

A Brief/Partial Introduction for R Users

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satRday Chicago Virtual Conference

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http://dirk.eddelbuettel.com/papers/satRday\_chicago2020\_rocker.pdf

## TODAY'S TALK

#### **Brief Outline**

- · Docker Intro: Appeal, Motivation, "Lego" blocks, ...
- · Brief Overview of Docker and its commands
- · Going Further: More about Rocker

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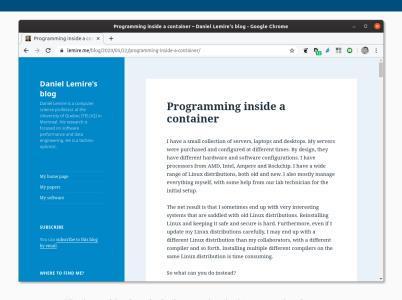
## **DOCKER**

#### 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
- Most recent talk at Chicago RUG Nov 2019

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#### MOTIVATION



#### **MOTIVATION**

## Excellent discussion by Daniel Lemire

The idea of a container approach is to always start from a pristine state. So you define the configuration that your database server needs to have, and you launch it, in this precise state each time. This makes your infrastructure predictable.

We can of course substitute "predictable" with "reproducible" ...

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## ON IN SIMPLER TERMS:

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## ON IN SIMPLER TERMS:



#### ON IN SIMPLER TERMS:

#### A box

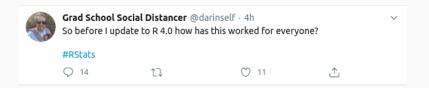
- · Standardized shape and form, identical for everyone
- · "Take it anywhere, useable by everyone"
- Genius of "if someone can run a box they can run your box"
- Examples or running
  - RStudio Server on an OS that RStudio does not provide it for
     (!!)
  - · Shiny Server on an OS that RStudio does not provide it for (!!)
  - other standardized setups your colleagues, PIs, students, ...
     cannot setup or maintain

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## Now why the fiddle do I care?

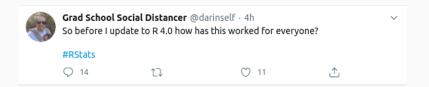
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## Now why the fiddle do I care?



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## Now why the fiddle do I care?



## Perfect for a pristine box:

- get R 4.0.0 "in a box"
- · put your code in

· check!

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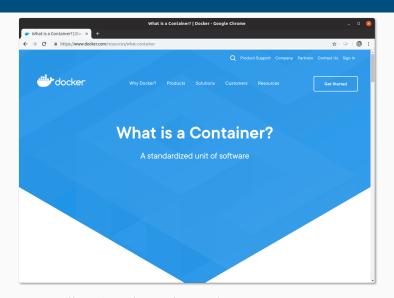
## **DOCKER**

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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:
  - · it requires only a very thin layer above the operating system
  - on macOS and Windows intermediating layer has to be provided
  - · hence very heavy Linux usage in cloud deployments
- · What is phenomenal are the
  - portability
  - encapsulation
  - security
  - reproducibility

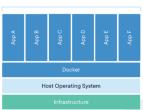
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Source: https://www.docker.com/resources/what-container

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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 to 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 settlings.

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.

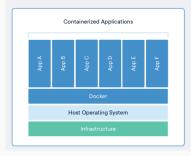
Source: https://www.docker.com/resources/what-container

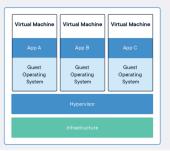
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#### **Comparing Containers and Virtual Machines**

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
  - not a virtual machine that is more like a whole computer system
- · So it helps to think of Docker encapsulating a single command
  - though that first 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,

...

## 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 sloppy and use container and image interchangeably
- · On the other hand, a virtual machine tends to be
  - · a heavier software layer providing a full virtual system
  - VMware and VirtualBox are two well-known systems.

