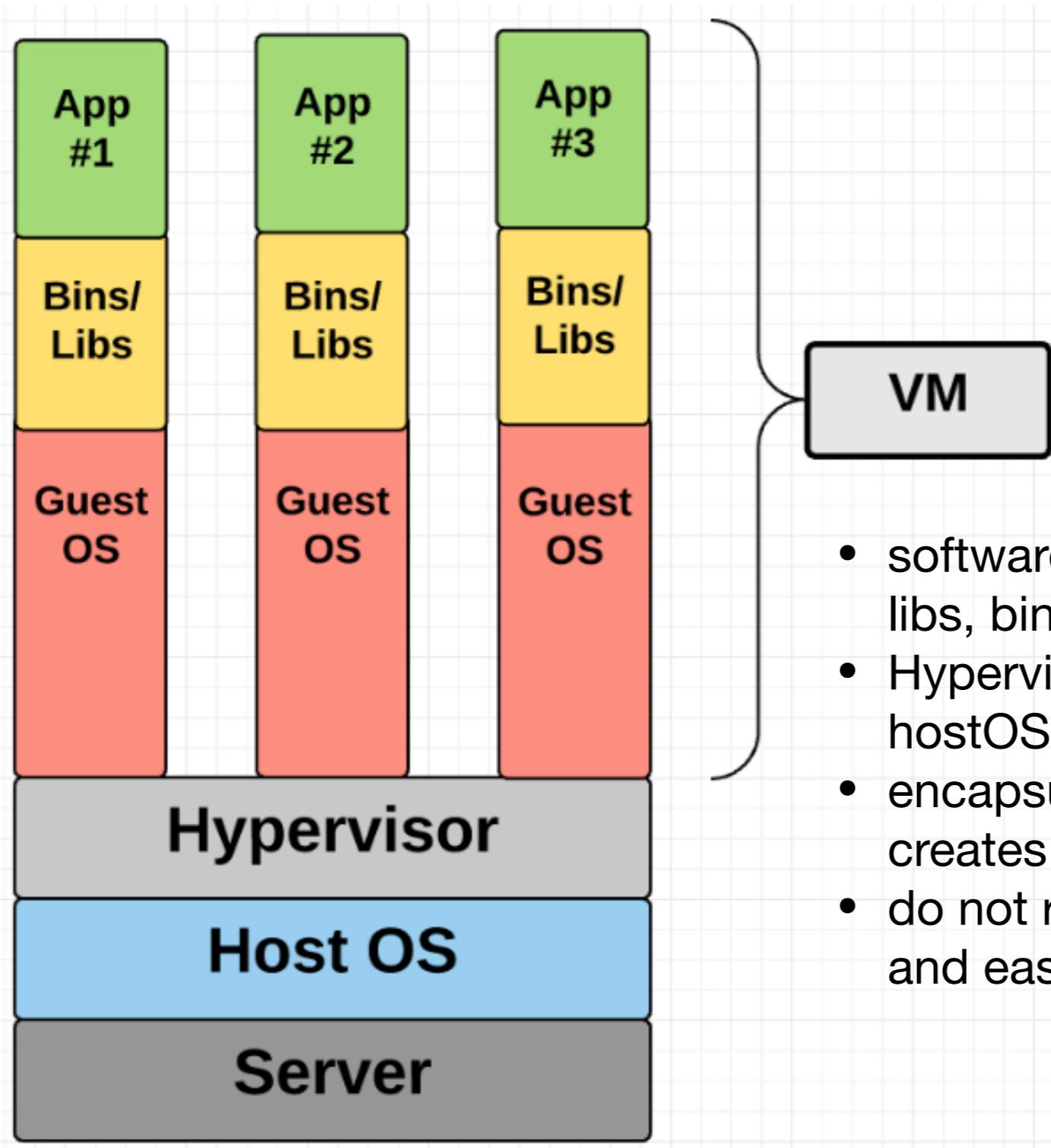


# Introduction to docker

*Chris Stricker, stricker@genetics-network.ch*

- Software needs to interact with other soft- and hardware to successfully run on a computer
  - we want to access the hard disk for file I/O, the printer, libraries for scientific computing, ...
  - interactions between software and/or software and hardware
  - dependencies may be different between different software products, creating incompatibilities (DLL incompatibilities in my old windows days)
  - even worse: we want our software to run on different hardware, different operating systems

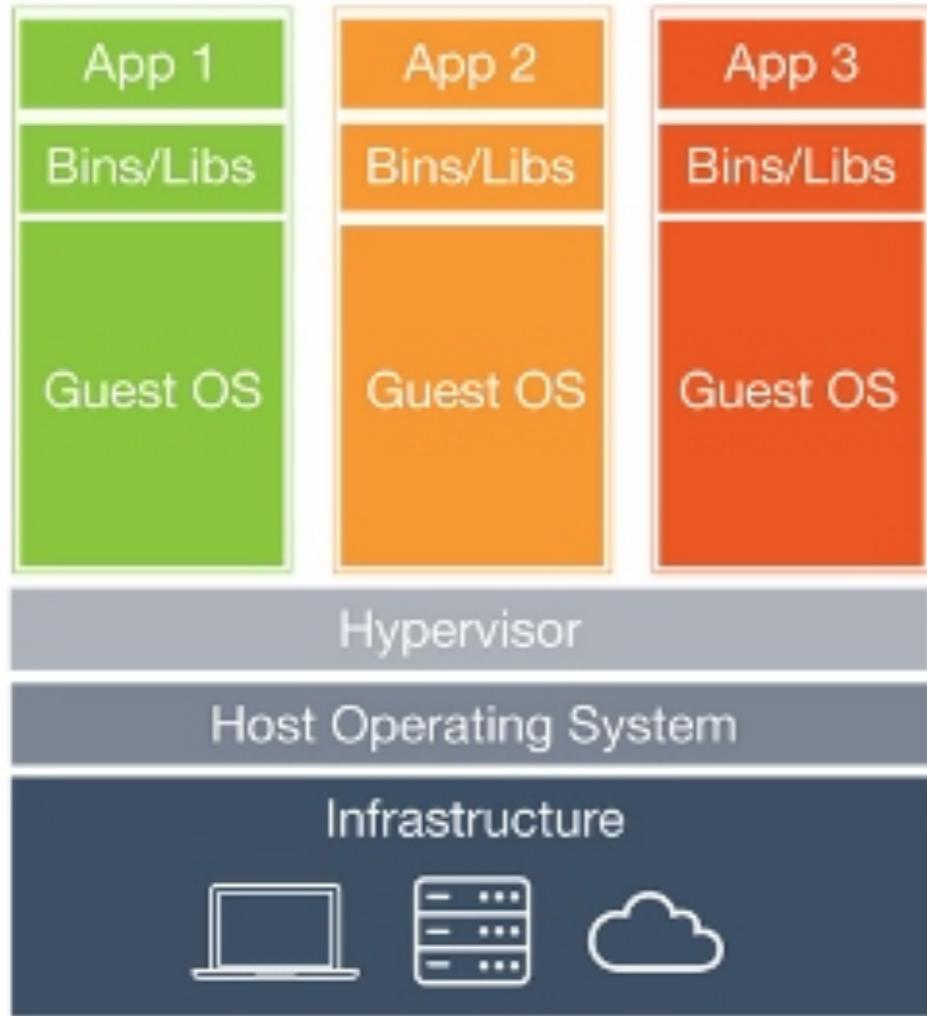
- What if we could encapsulate the software and isolate it as much as possible from other software?
  - virtual machines have been around for almost 20 years now
  - “computer within a computer”
  - provide maximum isolation at the expense of overhead



- software is encapsulated with specific libs, binaries and a guest OS
- Hypervisor as additional layer between hostOS and guestOS
- encapsulating software with guest OS creates large overhead
- do not really contribute to portability and ease of maintenance

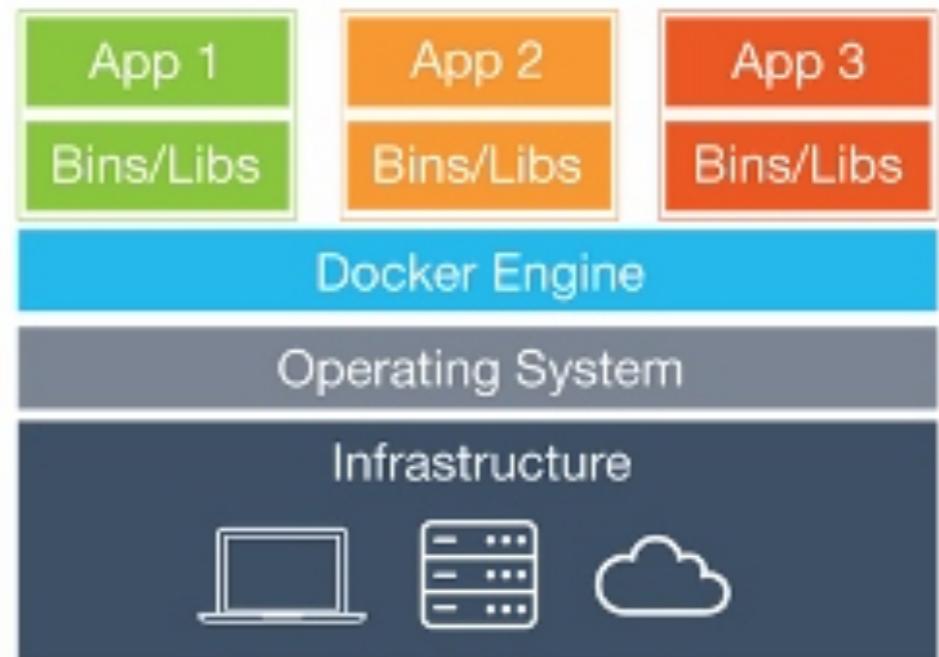
- <https://www.aquasec.com/wiki/display/containers/Docker+Containers+vs.+Virtual+Machines>

