

TODAY'S TALK

Brief Outline

- · Docker Intro: Appeal of Containers, "Lego" blocks, ...
- · Brief Overview of Docker and its commands
- Building and Customizing via two "blogged" examples
 - · Debug with gcc-9 on macOS
 - · Easy installation of "heavy" packages
- · Going Further: More about Rocker

Rocker, Nov'19 2/55

DOCKER

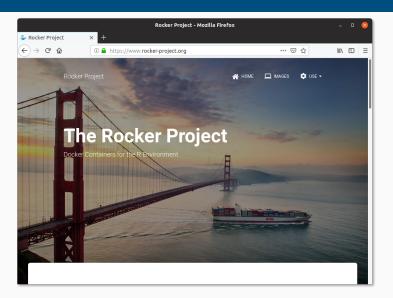
A Personal Timeline

- Docker itself started in 2013
- I started experimenting with it around spring of 2014
- Was convinced enough to say 'will change how we build and test' in keynote at useR! 2014 conference in mid-2014
- · Started the Rocker Project with Carl Boettiger fall 2014
- Gave three-hour tutorial at useR! in 2015
- · Active development of multiple (widely-used) containers

Introductory paper in R Journal, 2017

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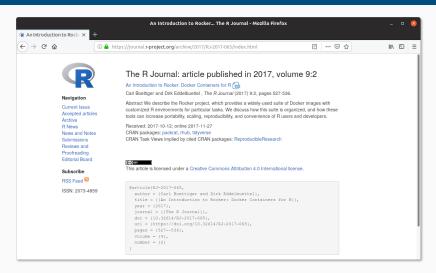
ROCKER PROJECT



Source: https://www.rocker-project.org

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ROCKER PAPER



Source: https://journal.r-project.org/archive/2017/RJ-2017-065/index.html

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CONTRIBUTED RESEARCH ARTICLE

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An Introduction to Rocker: Docker Containers for R

by Carl Boettiger, Dirk Eddelbuettel

Abstract We describe the Rocker project, which provides a widely-used suite of Docker images with customized R environments for particular tasks. We discuss how this suite is organized, and how these tools can increase portability, scaling, reproducibility, and convenience of R users and developers.

Introduction

The Rocker project was launched in October 2014 as a collaboration between the authors to provide high-quality Docker images containing the R environment (Boetige and Eddebuetle, 2014). Since that time, the project has seen both considerable uptake in the community and substantial development and evolution. Here we seek to document the project objectives and uses.

What is Docker?

Docker is a popular open-source tool to create, distribute, deploy, and run software applications using containers. Containers provide a virtual environment (see Clark et al. (2014) for an overview of common virtual environments) requiring all operating-system components an application needs to common virtual environments) requiring all operating-system components an application needs to the nun-Docker containers are lightweight as they share the operating system kernel, start instantly using a layered filesystem which minimizes disk footprint and download time, are built on open standards at run on all major platforms (Linux, Mao, Windows), and provide an added layer of security by running an application in an isolated environment (Docker, 2015). Familiarity with a few key terms is helpful in understanding this paper. The term' container' refers to an isolated software environment on a computer. R users can think of running a container as an analogous to loading an R package; a container is an active instance of a static Docker image. A Docker "image" is a binary article of that the container is an active instance of a static Docker image. A Docker "image" is a brinary active of that container is an active instance of a static Docker image. A Docker image is a brinary active of that container is an active instance of these Docker image. The public dy available through Docker thus, which plays a role for central distribution similar to CRAN in our analogy. Development and contributions to the Rocker project focus on the construction, organization and maintenance of these Dockerilles.

Source: https://journal.r-project.org/archive/2017/RJ-2017-065/index.html

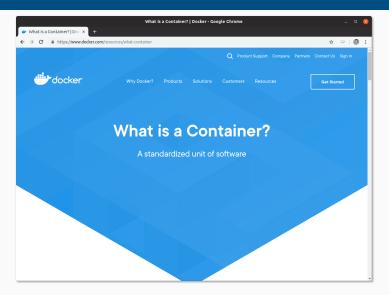
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DOCKER

So what is it?

