



Container-driven Reproducible Research Made Simple

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A little about me...



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- 3rd year PhD in Statistics & Applied Probability





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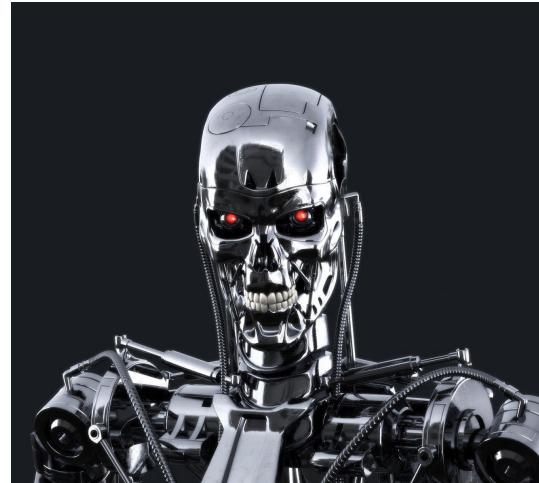
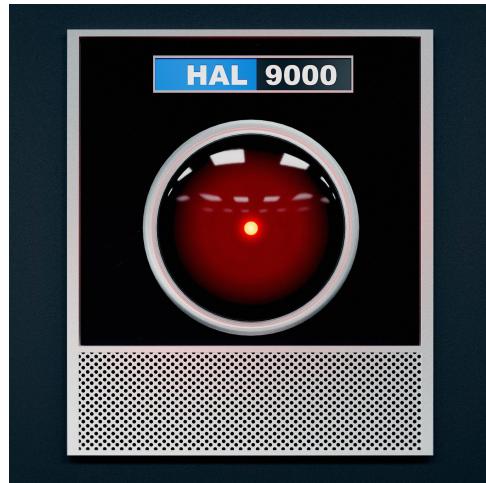
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- Background: Computer Science, Applied Mathematics





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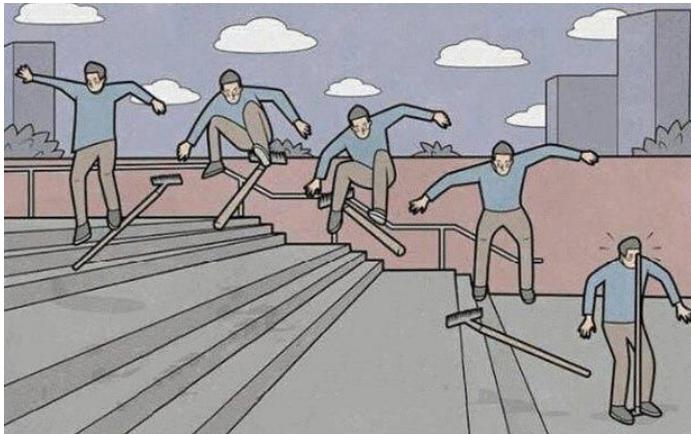
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- 3rd year PhD in Statistics & Applied Probability
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- As with most things, tripped, stumbled, and fell into this project by good fortune during my 2nd year





A little about me...

- 3rd year PhD in Statistics & Applied Probability
- Background: Computer Science, Applied Mathematics
- Interests: software development, reproducibility/explainability in ML
- As with most things, tripped, stumbled, and fell into this project by good fortune during my 2nd year
- Since then I have built tooling, created documentation, and ran workshops/trainings for the department to spread the good words of containerized research





Reproducibility

“An article about computational science in a scientific publication is not the scholarship itself, it is merely advertising of the scholarship. The actual scholarship is the complete software development environment and the complete set of instructions which generated the figures.”

Buckheit & Donoho [1]

Reproducibility

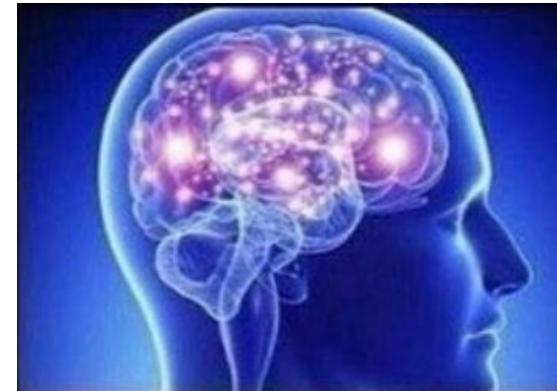
- An honorable task... one that requires effort and care in practice
- Simple truth: reproducibility is *hard*
- As a result, it is usually a burden or an afterthought