- What if we could encapsulate the software and isolate it as much as possible from other software ...
  - but can bundle it only with the necessary components, i.e. an ideal balance between isolation and overhead
  - containers
  - balance between isolation and overhead
  - containers share segments of the hostOS



## Virtual Machines

- software encapsulated with specific libs, binaries and a guest OS
- Hypervisor as additional layer between hostOS and guestOS
- encapsulating software with guest OS creates large overhead
- do not really contribute to portability and ease of maintenance



## Containers

- software encapsulated with specific libs, binaries
- container daemon interacts with kernel
- container isolated from OS
- portability and ease of maintenance
- stateless
- immutable
-

# Getting started with Docker

- you downloaded the docker client from <https://www.docker.com/get-started> and installed it

```
[al5:~] Chris% docker run hello-world
Unable to find image 'hello-world:latest' locally
latest: Pulling from library/hello-world
d1725b59e92d: Pull complete
Digest: sha256:0add3ace90ecb4adb7777e9aacf18357296e799f81cabc9fde470971e499788
Status: Downloaded newer image for hello-world:latest

Hello from Docker!
This message shows that your installation appears to be working correctly.
```

To generate this message, Docker took the following steps:

1. The Docker client contacted the Docker daemon.
2. The Docker daemon pulled the "hello-world" image from the Docker Hub.  
(amd64)
3. The Docker daemon created a new container from that image which runs the executable that produces the output you are currently reading.
4. The Docker daemon streamed that output to the Docker client, which sent it to your terminal.

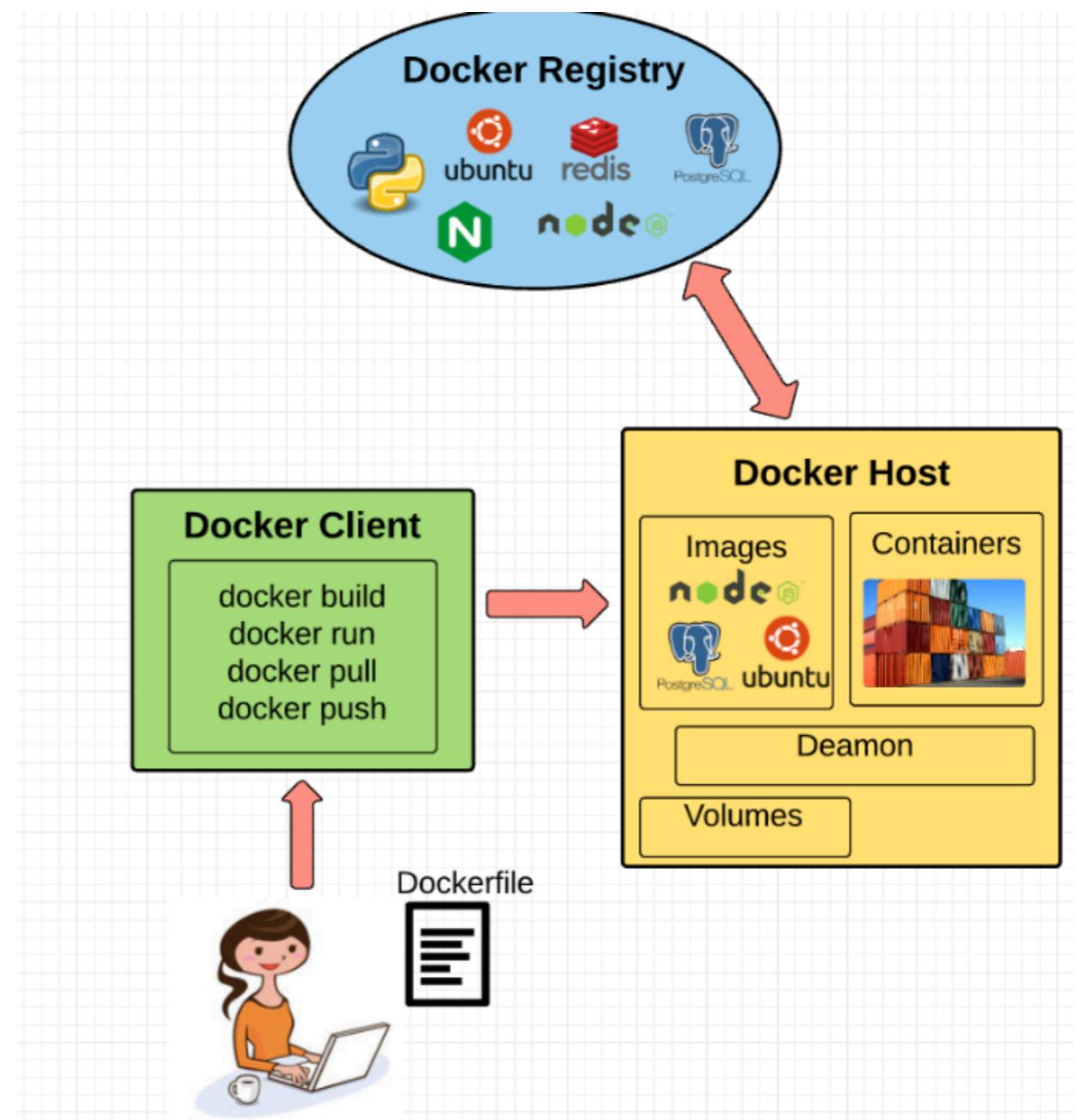
To try something more ambitious, you can run an Ubuntu container with:  
\$ docker run -it ubuntu bash

Share images, automate workflows, and more with a free Docker ID:  
<https://hub.docker.com/>

For more examples and ideas, visit:  
<https://docs.docker.com/get-started/>

# Fundamental Concepts

- docker client is the user interface
- docker daemon runs on host, executes the command coming from the client
- the docker file contains instructions to build a docker image
- a docker image is the blueprint of a container, it becomes a container, when the client requests to start the image. A container is an instance of an image.
- software is wrapped into a container with a file system, libs, tools, etc.
- images are read only, so read-write volumes are added also
- see <https://medium.freecodecamp.org/a-beginner-friendly-introduction-to-containers-vms-and-docker-79a9e3e119b>



# Available docker images

- what containers are currently on your system?

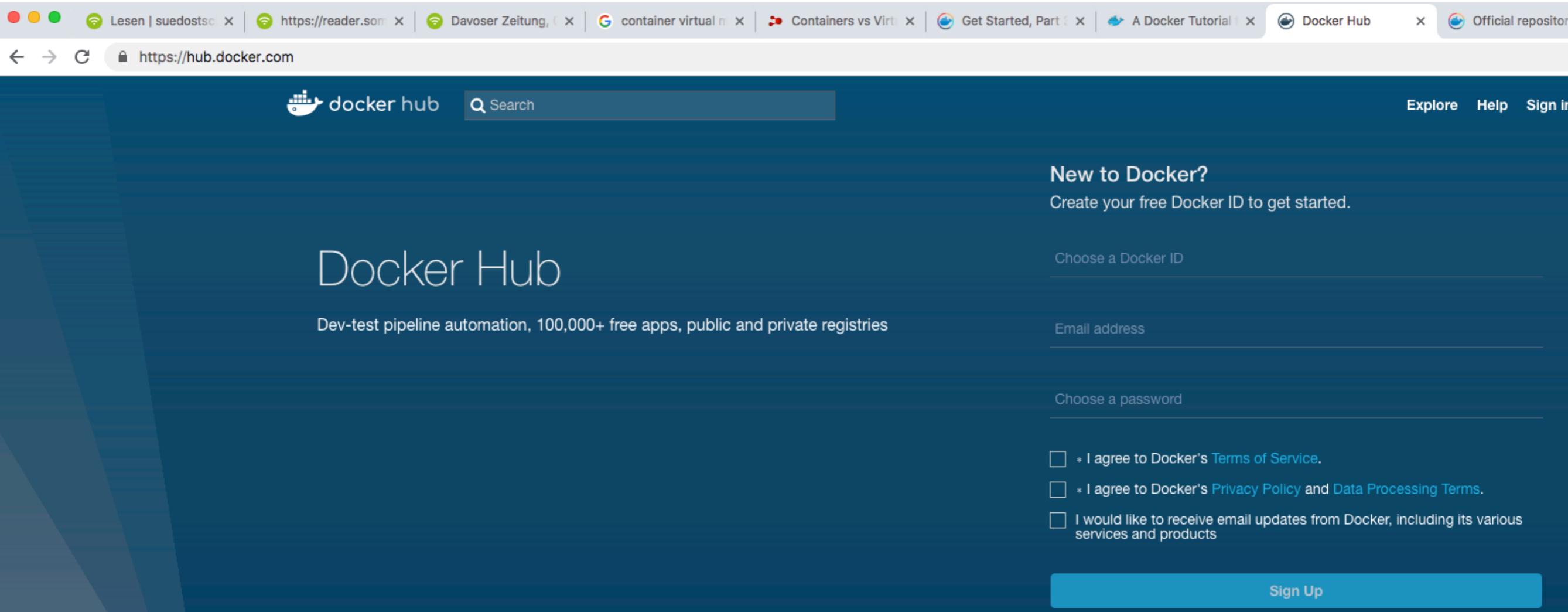
```
[[al5:~] Chris% docker ps -a
CONTAINER ID        IMAGE               COMMAND
08b7d4fec6a9      hello-world        "/hello"
                  CREATED   STATUS
                               17 hours ago   Exited (0) 17 hours ago
                                     PORTS
                                     NAMES
                                         quirky_tesla
```