- Think of its 'containers' as something portable like a zipfile
- · A 'container' allows you to execute code based on what is in it
- · Portable: same container used on Linux, Window, macOS
- However this really shines on Linux:
 - · as it requires only a very thin layer above the operating system
 - · on macOS and Windows intermediating layer has to be provided
 - · heavy usage in cloud deployments
- · Still, what is phenomenal are the
 - · portability
 - encapsulation
 - security
 - reproducibility

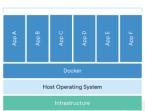
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Source: https://www.docker.com/resources/what-container

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Package Software into Standardized Units for Development, Shipment and Deployment

A container is a standard unit of software that packages up code and all its dependencies so the application runs quickly and reliably from one computing environment to another. A Docker container image is a lightweight, standalone, executable package of software that includes everything needed to run an application; code, runtime, system tools, system libraries and settling.

Container images become containers at runtime and in the case of Docker containers - images become containers when they run on Docker Engine. Available for both Linux and Windows-based applications, containerized software will always run the same, regardless of the infrastructure. Containers isolate software from its environment and ensure that it works uniformly despite differences for instance between development and staging.

Docker containers that run on Docker Engine:

- Standard: Docker created the industry standard for containers, so they could be portable anywhere
- Lightweight: Containers share the machine's OS system kernel and therefore do not require an OS per application, driving higher server efficiencies and reducing server and licensing costs
- Secure: Applications are safer in containers and Docker provides the strongest default isolation capabilities in the industry

Source: https://www.docker.com/resources/what-container

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Docker Containers Are Everywhere: Linux, Windows, Data center, Cloud, Serverless, etc.

Docker container technology was launched in 2013 as an open source Docker Engine.

It leveraged existing computing concepts around containers and specifically in the Linux world, primitives known as agroups and namespaces. Docker's technology is unique because it focuses on the requirements of developers and systems operators to separate application dependencies from infrastructure.

Success in the Linux world drove a partnership with Microsoft that brought Docker containers and its functionality to Windows Server (sometimes referred to as Docker Windows containers).

Technology available from Docker and its open source project, Moby has been leveraged by all major data center vendors and cloud providers. Many of these providers are leveraging Docker for their container-native laaS offerings. Additionally, the leading open source serverless frameworks utilize Docker container technology. Docker Today

Linux Windows Datacenter Cloud

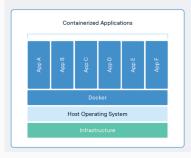
Source: https://www.docker.com/resources/what-container

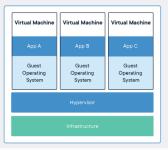
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Comparing Containers and Virtual Machines

Containers and virtual machines have similar resource isolation and allocation benefits, but function differently because containers virtualize the operating system instead of hardware.

Containers are more portable and efficient.





Source: https://www.docker.com/resources/what-container

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DOCKER IN SIMPLEST TERMS

Simplifying Somewhat:

- · A container can run a single process
 - (as opposed to a virtual machine behaving more like a whole computer system)
- · So it helps to think of Docker encapsulating a single command
 - · (though that command may spawn more commands)
- Docker containers can be orchestrated and combined
 - · each container can provide its services on a network port
 - · common pattern may be one for database, one for webserver, ...)

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DOCKER 'TERMINOLOGY'

Some Informal Definitions

- Image is a provided Docker run-time; can be built locally or downloaded
- Container is (possibly) stateful instance of a container, either running or suspended
- We will be a little sloppy and use container and image interchangeably
- On the hand, a virtual machine, on the hand, tends to be a heavier software layer provide a full virtual system. VMware and VirtualBox are two well-known systems.

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DOCKER: BASIC COMMANDS

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Basic commands

- · docker help lists the available commands
- docker images lists installed images
- docker run runs a container (with extra args, see below)
- · docker ps shows currently running containers
- docker pull someuser/somecontainer:version imports container (version optional; latest is default)
- docker build to create a new container
- · docker rm container removes a container
- docker rmi imageid removes an image

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docker images

- · list installed containers, versions, sizes
- very helpful for quick overview
- · can also list sub-sets per repository and/or tag