Reproducibility Options – Good

- Naïve solution: README with dependency instructions
 - e.g. sf package in R → relies on multiple manually configured dependencies (geos, gdal, proj)
 - Ok (at best): In depth test of reading comprehension
 - Con: Assumes in depth knowledge on the part of maintainer and user





Reproducibility Options – Better

- Naïve solution: README with dependency instructions
 - e.g. sf package in R → relies on multiple manually configured dependencies (geos, gdal, proj)
 - Ok (at best): In depth test of reading comprehension
 - Con: Assumes in depth knowledge on the part of maintainer and user
- Language Package Managers
 - e.g. requirements.txt, environment.yml, package-lock.json, etc.
 - Pro: Simple to use, usually built in with language or environment (Anaconda)
 - Con: Depends on underlying OS, not language agnostic, “works on mine, not on thine”





Reproducibility Options – Complete

- Naïve solution: README with dependency instructions
 - e.g. sf package in R → relies on multiple manually configured components
 - Ok (at best): In depth test of reading comprehension
 - Con: Assumes in depth knowledge on the part of maintainer and user
- Language Package Managers
 - e.g. requirements.txt, environment.yml, package-lock.json, etc.
 - Pro: Simple to use, usually built in with language or environment (Anaconda)
 - Con: Depend on underlying OS, not language agnostic, "works on mine, not on thine"
- Virtual Machines
 - Emulation/virtualization of a computer from hardware to software (computer in computer)
 - e.g. VirtualBox, VMWare
 - Pro: Portable via images, fully reproducible from ground up
 - Con: "If you wish to make an apple pie from scratch, you must first invent the universe."
~ Carl Sagan





Reproducibility Options – Just right...

- Containerization
 - Benefits of a VM, usage similar to a package manager
 - Access to full system resources – minimum overhead
 - No hypervisor needed to manage system resources
 - Contains *just* the required packages and configuration (OS/language(s)/packages/tools)
 - Only abstracts away software applications
 - Each container is isolated from the system and from each other (in some cases, other users)
 - e.g. 3 containers for separate projects with different language versions and dependencies
 - Easily shareable for other people to spin up and use
 - Widely used in software engineering for the specific purpose of isolating applications and development environments





Why use containers for research?

- Scenario 1:
 - Want two different versions of R
 - Non-trivial task – will likely require you to build R from source or use renv
 - Solution: Can use RStudio professional or Anaconda
- Scenario 2:
 - Attempting to install dependencies for a research project via a package manager...
 - ...only to realize it will *only* run on a Unix system
 - Solution: Shell out for a Macbook or install Linux
- Scenario 3:
 - A new student joins your lab and needs to get ramped up on an existing project
 - Will need to replicate language, package, and tool configurations...
 - Solution: Either leave them to their own devices or sit down and take time ironing out their configuration given their unique system
- Impossible to address all these scenarios at once



Why use containers for research?

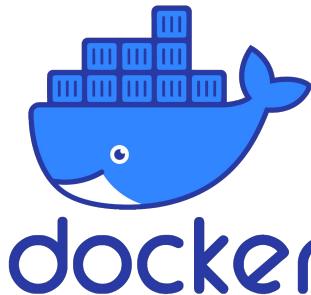
- Reproducibility should be something we simply do everyday
- Be able to configure a wide range of languages, packages, and development tools
- At the same time research should be available wherever you take or share it
- More than that it should be simple to use, run, and interface with
- ...as a result, we should dive straight into containers!





Containers for Reproducibility [2]

- Lightweight virtualization → Only requires a container engine (Docker/Podman/APPTAINER) for the underlying hardware
- Relies on a “Dockerfile” to completely define a working environment → easily portable between people and systems
- Can create arbitrary operating system, software, and language configurations





Containers for Reproducibility [2] (Example)

Dockerfile X

```
.devcontainer > Dockerfile
1  FROM ubuntu:latest
2
3  RUN apt-get update && apt-get install -y \
4      g++ \
5      git
6
7  WORKDIR /workspace
8
9  CMD ["bash"]
10
```

```
ronaldas > .devcontainer docker build -t my_awesome_container . &&
              docker run -it my_awesome_container
STEP 1/4: FROM ubuntu:latest
STEP 2/4: RUN apt-get update && apt-get install -y      g++      git
--> Using cache cdc10c83e5ae34f5220b5f9b7b1d5e22ed341f67a760de53b56bc63810199465
--> cdc10c83e5ae
STEP 3/4: WORKDIR /workspace
--> e3f5f9ea162d
STEP 4/4: CMD ["bash"]
COMMIT my_awesome_container
--> 4732f67f3271
Successfully tagged localhost/my_awesome_container:latest
4732f67f3271ab2dedf824632b5d71eeda18090c9b215abd00c273456507ed7b
root@7a3595cbcdb2:/workspace#
```