- what images are currently on your system?

```
[[al5:~] Chris% docker images
REPOSITORY          TAG      IMAGE ID            CREATED             SIZE
hello-world         latest   4ab4c602aa5e    2 months ago       1.84kB
jwas                latest   a0b8b84eb779    4 months ago       5GB
qtlrocks/jwas-docker latest   6d66776c87a7    5 months ago       999MB
```

# Available docker images

- what images are available on the docker hub?
  - \* <https://hub.docker.com>



The screenshot shows a web browser window with multiple tabs open at the top. The active tab is 'Docker Hub'. The page itself is the Docker Hub sign-up form. It features a dark blue header with the 'docker hub' logo and a search bar. Below the header, the text 'Docker Hub' is prominently displayed, followed by a subtext: 'Dev-test pipeline automation, 100,000+ free apps, public and private registries'. To the right, there's a 'New to Docker?' section with a 'Create your free Docker ID to get started.' button. This section includes fields for 'Choose a Docker ID' and 'Email address', both with placeholder text. Further down, there's a 'Choose a password' field with a placeholder. At the bottom of the form, there are three checkboxes: one agreeing to the 'Terms of Service', another to 'Privacy Policy and Data Processing Terms', and a third for receiving email updates. A large blue 'Sign Up' button is located at the very bottom right of the form.

New to Docker?  
Create your free Docker ID to get started.

Choose a Docker ID

Email address

Choose a password

\* I agree to Docker's [Terms of Service](#).

\* I agree to Docker's [Privacy Policy](#) and [Data Processing Terms](#).

I would like to receive email updates from Docker, including its various services and products

Sign Up

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https://hub.docker.com/search/?isAutomated=0&isOfficial=0&page=1&pullCount=0&q=ubuntu&starCount=1

Dashboard Explore Organizations Create cstricker

## Repositories (52973)

Stars

Repository	Type	Stars	Pulls	Actions
<a href="#">ubuntu/official</a>	official	8.7K STARS	10M+ PULLS	<a href="#">DETAILS</a>
<a href="#">phusion/baseimage</a>	public	1.5K STARS	5M+ PULLS	<a href="#">DETAILS</a>
<a href="#">alexeiled/docker-oracle-xe-11g</a>	public   automated build	276 STARS	100K+ PULLS	<a href="#">DETAILS</a>
<a href="#">dorowu/ubuntu-desktop-lxde-vnc</a>	public   automated build	241 STARS	1M+ PULLS	<a href="#">DETAILS</a>
<a href="#">williamyeh/ansible</a>	public   automated build	186 STARS	1M+ PULLS	<a href="#">DETAILS</a>
<a href="#">rastasheep/ubuntu-sshd</a>	public   automated build	180 STARS	1M+ PULLS	<a href="#">DETAILS</a>

```
[al5:~] Chris% docker run ubuntu
Unable to find image 'ubuntu:latest' locally
latest: Pulling from library/ubuntu
473ede7ed136: Pull complete
c46b5fa4d940: Pull complete
93ae3df89c92: Pull complete
6b1eed27cade: Pull complete
Digest: sha256:29934af957c53004d7fb6340139880d23fb1952505a15d69a03af0d1418878cb
Status: Downloaded newer image for ubuntu:latest
[al5:~] Chris%
```

image started as container but immediately exited

```
[[al5:~] Chris% docker ps -a
CONTAINER ID        IMAGE               COMMAND             CREATED            STATUS
3cbbb3db66fa      ubuntu              "/bin/bash"         About a minute ago   Exited (0) 59 seconds ago
[al5:~] Chris%
```

- now try

```
[[al5:~] Chris% docker run -itd ubuntu  
c866e65f29788ef0247bb79ca67392800def276bebd17114d431c9a9c87be04b  
[[al5:~] Chris% docker ps -a  
CONTAINER ID        IMAGE               COMMAND             CREATED            STATUS              PORTS  
c866e65f2978        ubuntu              "/bin/bash"         10 seconds ago   Up 8 seconds  
3cbbb3db66fa        ubuntu              "/bin/bash"         2 minutes ago    Exited (0) 2 minutes ago  
[al5:~] Chris% 
```

- spawns a new ubuntu container from the ubuntu image, keeps it alive (-i), connects it to a terminal (-t) but detaches it from the current terminal (-d).

- Now login to that container and do something...

```
[[al5:~] Chris% docker exec -it c866e65f2978 bash  
[root@c866e65f2978:/# ls  
bin  boot  dev  etc  home  lib  lib64  media  mnt  opt  proc  root  run  sbin  srv  sys  tmp  usr  var  
[root@c866e65f2978:/# mkdir MYDIR  
[root@c866e65f2978:/# ls  
MYDIR  bin  boot  dev  etc  home  lib  lib64  media  mnt  opt  proc  root  run  sbin  srv  sys  tmp  usr  var  
[root@c866e65f2978:/# exit  
exit  
[[al5:~] Chris% docker ps -a  
CONTAINER ID        IMAGE               COMMAND             CREATED            STATUS              PORTS  
c866e65f2978        ubuntu              "/bin/bash"         2 minutes ago   Up 2 minutes  
3cbbb3db66fa        ubuntu              "/bin/bash"         4 minutes ago    Exited (0) 4 minutes ago  
[[al5:~] Chris% docker exec -it c866e65f2978 bash  
[root@c866e65f2978:/# ls  
MYDIR  bin  boot  dev  etc  home  lib  lib64  media  mnt  opt  proc  root  run  sbin  srv  sys  tmp  usr  var  
[root@c866e65f2978:/# exit  
exit  
[al5:~] Chris% 
```

**Changes are persistent, as long as container exists!**

- can verify this, stop and restart the container

```
[al5:~] Chris% docker stop c866e65f2978
c866e65f2978
[al5:~] Chris% docker ps -a
CONTAINER ID        IMAGE               COMMAND             CREATED            STATUS              PORTS
c866e65f2978        ubuntu              "/bin/bash"         4 minutes ago     Exited (0) 6 seconds ago
3cbbb3db66fa        ubuntu              "/bin/bash"         7 minutes ago     Exited (0) 7 minutes ago
```

- Now start it again...

```
[al5:~] Chris% docker start -i c866e65f2978
root@c866e65f2978:/# ls
MYDIR  bin  boot  dev  etc  home  lib  lib64  media  mnt  opt  proc  root  run  sbin  srv  sys  tmp  usr  var
root@c866e65f2978:/#
```

**Changes are persistent, as long as container exists!**  
**However, starting a new container from the ubuntu image will not have MYDIR in it**

- create a new ubuntu container

```
[root@c866e65f2978:/# exit
exit
[[al5:~] Chris% docker ps -a
CONTAINER ID        IMAGE               COMMAND             CREATED            STATUS              PORTS
c866e65f2978        ubuntu              "/bin/bash"         17 minutes ago    Exited (0) 13 seconds ago
3cbbb3db66fa        ubuntu              "/bin/bash"         19 minutes ago    Exited (0) 19 minutes ago
[[al5:~] Chris% docker run -itd ubuntu
ad96279dd9423e3cd8548e05418b87f20adfbfed86a33c955392fbb2f0fc9df9
[[al5:~] Chris% docker ps -a
CONTAINER ID        IMAGE               COMMAND             CREATED            STATUS              PORTS
ad96279dd942        ubuntu              "/bin/bash"         14 seconds ago   Up 12 seconds
c866e65f2978        ubuntu              "/bin/bash"         17 minutes ago   Exited (0) 50 seconds ago
3cbbb3db66fa        ubuntu              "/bin/bash"         20 minutes ago   Exited (0) 20 minutes ago
```