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docker run

- Bread and butter command to use Docker
- · Common arguments
 - · --rm to remove artifacts after run ("clean up")
 - · -ti to add terminal and interactive use
 - · -v LocalDir:MountedDir to make local dir available
 - · -w WorkDir to switch to workdir
 - · -р 8787:8787 to publish container port 8787 as host port 8787
 - · container/tag:version
 - · cmdline arguments for container application
 - · plus many more options so see documentation

· When named container is not locally installed it is pulled

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docker pull (and docker commit)

- · Main command to obtain images from repository / registry
- By default uses hub.docker.com / cloud.docker.com registries
- Note that pulled containers can be altered and saved via docker commit

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docker pull (and docker commit)

- · Main command to obtain images from repository / registry
- By default uses hub.docker.com / cloud.docker.com registries
- Note that pulled containers can be altered and saved via 'docker commit'

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docker build

- Principal command to create new images
- · Containers are 'layered':
 - easy to start from existing container making small change
 - · creating new augmented or adapted container
- · Input is a text file Dockerfile
- Many tutorials available to get started

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USE CASE ILLUSTRATIONS

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SIMPLE DOCKER EXAMPLES

Use multiple R versions

- E.g. test an R package against multiple R releases
- test code against current and development versions of tools
- \cdot access to different R versions via different $r ext{-base}$ containers
- just specify different tags for different R versions
- · (Rocker also has another stack for explicitly versioned images)

```
$ docker run --rm -ti r-base:latest R --version | head -1
R version 3.6.1 (2019-07-05) -- "Action of the Toes"
$ docker run --rm -ti r-base:3.5.3 R --version | head -1
R version 3.5.3 (2019-03-11) -- "Great Truth"
$ docker run --rm -ti r-base:3.4.2 R --version | head -1
R version 3.4.2 (2017-09-28) -- "Short Summer"
$
```

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SIMPLE DOCKER EXAMPLES

Test against development versions

- · Sometimes we want to test against new development versions
- These versions may still be unfinished and undergo changes
- This makes using them in a 'sandbox' ideal great container use

```
edd@rob:~$ docker run --rm -ti rocker/drd:latest RD --version | head -4
R Under development (unstable) (2019-11-23 r77455) -- "Unsuffered Consequences"
Copyright (C) 2019 The R Foundation for Statistical Computing
Platform: x86_64-pc-linux-gnu (64-bit)
edd@rob:~$
```

(This shows the November 23 sources of R-devel. So with very little effort we get access to recent development versions—as the container builds are triggered weekly by a a **crontab** entry invoking a web trigger at hub.docker.com.)

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SIMPLE DOCKER EXAMPLES

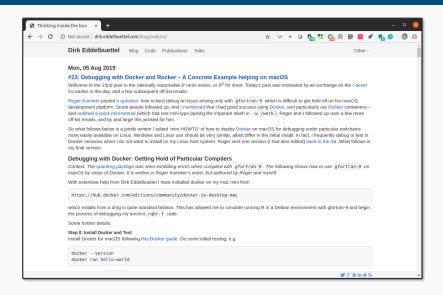
Test with special versions

- · We have R containers for 'undefined behavior sanitizer' (UBSAN)
- This uses R built with particular compilation options which can detect 'undefined behavior'
- · Similarly, R has another checker 'rchk' and a container

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MOTIVATING EXAMPLES

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Context

- · Roger Koenker gets CRAN email about issue with a new compiler
- · He works on macOS without easy access to new gcc versions
- · Building gcc from source a bit painful
- But what if we could just run it?
- I email Roger, give some pointers and hints ...
- · ... and he fixed the issue
- · So we wrote a blog post

Rocker, Nov'19 27/5:

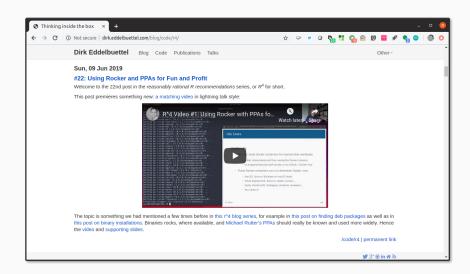
More detail (see the blog post for more)