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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
  - -p 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 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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## 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
- more advanced use use of different R builds is also possible

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## Use multiple R versions

```
$ docker run --rm -ti r-base:latest R --version | head -1
R version 4.0.0 (2020-04-24) -- "Arbor Day"
$ docker run --rm -ti r-base:3.6.3 R --version | head -1
R version 3.6.3 (2020-02-29) -- "Holding the Windsock"
$ 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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## Use multiple R versions (and an alias dkrr)

```
$ dkrr r-base:latest R --version | head -1
R version 4.0.0 (2020-04-24) -- "Arbor Day"
$ dkrr r-base:3.6.3 R --version | head -1
R version 3.6.3 (2020-02-29) -- "Holding the Windsock"
$ dkrr r-base:3.5.3 R --version | head -1
R version 3.5.3 (2019-03-11) -- "Great Truth"
$ dkrr r-base:3.4.2 R --version | head -1
R version 3.4.2 (2017-09-28) -- "Short Summer"
$
```

which generalizes to the the triplet:

## dockerCommand dockerContainer args

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## Test against development versions

- Sometimes we want to test against new development versions
- These versions may still be unfinished and undergo changes
- · Containers provide ideal use via a 'sandbox'

```
edd@rob:~$ docker run --rm -ti rocker/drd:latest RD --version | head -4
R Under development (unstable) (2020-05-23 r78555) -- "Unsuffered Consequences"
Copyright (C) 2020 The R Foundation for Statistical Computing
Platform: x86_64-pc-linux-gnu (64-bit)
edd@rob:~$
```

(This shows the May 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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## **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 (coming soon!)

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#### REPRODUCIBILITY

## Some Examples

- · Key part of Rocker are versioned containers
  - · use dated snapshots of CRAN archives
  - · gives ability to 'freeze' container at a given release point

#### Allows for add-ons

- Reproducibility: 'turn research study into container'
  - e.g. containerit does that
  - or mybinder.org is another possibility using holepunch

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## 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...

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So ...

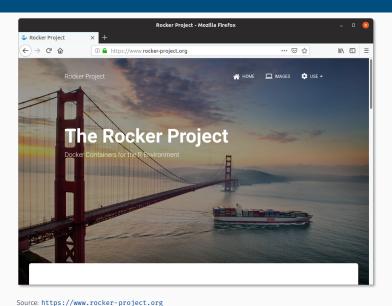
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## THAT BOX ANALOGY

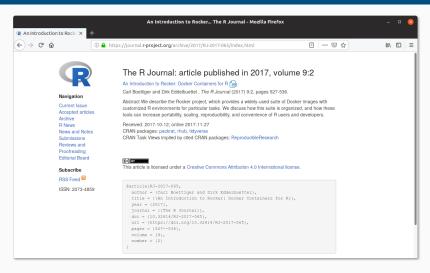


 $Source: \verb|https://commons.wikimedia.org/wiki/File:Pralinenteller_-_box_of_chocolates.jpg| satRday Chicago 2020$ 

## **ROCKER PROJECT**



#### **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 that 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 of 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 statle Docker image. A Docker 'image' is a binary article of the base of the container is an extensive of that the container is an extensive of that the container is an extensive of the container is an extensive of the container of the container of the property of the control of the container of the container of the property of the control of the container of the

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

## **ROCKER TEAM**

## Team







The Rocker project was created by Carl Boettiger and Dirk Eddelbuettel, and is now maintained by Carl, Dirk, and Noam Ross, with significant contributions from a broad community of users and developers. Get in touch on GitHub issues with bug reports, feature requests, or other feedback.

Source: https://rocker-project.org

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#### LEARN MORE ABOUT DOCKER

#### Some Pointers

- A Docker 101 course
- Several usage samples
- R on Docker tutorial from rOpenSci
- My (maybe dated in parts) three hour tutorial from useR! 2015
- For Rocker: Boettiger and Eddelbuettel, 2017, RJournal

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## Julia Evans

#### **New zine: How Containers Work!**

On Friday I published a new zine: "How Containers Work!". I also launched a fun redesign of wizardzines.com.

You can get it for \$12 at https://wizardzines.com/zines/containers. If you buy it, you'll get a PDF that you can either print out or read on your computer. Or you can get a pack of all 8 zines so far.

Here's the cover and table of contents:



#### table of contents

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## Zine by Julia Evans

\$12 likely well-spent

have not seen zine

but have enjoyed several posts

See https://jvns.ca/blog/ 2020/04/27/new-zine-howcontainers-work/

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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
```