- see whether it has MYDIR?

```
[a15:~] Chris% docker exec -it ad96279dd942 bash
root@ad96279dd942:/# ls
bin  boot  dev  etc  home  lib  lib64  media  mnt  opt  proc  root  run  sbin  srv  sys  tmp  usr  var
root@ad96279dd942:/# exit
exit
[a15:~] Chris% docker rm ad96279dd942
Error response from daemon: You cannot remove a running container ad96279dd9423e3cd8548e05418b87f20adfbfed
[a15:~] Chris% docker stop ad96279dd942
ad96279dd942
[a15:~] Chris% docker rm ad96279dd942
ad96279dd942
[a15:~] Chris% docker ps -a
CONTAINER ID        IMAGE               COMMAND             CREATED            STATUS
c866e65f2978        ubuntu              "/bin/bash"         19 minutes ago    Exited (0) 2 minutes ago
3cbbb3db66fa        ubuntu              "/bin/bash"         21 minutes ago    Exited (0) 21 minutes ago
[a15:~] Chris%
```

**Changes are persistent, as long as container exists!  
However, starting a new container from the ubuntu  
image will not have MYDIR in it**

**—> Containers are immutable & stateless**

- equivalently, try

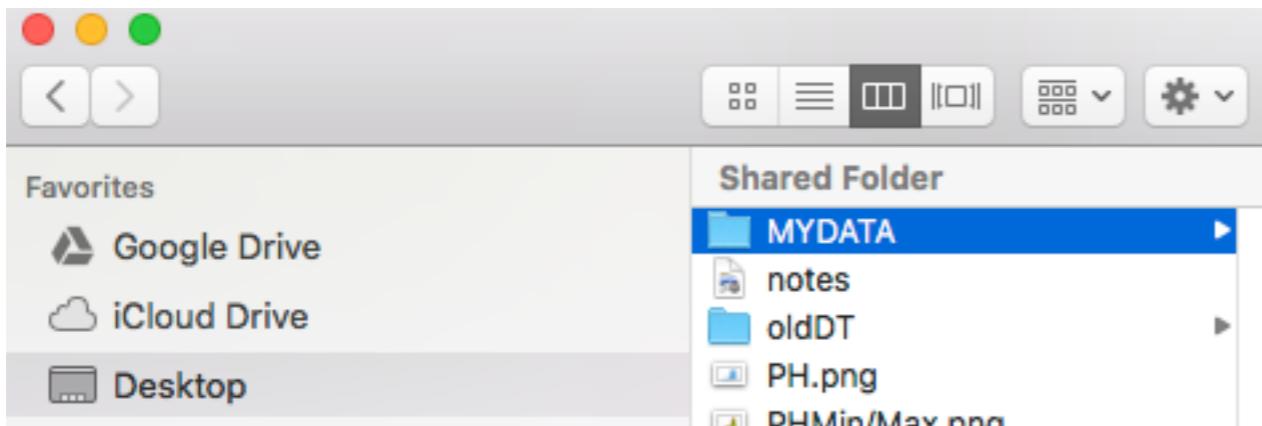
```
[al5:~] Chris% docker ps -a
CONTAINER ID        IMAGE               COMMAND                  CREATED             STATUS              PORTS
c866e65f2978        ubuntu              "/bin/bash"            26 minutes ago    Exited (0) 9 minutes ago
3cbbb3db66fa        ubuntu              "/bin/bash"            28 minutes ago    Exited (0) 28 minutes ago
[al5:~] Chris% docker run --rm -it ubuntu bash
root@91ec62e5458f:/# ls
bin  boot  dev  etc  home  lib  lib64  media  mnt  opt  proc  root  run  sbin  srv  sys  tmp  usr  var
root@91ec62e5458f:/# mkdir MYDIR
root@91ec62e5458f:/# ls
MYDIR  bin  boot  dev  etc  home  lib  lib64  media  mnt  opt  proc  root  run  sbin  srv  sys  tmp  usr  var
root@91ec62e5458f:/# exit
exit
[al5:~] Chris% docker ps -a
CONTAINER ID        IMAGE               COMMAND                  CREATED             STATUS              PORTS
c866e65f2978        ubuntu              "/bin/bash"            27 minutes ago    Exited (0) 10 minutes ago
3cbbb3db66fa        ubuntu              "/bin/bash"            30 minutes ago    Exited (0) 30 minutes ago
[al5:~] Chris%
```

**Changes are lost, when the container is removed!**  
→ Container images are immutable & stateless

- how can we save our work, the data we created?

```
[al5:~] Chris% docker run --rm -it -v ~/Desktop/MYDATA:/MYDir ubuntu bash
[root@bcb6276780df:/# ls
MYDir bin boot dev etc home lib lib64 media mnt opt proc root run sbin srv sys tmp usr var
```

- the new dir MYDir in the container is linked to MYDATA on the local desktop



- after exiting the container...

```
[root@bcb6276780df:/# exit
exit
[[al5:~] Chris% cat ~/Desktop/MYDATA/listing
total 72
drwxr-xr-x 1 root root 4096 Nov 16 11:19 .
drwxr-xr-x 1 root root 4096 Nov 16 11:19 ..
-rw xr-xr-x 1 root root 0 Nov 16 11:19 .dockerenv
drwxr-xr-x 3 root root 102 Nov 16 09:49 MYDir
drwxr-xr-x 2 root root 4096 Oct 18 21:03 bin
drwxr-xr-x 2 root root 4096 Apr 24 2018 boot
drwxr-xr-x 5 root root 360 Nov 16 11:19 dev
drwxr-xr-x 1 root root 4096 Nov 16 11:19 etc
drwxr-xr-x 2 root root 4096 Apr 24 2018 home
drwxr-xr-x 8 root root 4096 Oct 18 21:02 lib
drwxr-xr-x 2 root root 4096 Oct 18 21:02 lib64
drwxr-xr-x 2 root root 4096 Oct 18 21:02 media
drwxr-xr-x 2 root root 4096 Oct 18 21:02 mnt
drwxr-xr-x 2 root root 4096 Oct 18 21:02 opt
dr-xr-xr-x 317 root root 0 Nov 16 11:19 proc
drwx----- 2 root root 4096 Oct 18 21:03 root
drwxr-xr-x 1 root root 4096 Oct 19 00:47 run
drwxr-xr-x 1 root root 4096 Oct 19 00:47 sbin
drwxr-xr-x 2 root root 4096 Oct 18 21:02 srv
dr-xr-xr-x 13 root root 0 Nov 15 12:14 sys
drwxrwxrwt 2 root root 4096 Oct 18 21:03 tmp
drwxr-xr-x 1 root root 4096 Oct 18 21:02 usr
drwxr-xr-x 1 root root 4096 Oct 18 21:03 var
```

```
[root@bcb6276780df:/# ls -al > MYDir/listing
[root@bcb6276780df:/# cat MYDir/listing
total 72
drwxr-xr-x 1 root root 4096 Nov 16 11:19 .
drwxr-xr-x 1 root root 4096 Nov 16 11:19 ..
-rw xr-xr-x 1 root root 0 Nov 16 11:19 .dockerenv
drwxr-xr-x 3 root root 102 Nov 16 09:49 MYDir
drwxr-xr-x 2 root root 4096 Oct 18 21:03 bin
drwxr-xr-x 2 root root 4096 Apr 24 2018 boot
drwxr-xr-x 5 root root 360 Nov 16 11:19 dev
drwxr-xr-x 1 root root 4096 Nov 16 11:19 etc
drwxr-xr-x 2 root root 4096 Apr 24 2018 home
drwxr-xr-x 8 root root 4096 Oct 18 21:02 lib
drwxr-xr-x 2 root root 4096 Oct 18 21:02 lib64
drwxr-xr-x 2 root root 4096 Oct 18 21:02 media
drwxr-xr-x 2 root root 4096 Oct 18 21:02 mnt
drwxr-xr-x 2 root root 4096 Oct 18 21:02 opt
dr-xr-xr-x 317 root root 0 Nov 16 11:19 proc
drwx----- 2 root root 4096 Oct 18 21:03 root
drwxr-xr-x 1 root root 4096 Oct 19 00:47 run
drwxr-xr-x 1 root root 4096 Oct 19 00:47 sbin
drwxr-xr-x 2 root root 4096 Oct 18 21:02 srv
dr-xr-xr-x 13 root root 0 Nov 15 12:14 sys
drwxrwxrwt 2 root root 4096 Oct 18 21:03 tmp
drwxr-xr-x 1 root root 4096 Oct 18 21:02 usr
drwxr-xr-x 1 root root 4096 Oct 18 21:03 var
```

# Where are we?

- we learned:
  - \* docker is a way to isolate software into a self-contained box, a container
  - \* there are basic containers available on a docker hub
  - \* can download and run such a container
  - \* can add functionality to a container
- \* next: we want to save those changes and upload such a container

- Note that by

```
[al5:~] Chris% docker run --rm -it -v ~/Desktop/MYDATA/:/MYDir ubuntu bash
[root@bcb6276780df:/# ls
MYDir bin boot dev etc home lib lib64 media mnt opt proc root run sbin srv sys tmp usr var
```