- Step 0: Get Docker installed (which is easy-ish on mac/win/lin)
- Step 1: Install Rocker's r-base container with current R
- Step 2: Use Docker options -v0:I -wI to
 - map 'outer' dir O, say, ~/proj/abc to 'inner' I, say /work
 - start Docker session in 'inner' dir, say /work
- Step 3: Update with apt, install gcc-9 + gfortran-9
- · Step 4: Deal with build dependencies for the package
- Step 5: Set compiler flags in ~/.R/Makevars
- Step 6: Install R source package in question (here: quantreg)

Step 7: Debug issue at hand and solve problem

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USING ROCKER WITH PPAS



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More detail

- · This illustrates what we touched upon earlier
- · Installing, say, r-cran-rstan from binary is
 - · a single and fast step
 - as opposed to compiling from source
- · Another famous example also shown: r-cran-tidyverse
- Several blog posts describe approaches
- "Seeing is believing" so I made a video and slides
- Video demonstrates installation "live" and backed by slides

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DETAILED EXAMPLE: RSTAN

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We fire up our **r-base** container for a working basic R installation:

```
edd@rob:~$ docker run --rm -ti r-base
R version 3.5.3 (2019-03-11) -- "Great Truth"
Copyright (C) 2019 The R Foundation for Statistical Computing
Platform: x86 64-pc-linux-gnu (64-bit)
R is free software and comes with ABSOLUTELY NO WARRANTY.
You are welcome to redistribute it under certain conditions.
Type 'license()' or 'licence()' for distribution details.
  Natural language support but running in an English locale
R is a collaborative project with many contributors.
Type 'contributors()' for more information and
'citation()' on how to cite R or R packages in publications.
Type 'demo()' for some demos, 'help()' for on-line help, or
'help.start()' for an HTML browser interface to help.
Type 'q()' to quit R.
```

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Interactively, we ask R to install rstan

```
> install.packages("rstan")
Installing package into '/usr/local/lib/R/site-library'
(as 'lib' is unspecified)
'stringr', 'labeling', 'munsell', 'RColorBrewer', 'fansi', 'pillar', 'pkgconfig',
'backports', 'processx', 'assertthat', 'magrittr', 'digest', 'gtable', 'lazyeval',
'plyr', 'reshape2', 'rlang', 'scales', 'tibble', 'viridisLite', 'withr',
'matrixStats', 'checkmate', 'callr', 'cli', 'crayon', 'desc', 'prettyunits', 'R6',
'rprojroot', 'ggplot2', 'StanHeaders', 'inline', 'gridExtra', 'Rcpp', 'loo',
'pkgbuild', 'RcppEigen', 'BH'
trying URL 'https://cloud.r-project.org/src/contrib/glue 1.3.1.tar.gz'
Content type 'application/x-gzip' length 122950 bytes (120 KB)
downloaded 120 KB
trying URL 'https://cloud.r-project.org/src/contrib/stringi_1.4.3.tar.gz'
Content type 'application/x-gzip' length 7290890 bytes (7.0 MB)
downloaded 7.0 MB
[... many more downloads omitted ...]
```

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We ask R to install **rstan** (continued)

```
[... quite a bit of compilation later ...]
g++ -std=gnu++14 -shared -L/usr/lib/R/lib -Wl,-z,relro -o rstan.so chains.o init.o lang ast def.o
lang_grammars_bare_type_grammar_inst.o lang_grammars_expression07_grammar_inst.o
lang grammars expression grammar inst.o lang grammars functions grammar inst.o
lang grammars indexes grammar inst.o lang grammars program grammar inst.o
lang_grammars_semantic_actions.o lang_grammars_statement_2_grammar_inst.o
lang_grammars_statement_grammar_inst.o lang_grammars_term_grammar_inst.o
lang grammars var deccls grammar inst.o lang grammars whitespace grammar inst.o misc.o
pointer-tools.o sparse extractors.o stanc.o -L/usr/lib/R/lib -lR
installing to /usr/local/lib/R/site-library/rstan/libs
** R
** inst
** byte-compile and prepare package for lazy loading
** help
*** installing help indices
*** copving figures
** building package indices
** installing vignettes
** testing if installed package can be loaded
* DONE (rstan)
The downloaded source packages are in '/tmp/Rtmpo38sEg/downloaded packages'
5
```

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We ask R to install rstan (continued)

```
> library(rstan)
Loading required package: ggplot2
Use suppressPackageStartupMessages() to eliminate package startup
messages.
Loading required package: StanHeaders
rstan (Version 2.18.2, GitRev: 2e1f913d3ca3)
For execution on a local, multicore CPU with excess RAM we recommend calling
options(mc.cores = parallel::detectCores()).
To avoid recompilation of unchanged Stan programs, we recommend calling
rstan_options(auto_write = TRUE)
>
```

Now we run **rstan** in this interactive R session. Can we persist it?