⚠️ Challenges – Docker CLI

- As you can see, we are interacting with terminal which is not ideal
- A more complex configuration using a Jupyter container:

```
docker run -it --rm -p 1000:8888 -v "${PWD}":/home/jovyan/work  
quay.io/jupyter/r-notebook:2024-10-07
```

- No easy way to manage containers other than learning yet another CLI tool
- Cumbersome! (and not even the most complicated configuration)
- Writing the actual configs can get complicated as well (more on that later)



Development Containers with Visual Studio Code

- “Development containers” (devcontainers) [3] simplify the process of interacting with and managing your containers
- Adds one additional spec file: devcontainer.json in it...
 - ...we can specify either a pullable image or a Dockerfile
 - ...configure build and run arguments
 - ...add development environment customizations through extensions
- This interfaces with Visual Studio Code (VS Code), a powerful integrated development environment that helps manage our containers, remote servers, and GitHub repositories through convenient extensions
- Our project software *and* development tools are now made easily reproducible, shareable, and (most importantly) interactive



Devcontainers with VS Code (Example)

Dockerfile X

```
.devcontainer > Dockerfile
1  FROM ubuntu:latest
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3  RUN apt-get update && apt-get install -y \
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```
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--> Using cache cdc10c83e5ae34f5220b5f9b7b1d5e22ed341f67a760de53b56bc63810199465
--> cdc10c83e5ae
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root@7a3595cbcdb2:/workspace#
```



Devcontainers with VS Code (Example)

Dockerfile X

```
.devcontainer > Dockerfile
1  FROM ubuntu:latest
2
3  RUN apt-get update && a
4      g++ \
5      git
6
7  WORKDIR /workspace
8
9  CMD ["bash"]
10
```

{} devcontainer.json X

```
.devcontainer > {} devcontainer.json > ...
1  {
2      "name": "My Dev Container",
3      "build": {
4          "dockerfile": "Dockerfile"
5      },
6      "customizations": {
7          "settings": {
8              "terminal.integrated.shell.linux": "/bin/bash"
9          },
10         "extensions": [
11             "ms-vscode.cpptools",
12             "ms-python.python"
13         ]
14     }
15 }
```



Devcontainers with VS Code (Example)

Dockerfile X

```
.devcontainer > Dockerfile
1  FROM ubuntu:latest
2
3  RUN apt-get update && a
4      g++ \
5      git
6
7  WORKDIR /workspace
8
9  CMD ["bash"]
10
```

{ devcontainer.json >

```
.devcontainer > { de
```

```
1  {
2      "name": "My Dev Container",
3      "build": {
4          "dockerfile": "Dockerfile"
5      },
6      "customizations": {
7          "settings": {
8              "terminal.integrated.shell.linux": "/bin/bash"
9          },
10         "extensions": [
11             "ms-vscode.cpptools",
12             "ms-python.python"
13         ]
14     }
15 }
```

i Folder contains a Dev Container configuration file. Reopen folder to develop in a container (learn more).

Source: Dev Containers

Reopen in Container

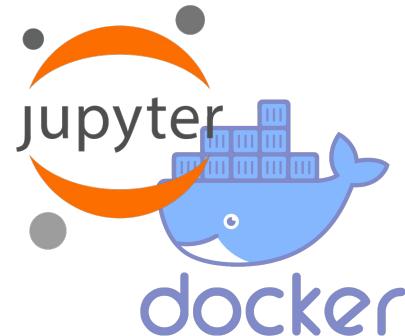
Don't Show Again...