- we were spawning a new container from the ubuntu image, created the new directory “MYDIR” in the container and linked it to a directory on our desktop.
- However, the container was deleted after exiting. Therefore, let's do it again, but this time without ‘–rm’...

```
[al5:~] Chris% docker run -it -v ~/Desktop/MYDATA/:/MYDir ubuntu bash
[root@b18e135cbd91:/# ls
MYDir bin boot dev etc home lib lib64 media mnt opt proc root run sbin srv sys tmp usr var
[root@b18e135cbd91:/# ls MYDir/
listing
[root@b18e135cbd91:/# exit
exit
[al5:~] Chris%
```

- now the new container is still available

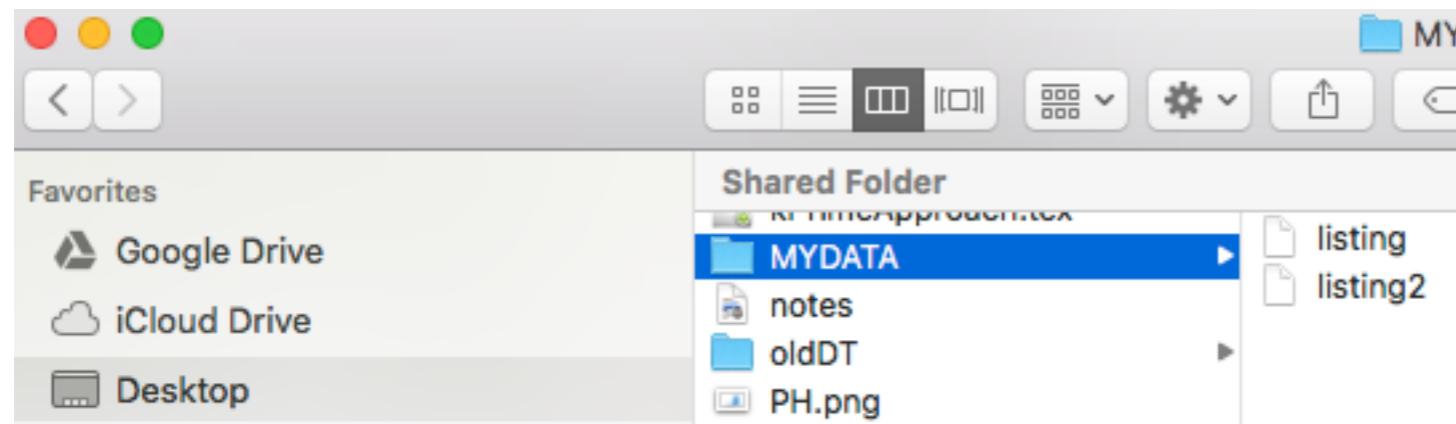
CONTAINER ID	IMAGE	COMMAND	CREATED	STATUS	PORTS
b18e135cbd91	ubuntu	"bash"	27 minutes ago	Exited (0) 4 minutes ago	
c866e65f2978	ubuntu	"/bin/bash"	2 days ago	Exited (0) 27 minutes ago	
3cbbb3db66fa	ubuntu	"/bin/bash"	2 days ago	Exited (0) 2 days ago	

- and the directory MYDir has persisted and is linked to to MYDATA on the desktop!

- and the directory MYDir has persisted and is linked to MYDATA on the desktop!

```
[al5:~] Chris% docker ps -a
CONTAINER ID        IMAGE               COMMAND             CREATED            STATUS              PORTS
b18e135cbd91        ubuntu              "bash"              3 hours ago       Exited (0) 3 seconds ago
c866e65f2978        ubuntu              "/bin/bash"         3 days ago        Exited (0) 3 hours ago
3cbbb3db66fa        ubuntu              "/bin/bash"         3 days ago        Exited (0) 3 days ago
[al5:~] Chris% docker start -i b18e135cbd91
[root@b18e135cbd91:/# ls
MYDir  bin  boot  dev  etc  home  lib  lib64  media  mnt  opt  proc  root  run  sbin  srv  sys  tmp  usr  var
[root@b18e135cbd91:/# ls >MYDir/listing2
[root@b18e135cbd91:/# cat MYDir/listing2
MYDir
bin
boot
dev
etc
home
```

- and MYDATA on my Desktop looks like



- now let's commit those changes to a new image

- now let's commit those changes to a new image

```

[[al5:~] Chris% docker ps -a
CONTAINER ID        IMAGE               COMMAND             CREATED            STATUS              PORTS
b18e135cbd91      ubuntu              "bash"              3 hours ago       Exited (0) 9 minutes ago
c866e65f2978      ubuntu              "/bin/bash"         3 days ago        Exited (0) 3 hours ago
3cbbb3db66fa      ubuntu              "/bin/bash"         3 days ago        Exited (0) 3 days ago
[[al5:~] Chris% docker images
REPOSITORY          TAG                 IMAGE ID            CREATED           SIZE
ubuntu              latest              ea4c82dcd15a      4 weeks ago      85.8MB
hello-world         latest              4ab4c602aa5e      2 months ago     1.84kB
jwas                latest              a0b8b84eb779      5 months ago     5GB
qtlrocks/jwas-docker latest              6d66776c87a7      5 months ago     999MB
[[al5:~] Chris% docker commit b18e135cbd91 chris-ubuntu
sha256:0bce066c853a720c7a4e3799cc0c2a64db1e0b415329465632de674360db3ae1
[[al5:~] Chris% docker run -it chris-ubuntu
[root@9c24685c01c5:/# ls
MYDir  bin  boot  dev  etc  home  lib  lib64  media  mnt  opt  proc  root  run  sbin  srv  sys  tmp  usr  var

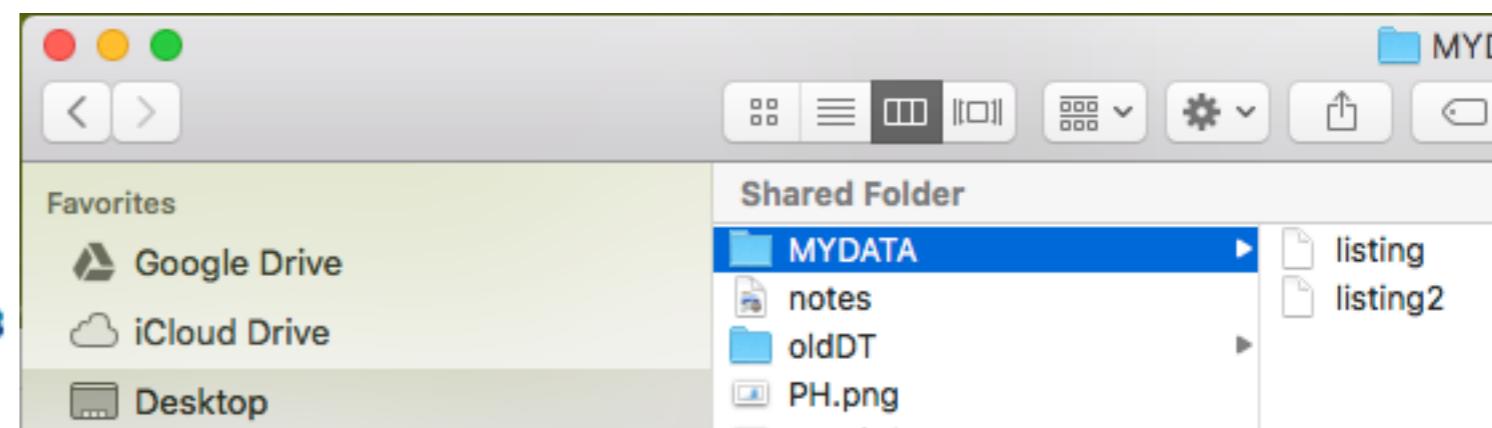
```

- spawning a new container from the modified images reveals that the changes are still there (dir MYDir), BUT

```

[root@9c24685c01c5:/# cd MYDir/
[root@9c24685c01c5:/MYDir# ls -al
total 8
drwxr-xr-x 2 root root 4096 Nov 19 09:34 .
drwxr-xr-x 1 root root 4096 Nov 19 12:29 ..
[root@9c24685c01c5:/MYDir# cd ..
[root@9c24685c01c5:/# ls /usr > MYDir/listing3
[root@9c24685c01c5:/# ls MYDir/
listing3

```



- the link between the dir MYDir in the container and our local MYDATA-directory is not saved with to the newly committed image.
- we need to re-establish that link upon spawning the new container

```
[al5:~] Chris% docker run -it -v ~/Desktop/MYDATA/:/MYDir chris-ubuntu
[root@50b58ccf6732:/# ls MYDir/
listing listing2
root@50b58ccf6732:/# ]
```

- now we can push our modified image to the docker hub for others to download

- now we can push our modified image to the docker hub for others to download

```
[[al5:~] Chris% docker push chris-ubuntu
The push refers to repository [docker.io/library/chris-ubuntu]
3ba479ced88d: Preparing
76c033092e10: Preparing
2146d867acf3: Preparing
ae1f631f14b7: Preparing
102645f1cf72: Preparing
denied: requested access to the resource is denied
```