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We are in a docker container. Let's ask docker ps:

```
edd@rob:~$ docker ps
CONTAINER ID IMAGE
                        COMMAND
                                   CREATED
                                                    STATUS
                                                                      PORTS
                                                                               NAMES
b236f06518b5 r-base
                                   29 minutes ago Up 29 minutes
                                                                               loving neumann
edd@rob:~$
edd@rob:~$ docker commit --author "<dirk@eddelbuettel.com>" --message "rstan demo container" \
     b236f06518b5 local-rstan
                                  ## continer id here key, refers back to the running container
sha256 d72f105h396ff99400618h2d527332af2ah5fa4h45ce88ea7aaa7a5e813a9c87
edd@rob:~$
edd@rob:~$ docker images | grep stan
local-rstan
                                                d72f105b396f
                            latest
                                                                    19 seconds ago
                                                                                         1.23GB
edd@rob:~$
```

So **docker** commit can create a new container image under a new name – perfect for interactively modifying containers.

NB: Some whitespace removed, and lines reindented for display

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```
edd@rob:~$ docker run --rm -ti local-rstan
R version 3.5.3 (2019-03-11) -- "Great Truth"
Copyright (C) 2019 The R Foundation for Statistical Computing
Platform: x86 64-pc-linux-gnu (64-bit)
[...1
Type 'demo()' for some demos, 'help()' for on-line help, or
'help.start()' for an HTML browser interface to help.
Type 'a()' to quit R.
> library(rstan)
Loading required package: ggplot2
Loading required package: StanHeaders
rstan (Version 2.18.2. GitRev: 2e1f913d3ca3)
For execution on a local, multicore CPU with excess RAM we recommend calling
options(mc.cores = parallel::detectCores()).
To avoid recompilation of unchanged Stan programs, we recommend calling
rstan_options(auto_write = TRUE)
```

Run the new one

We containerized an application!

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ALTERNATIVE: USE A DOCKERFILE

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A 'Dockerfile' is the standard way to build a container

```
## Start from rocker's r-base or official r-base
FROM rocker/r-base:latest
## Handle for maintainer; these days using LABEL is preferred
MAINTAINER "Dirk Eddelbuettel" dirk@eddelbuettel.com
## Install rstan (downloads and builds all dependencies)
RUN Rscript -e 'install.packages("rstan")'
## Make R the default
CMD ["R"]
```

Rocker, Nov'19 39/55

Building it

· Usually in a directory containing a Dockerfile

docker build --tag rocker-rstan .

- Lots of other options
- Once built we can push to a repository
- Excellent alternative:
 - · Dockerfile at GitHub
 - · Build setup at cloud.docker.com (or hub.docker.com)

· Automatic build and provisioning by Docker

Rocker, Nov'19 40/55

Building it from .deb binaries – "Lego" again as we reuse binaries

- A useful (if little known) alternative is to lean on the binaries
- Mentioned in my blogposts from Dec 2017 and June 2019
- · Simpler, faster & more failsafe as binaries and deps *pre-built*

```
## Start from Rocker container bsaed around Rutter PPAs
FROM rocker/r-ubuntu:18.04