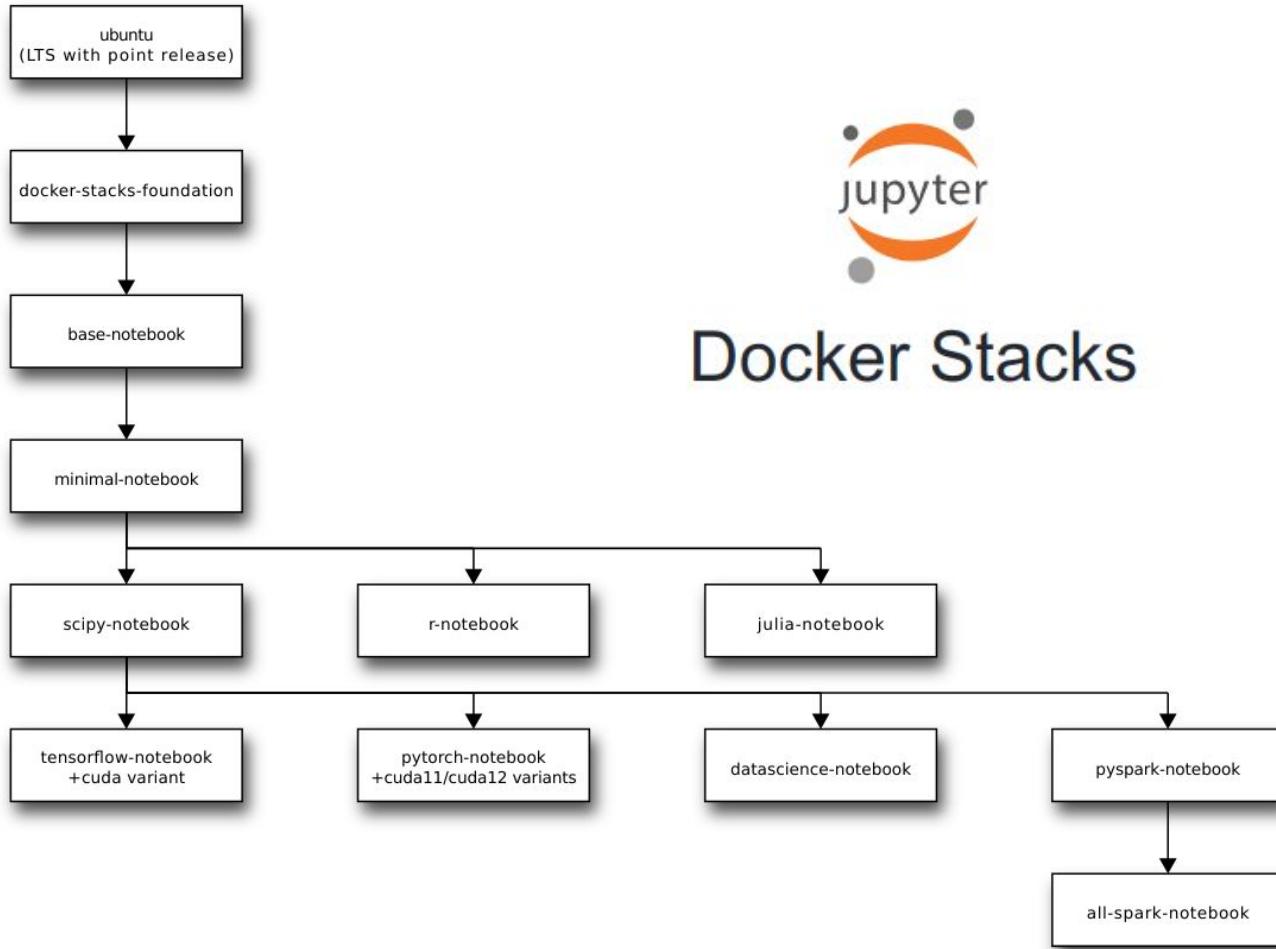




Devcontainers with VS Code (Jupyter Stacks)

- Previous container isn't too exciting so let's check out one with a built in RStudio server
- To do this we will use Jupyter Docker Stacks [4], a set of Docker images containing Jupyter apps and tools
- If you or your institution uses JupyterHub instances for students then you may have been using this the entire time without realizing it!