- we need to tag the image and login to docker hub

```
[[al5:~] Chris% docker tag chris-ubuntu cstricker/chris-ubuntu
[[al5:~] Chris% docker images
REPOSITORY          TAG      IMAGE ID      CREATED       SIZE
chris-ubuntu        latest   0bce066c853a  About an hour ago  85.8MB
cstricker/chris-ubuntu  latest   0bce066c853a  About an hour ago  85.8MB
ubuntu              latest   ea4c82dcd15a  4 weeks ago    85.8MB
hello-world         latest   4ab4c602aa5e  2 months ago   1.84kB
jwas                latest   a0b8b84eb779  5 months ago   5GB
qtlrocks/jwas-docker  latest   6d66776c87a7  5 months ago   999MB
```

```
[[al5:~] Chris% docker login
Login with your Docker ID to push and pull images from Docker Hub. If you don't have a Docker ID, head over
Username: cstricker
[Password:
Login Succeeded
[[al5:~] Chris%
```

- now, uploading works

```
[al5:~] Chris% docker push cstricker/chris-ubuntu
The push refers to repository [docker.io/cstricker/chris-ubuntu]
3ba479ced88d: Pushed
76c033092e10: Pushed
2146d867acf3: Pushed
ae1f631f14b7: Pushed
102645f1cf72: Pushed
latest: digest: sha256:2295a0d59e78a80bdee35a471adc52454eb1a05aaffe1551ac129e55381386ce size: 1357
```

- docker uploads layers of modifications, not the whole modified image
- can create a new image from scratch by a docker file
  - ▶ we may need to update the software in our container
  - ▶ cookbook of our image

# Docker file for JWAS image

(<https://github.com/reworkhow/JWAS-Docker/blob/master/dockerfile-jwas-large/Dockerfile>)

```
1 ARG BASE_CONTAINER=jupyter/datascience-notebook
2 FROM $BASE_CONTAINER
3
4 LABEL maintainer="Hao Cheng <qtlcheng@ucdavis.edu>"
5
6 # Add JWAS, XSim and PyPlot packages.
7 RUN julia -e 'using Pkg; Pkg.update()' && \
8     julia -e 'using Pkg; Pkg.add("PyPlot")' && \
9     julia -e 'using Pkg; Pkg.add("Plots")' && \
10    julia -e 'using Pkg; Pkg.add("DataFrames")' && \
11    julia -e 'using Pkg; Pkg.add("CSV")' && \
12    julia -e 'using Pkg; Pkg.add("Distributions")' && \
13    julia -e 'using Pkg; Pkg.add("JWAS")' && \
14    julia -e 'using Pkg; Pkg.add("XSim")' && \
15    # Precompile JWAS \
16    julia -e 'using Pkg; using JWAS' && \
17    julia -e 'using Pkg; using XSim' && \
18    julia -e 'using Pkg; using Plots' && \
19    julia -e 'using Pkg; using CSV' && \
20    julia -e 'using Pkg; using DataFrames' && \
21    fix-permissions $JULIA_PKGDIR $CONDA_DIR/share/jupyter
22
23 ADD --chown=jovyan:users ./notebooks /home/jovyan/notebooks
```

# what did we learn?

- \* docker is a way to isolate software into a self-contained box, a container
- \* there are basic containers available on a docker hub
- \* download and run such a container
- \* add functionality to a container
- \* save those changes to an image
- \* upload to docker hub
- \* create our own containers via docker files
- \* automated connection between docker hub and GitHub possible

# what did we learn?

- \* most useful docker commands
  - docker ps -a
  - docker pull
  - docker build
  - docker run
  - docker logs
  - docker volume ls
  - docker rm
  - docker rmi
  - docker stop / start
- lots of tutorials online, e.g. <https://docker-curriculum.com/>

# Using the JWAS docker container...

*but Jupyter first....*

*Chris Stricker, stricker@genetics-network.ch*

# Pulling the container from docker hub

```
[al5:~] Chris% docker pull qtlrocks/jwas-docker
Using default tag: latest
latest: Pulling from qtlrocks/jwas-docker
a48c500ed24e: Already exists
1e1de00ff7e1: Already exists
0330ca45a200: Already exists
471db38bcfbf: Already exists
0b4aba487617: Already exists
27261a5cbf78: Pull complete
2773b009b29a: Pull complete
0915dfd6dae3: Pull complete
ee7dca77f9ed: Pull complete
cf5be5e11621: Pull complete
33aa38e94d28: Pull complete
68f4b2245d2a: Pull complete
f5ab1b831f77: Pull complete
7ba257ca073a: Pull complete
0eb8f950b3ea: Pull complete
7774c2ec4751: Pull complete
2b9f5766a263: Pull complete
e4052009a673: Pull complete
f9e7255ce189: Pull complete
267a2399516f: Pull complete
3b54695138ea: Pull complete
d23336e5273c: Pull complete
e612b1583510: Pull complete
35ccca5c04fe: Pull complete
89cf804a40ff: Pull complete
81cdf7ccfcfd1: Pull complete
2d79f9fc672b: Pull complete
e68a6f6ec56b: Pull complete
889930c80fd2: Pull complete
4c9509f294c8: Pull complete
14e58f71fd50: Pull complete
Digest: sha256:7a6d83f972ed725385d146a765f816d0d02330917446becfe1fc9a00b13a4408
Status: Downloaded newer image for qtlrocks/jwas-docker:latest
[al5:~] Chris%
```

# starting the container from the pulled image

```
[al5:~] Chris% docker images
```

REPOSITORY	TAG	IMAGE ID	CREATED	SIZE
chris-ubuntu	latest	0bce066c853a	22 hours ago	85.8MB
qtlrocks/jwas-docker	latest	96dc980a3a55	5 days ago	6.26GB
ubuntu	latest	ea4c82dcd15a	4 weeks ago	85.8MB
hello-world	latest	4ab4c602aa5e	2 months ago	1.84kB
jwas	latest	a0b8b84eb779	5 months ago	5GB
qtlrocks/jwas-docker	<none>	6d66776c87a7	5 months ago	999MB

```
[al5:~] Chris%
```

```
[al5:~] Chris% docker run -it --rm -p 8888:8888 -v /Users/Chris/agn/TUM/JuliaCourse/dataDay1:/home/jovyan/work qtlrocks/jwas-docker
```

Container must be run with group "root" to update passwd file

Executing the command: jupyter notebook

```
[I 13:23:20.023 NotebookApp] Writing notebook server cookie secret to /home/jovyan/.local/share/jupyter/runtime/notebook_cookie_secr
[I 13:23:20.380 NotebookApp] JupyterLab extension loaded from /opt/conda/lib/python3.6/site-packages/jupyterlab
[I 13:23:20.380 NotebookApp] JupyterLab application directory is /opt/conda/share/jupyter/lab
[I 13:23:20.392 NotebookApp] Serving notebooks from local directory: /home/jovyan
[I 13:23:20.393 NotebookApp] The Jupyter Notebook is running at:
[I 13:23:20.393 NotebookApp] http://(3a7300f0e64d or 127.0.0.1):8888/?token=86f15cc77730d704ac931052cc66cd5ef0a390064eb4a2e7
[I 13:23:20.393 NotebookApp] Use Control-C to stop this server and shut down all kernels (twice to skip confirmation).
[C 13:23:20.394 NotebookApp]
```

Copy/paste this URL into your browser when you connect for the first time,  
to login with a token:

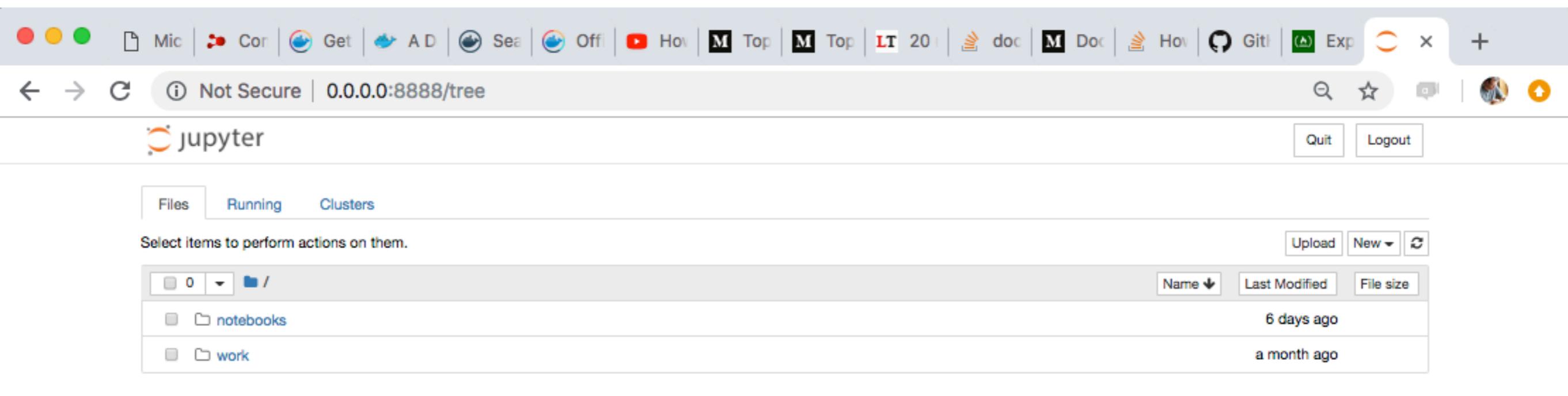
```
http://(3a7300f0e64d or 127.0.0.1):8888/?token=86f15cc77730d704ac931052cc66cd5ef0a390064eb4a2e7
```

- exposing port 8888 to local host
- mounting local dir to docker dir
- container executes jupyter notebook mapped to port 8888

- \* paste

`http://127.0.0.1:8888?token=86f15cc77730d704ac931052cc66cd5ef0a390064eb4a2e7`

in browser



- \* we interact with the running container by a jupyter notebook through the exposed port 8888

# But what is jupyter notebook?

- loose acronym meaning **Julia**, **Python** and **R**
- a web-based frontend to create, run, document, plot and manage source code in various programming languages (Julia, Python, R, C/C++, Fortran,.....)
- it comes free with the anaconda distribution
- Anaconda is an open source distribution for python and R. It includes packages for data management and large scale data processing and scientific computing. It has its own package manager.