## Handle for maintainer; these days using LABEL is preferred
MAINTAINER "Dirk Eddelbuettel" dirk@eddelbuettel.com

## Update and install rstan -- from binary
RUN apt-get update && apt-get install -y --no-install-recommends r-cran-rstan

## Make R the default
CMD ["R"]
```

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More to know

- · You can include multiple RUN commands:
 - · each produces a separate 'layer' cached during build
 - · layers are applied consecutively and can be reused
- Other arguments:
 - · COPY to transfer file from build area into container
 - ENV to set environment variables
 - PORT to provide network access to a given port (great for 'backend' services like databases or other servers)
 - · ... and much much more
- · More details at Best practices for writing Dockerfile

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DOCKER HUB / DOCKER CLOUD

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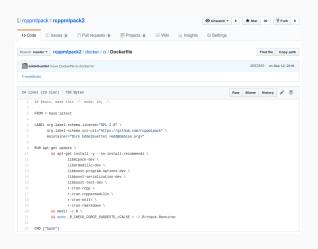
DOCKER HUB / DOCKER CLOUD

Clould Support for Building Docker Containers

- · Branding is a little inconsistent and flips back and forth
- · But in essence another excellent and free service:
 - · Create a repo on GitHub
 - · Create an account Docker Hub / Docker Cloud
 - · Define an automated build linking Docker Hub to GitHub
- Then (easiest setting) each commit at GitHub triggers new build
- Very useful (though at times 'laggy' / buys queue)

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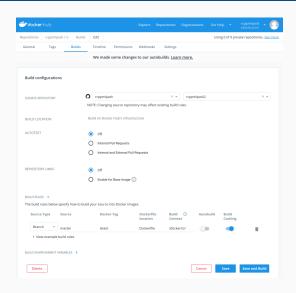
DOCKER HUB / DOCKER CLOUD: GITHUB REPO



GitHub source repository (for R package requiring external MLPACK machine learning library) with definition for Dockerfile used for testing same repository.

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DOCKER HUB / DOCKER CLOUD: DOCKER HUB

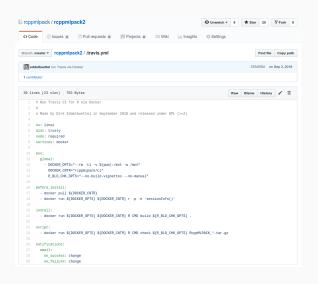


Simple Docker Hub setup to tie automatic builds to a GitHub repository.

More complicated dependency-triggered builds also possible.

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DOCKER HUB / DOCKER CLOUD: USE IN TRAVIS CI



In essence, we use the Docker container (defined in this repo but built by the Docker Hub) to run continuous integration via Travis CI.

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ROCKER USE CASES

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CONTAINERIZATION

Some Examples

- 'Difficult' or 'Large' Things: Rocker Project has long maintained large 'tidyverse', geospatial, … containers and more
- · 'Applications' as for example RStudio Server or Shiny Server
- · 'Frameworks' adding Machine Learning / Tensorflow containers

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REPRODUCIBILITY

Some Examples

- One key part of Rocker are the versioned containers using the snapshot 'MRAN' archive provided by Microsoft
- This gives the ability to 'freeze' a container with software at a given release point
- Reproducibility: 'turn research study into container'; and containerit does that
- · Using mybinder.org is another possibily using holepunch

Rocker, Nov'19 50/5:

OTHER TOPICS

Rocker, Nov'19 51/55

More Docker

Things we did not cover

- Composition: Orchestrating multiple containers has become a big topic, Kubernetes is a key application here (c.f. next talk)
- Docker variants and spin-offs: containerd is part of the Docker backend and has been spun off; there is a fair amount going on but Docker has first-mover advantage and mind-share
- Docker for science: a somewhat simpler approach called singularity has made inroads

· And much much more...

Rocker, Nov'19 52/55

LEARN MORE ABOUT DOCKER

Some Pointers

- · A Docker 101 course
- Several usage samples
- · R on Docker tutorial from rOpenSci
- My (possibly dated in parts) three hour tutorial from useR! 2015

· For Rocker: Boettiger and Eddelbuettel, 2017, RJournal

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LEARNING BY DOING





Details

https://events.docker.com/events/details/docker-chicago-presents-hands-on-workshop-introduction-to-docker-for-developers/

Join us for the Chicago local edition of this season's global hands-on workshop series! Food and drinks will be provided! Bring your laptop and #LearnDocker. There will be swag!

Docker has (or had) some meetups in Chicago; this is AFAIK the first in a while.

Give it a go!

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THANK YOU!

```
slides http://dirk.eddelbuettel.com/presentations/
  web http://dirk.eddelbuettel.com/
  mail dirk@eddelbuettel.com
github @eddelbuettel
twitter @eddelbuettel
```

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