# Components of jupyter

- ***notebook document (“notebooks”):***
  - ◆ your source code including the description of the analysis (markdown language) and the results of your analysis
- ***notebook app:***
  - ◆ server-client application that allows editing and running notebooks via web browser. Can run locally or remotely
- ***kernel:***
  - ◆ “computational engine” executing the code, a notebook is associated with a kernel
- ***dashboard***
  - ◆ jupyters “file manager”

# Let's start

## jupyter notebook

- without our docker container, after having installed Julia, Anaconda and IJulia, then the above command will start the jupyter server
- our docker-jwas container has all necessary software installed and starts the server automatically which the cmd

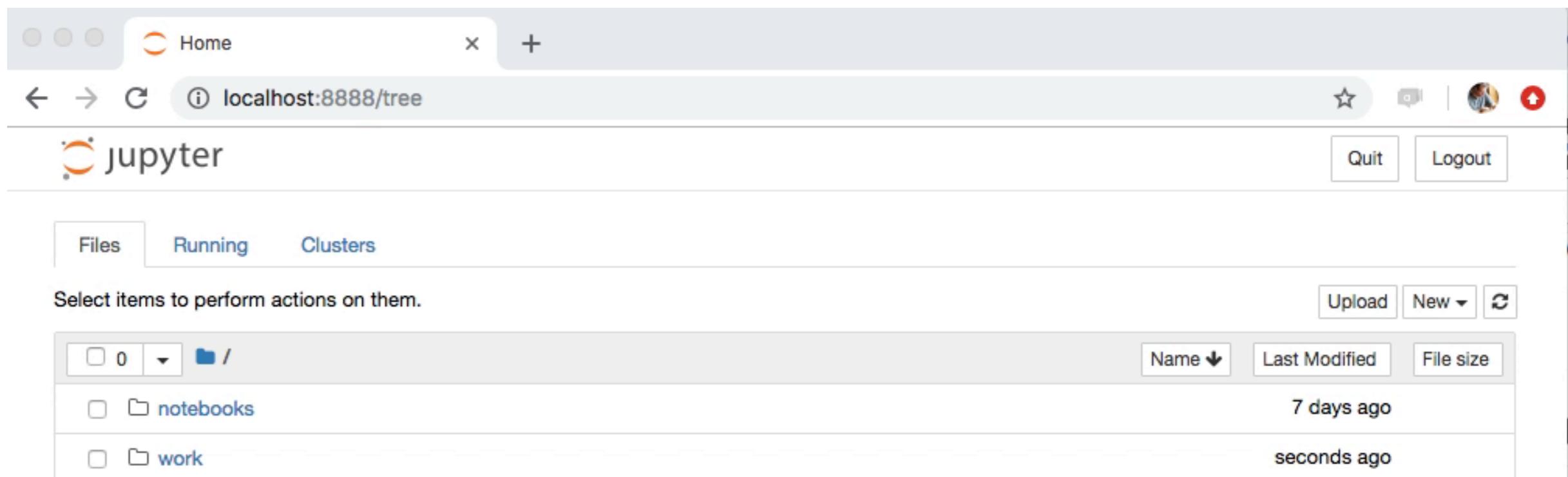
```
docker run -it -rm -p 8888:8888 -v /Users/Chris/agn/TUM/JuliaCourse/dataDay1:/home/ubuntu/work qt1rocks/jwas-docker
```

Copy/paste this URL into your browser when you connect for the first time, to login with a token:

[http://\(80b2e434cd65 or 127.0.0.1\):8888/?token=e672dec4624214a8a2da817d541c9b5ebef5f27fef0af73b](http://(80b2e434cd65 or 127.0.0.1):8888/?token=e672dec4624214a8a2da817d541c9b5ebef5f27fef0af73b)

# Using jupyter notebook

creating a new notebook from the dashboard



The screenshot shows the Jupyter Notebook dashboard at `localhost:8888/tree`. The interface includes a top bar with a logo, a title bar, and user profile icons. Below the title bar are navigation buttons for back, forward, and search, along with links for 'Quit' and 'Logout'. A menu bar offers 'Files', 'Running', and 'Clusters' options. The main area displays a file tree with two entries: 'notebooks' (modified 7 days ago) and 'work' (modified seconds ago). There are also buttons for 'Upload', 'New', and a refresh icon.

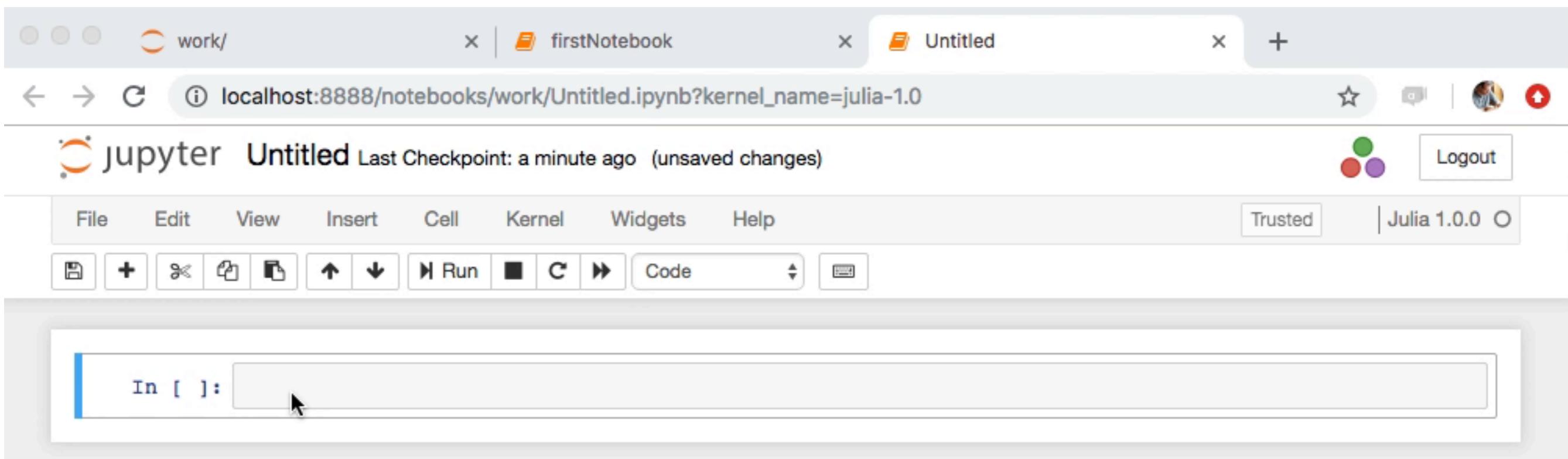
Name	Last Modified	File size
notebooks	7 days ago	
work	seconds ago	

# Using jupyter notebook

2 different modes in a jupyter notebook

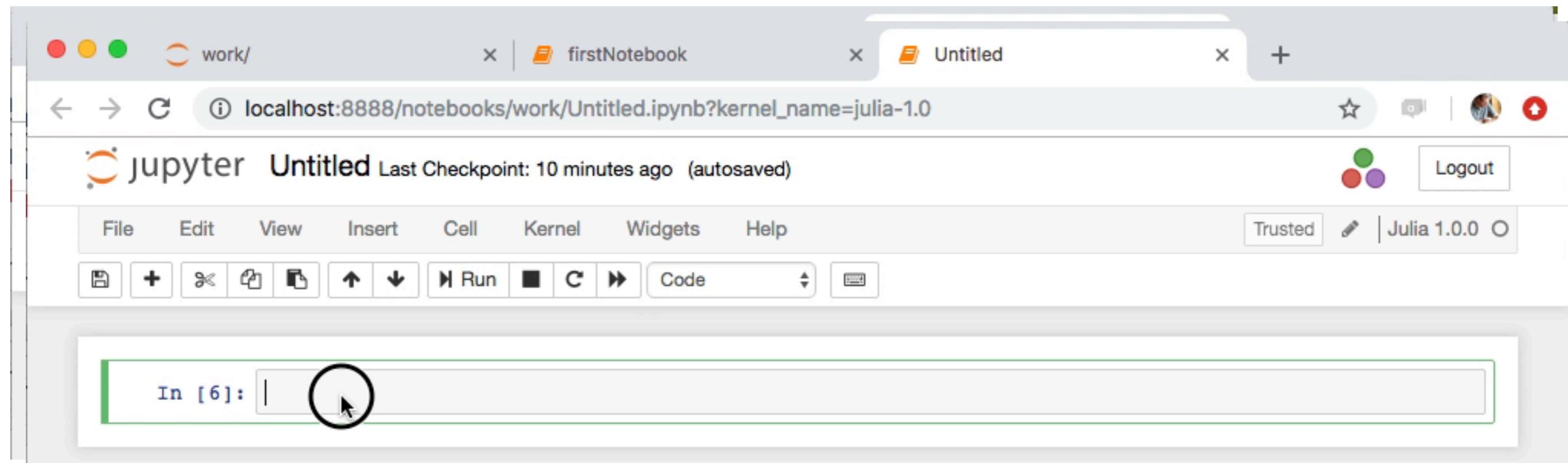
- green cell border = edit mode
- blue cell border = cmd mode

Switch between these modes with the mouse  
(esc switched from edit to cmd mode)



# Using jupyter notebook

- ◆ switch between edit and cmd mode
- ◆ execute a cell by dropdown menu, ctrl-return or shift-return
- ◆ execute several cells via drop-down menu
- ◆ by default, output from last line of a cell is printed to stdout (; at the end suppresses that)

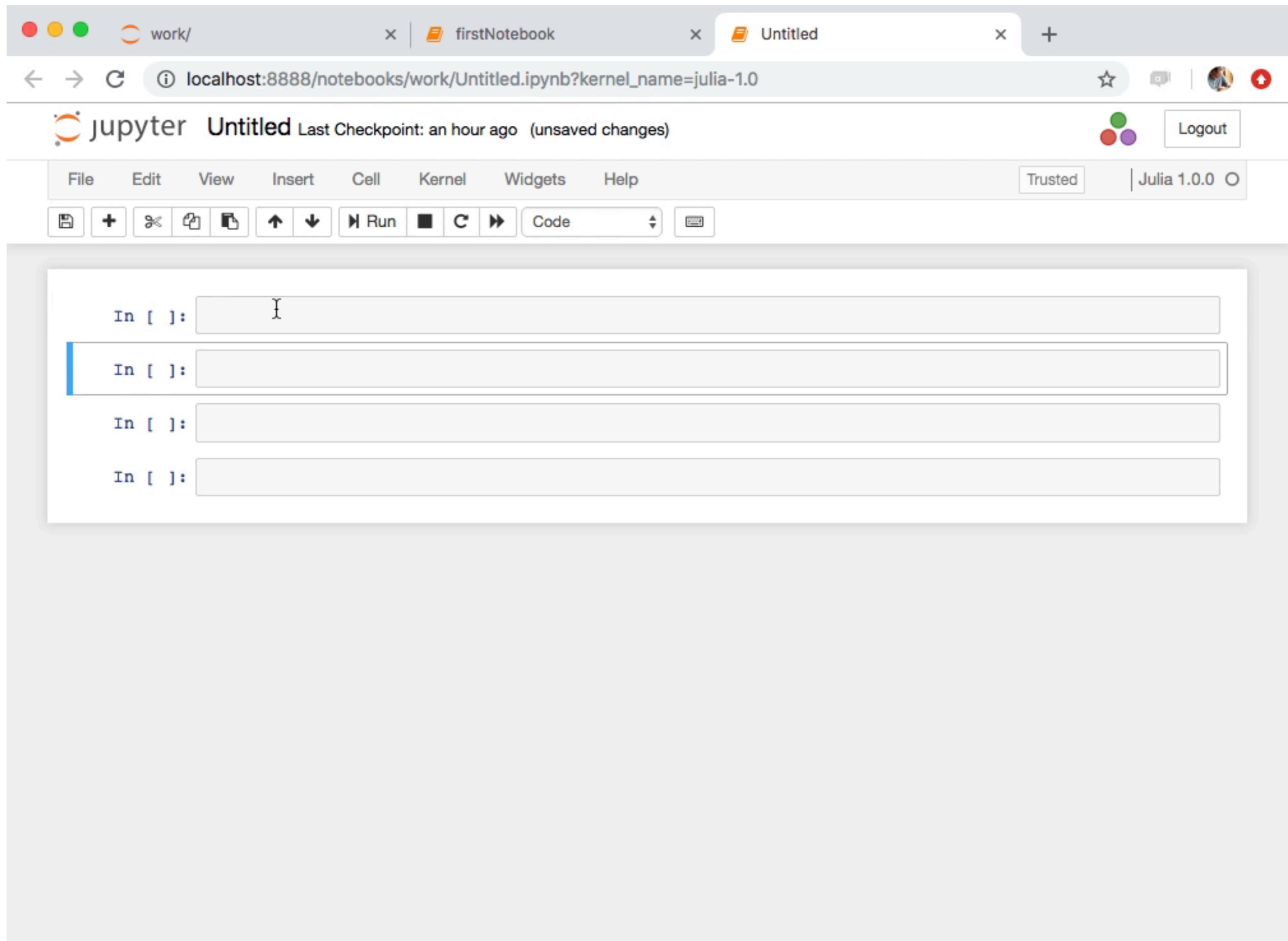


# Shortcuts in jupyter notebook

(try this in notebook\_JupyterCMDs)

- ◆ **ESC** to go into cmd mode
- ◆ **M** changes cell to Markdown, **Y** back to code
- ◆ **X** or **DD** deletes a cell, **a** adds above **b** adds below
- ◆ **Shift+Tab** will show short info on method on that line
- ◆ **?<cmd>** will show help for <cmd>
- ◆ **Crtl+Shift+-** split cell at cursor pos
- ◆ **Shift+down/up** to select cells down/upwards, then **Shift+M** to merge
- ◆ **ESC+O** to toggle cell output
- ◆ <https://jupyter-notebook.readthedocs.io/en/stable/notebook.html>

- ❖ no need to declare type of variable explicitly



# Basics in Julia

- ◆ # is used for comments, #= ....=# for mulit-line comments
- ◆ simple math is straightforward (+-\*%^%)
- ◆ strings are declared by “string” or “””string”””
  - ◆ can be concatenated, indexed like arrays
- ◆ Test this with the notebook “notebookJupyterCMDs”

The screenshot shows a Jupyter Notebook interface running on a Mac OS X system. The top bar includes tabs for 'work/' (active), 'firstNotebook', and 'Untitled'. The address bar indicates the URL is `localhost:8888/notebooks/work/Untitled.ipynb?kernel_name=julia-1.0#String-concatenation`. The title bar says 'jupyter Untitled Last Checkpoint: 2 hours ago (unsaved changes)'. The toolbar includes File, Edit, View, Insert, Cell, Kernel, Widgets, Help, Trusted (status), and Julia 1.0.0 (status). Below the toolbar is a toolbar with icons for file operations like new, open, save, and run.

The notebook content consists of several code cells:

- In [ ]: 

```
myFirstName = "Chris"
myLastName = "Stricker"
myCountry = "Switzerland"
numberParticipants=28
numberInstructors=3;
```
- In [ ]: 

```
# $ is used for string interpolation
println("My name is $myFirstName, and I live in $myCountry.")
```
- In [ ]: 

```
# without string interpolation
println("My name is ",myFirstName," and I live in ", myCountry,".)")
```
- In [ ]: 

```
# Interpolating other types of variables works too
println("There are currently $(numberParticipants+numberInstructors) people in this room.")
```
- ### ### String concatenation and indexing
- In [ ]: 

```
string(myFirstName, " ",myLastName)
```
- In [ ]: 

```
myFirstName*" "*myLastName
```
- In [ ]: 

```
"$myFirstName $myLastName"
```
- In [ ]: 

```
myFirstName[1]
```
- In [ ]: 

```
myFirstName[end]
```
- In [ ]: (empty cell)

# Basics in Julia (<https://julialang.org/>)

- ◆ File I/O (*notebook\_IO\_DataFrames*)
- ◆ adding packages
  - ◆ Pkg.add(), Pkg.update()
  - ◆ using <pkgName>
- ◆ **DataFrames** (*notebook\_IO\_DataFrames*)
- ◆ strings, arrays, dictionaries, tuples (*notebook\_StringsArraysDictPlotting*)
- ◆ plotting (*notebook\_StringsArraysDictPlotting*)
  - ◆ many plotting packages available (*PyPlot*, *Gadfly*, *Plots*, *Winston*, *StatPlots*, *Vega*, *Plotly*, *Plotlyjs*,....), not all of them ported to Julia 1.0 yet
  - ◆ will show how to use plots and gadfly by example

# References

- ◆ <https://docs.julialang.org/en/v1/index.html>
- ◆ <https://juliabyexample.helpmanual.io/>
- ◆ <https://syl1.gitbook.io/julia-language-a-concise-tutorial/>
- ◆ <https://jupyter-notebook.readthedocs.io/en/stable/notebook.html>