Docker Stacks

```
1 FROM quay.io/jupyter/r-notebook:r-4.3.1
2
3 ENV GITHUB_CLI_VERSION 2.30.0
4 ENV R_STUDIO_VERSION 2023.12.1-402
5
6 USER root
7
8 RUN apt-get update && \
9     apt-get install -y --no-install-recommends \
10    lmodern \
11    file \
12    curl \
13    g++ \
14    tmux \
15    psmisc \
16    libssl-dev \
17    libclang-dev \
18    libpq5 \
19    libtiff-dev \
20    && \
21
22 apt-get clean -y && \
23 rm -rf /var/lib/apt/lists/* /tmp/library-scripts
24
25 RUN R -e "dotR <- file.path(Sys.getenv('HOME'), '.R'); if(!file.exists(dotR)){ dir.create(dotR) }; Makevars <- file.path(dotR, 'Makevars'); file.create(Makevars); file.write(Makevars, 'CC=gcc CXX=g++')"; \
26 RUN R -e "dotRprofile <- file.path(Sys.getenv('HOME'), '.Rprofile'); if(!file.exists(dotRprofile)){ file.create(dotRprofile) }; file.write(dotRprofile, 'options(repr.plot.width=12, repr.plot.height=8)')"; \
27
28 RUN wget -q https://download2.rstudio.org/server/jammy/amd64/rstudio-server-${R_STUDIO_VERSION}-amd64.deb && \
29     apt-get install -yq --no-install-recommends ./rstudio*.deb && \
30     rm -f ./rstudio*.deb && \
31     apt-get clean && \
32     chmod 777 /var/run/rstudio-server && \
33     chmod +t /var/run/rstudio-server
34
35 USER ${NB_USER}
36
37 RUN mamba install -y -c conda-forge --freeze-installed \
38    jupyter-server-proxy=4.1.0 \
39    jupyter-rsession-proxy=2.2.0 \
40    && \
41 mamba clean --all
42
43 RUN pip install \
44    nbgitpuller radian==0.6.11 \
45    && \
46 jupyter labextension enable nbgitpuller
47
48 RUN R -q -e 'remotes::install_version("markdown", version="1.12", repos="cloud.r-project.org")' && \
49 R -q -e 'remotes::install_version("languageserver", version="0.3.16", repos="cloud.r-project.org")' && \
50 R -q -e 'remotes::install_version("httpgd", version="2.0.1", repos="cloud.r-project.org")' && \
51 R -q -e 'remotes::install_github("ManuelHentschel/vscDebugger")' && \
52 R -q -e 'remotes::install_version("syuzhet", version="1.0.7", repos="cloud.r-project.org")' && \
53 echo
54
55 RUN wget https://github.com/cli/cli/releases/download/v${GITHUB_CLI_VERSION}/gh_${GITHUB_CLI_VERSION}_linux_amd64.tar.gz -O - | \
56 tar xvzf - -C /opt/conda/bin gh_${GITHUB_CLI_VERSION}_linux_amd64/bin/gh --strip-components=2
57
58 RUN echo "echo \"Jupyter server token: \$(jupyter server list 2>&1 | grep -oP '(?=<token=)[[:alnum:]]*\')\" > ${HOME}/.get-jupyter-token" > ${HOME}/.bashrc
59 echo "sh ${HOME}/.get-jupyter-url.sh" >> ${HOME}/.bashrc
```

```
FROM quay.io/jupyter/r-notebook:r-4.3.1

ENV GITHUB_CLI_VERSION 2.30.0
ENV R_STUDIO_VERSION 2023.12.1-402

USER root

RUN apt-get update && \
    apt-get install -y --no-install-recommends \
        lmodern \
        file \
        curl \
        g++ \
        tmux \
        psmisc \
        lsb-release \
        libssl-dev \
        libclang-dev \
        libpq5 \
        libtiff-dev \
        && \
    apt-get clean -y && \
    rm -rf /var/lib/apt/lists/* /tmp/library-scripts

RUN R -e "dotR <- file.path(Sys.getenv('HOME'), '.R'); if(!file.exists(dotR)){ dir.create(dotR) }; Makevars <- file.path(dotR, \
RUN R -e "dotRprofile <- file.path(Sys.getenv('HOME'), '.Rprofile'); if(!file.exists(dotRprofile)){ file.create(dotRprofile) }";"

RUN wget -q https://download.rstudio.org/Windows/R-4.3.1/r-4.3.1-win.exe \
    apt-get install -yq --no-install-recommends \
    rm -f ./rstudio*.deb & \
    apt-get clean && \
    chmod 777 /var/run/rstudio-server && \
    chmod +t /var/run/rstudio-server

USER ${NB_USER}

RUN mamba install -y -c conda-forge --freeze-installed \
    jupyter-server-proxy=4.1.0 \
    jupyter-rsession-proxy=2.2.0 \
    && \
    mamba clean --all

RUN pip install \
    nbgitpuller \radian==0.6.11 \
    && \
    jupyter labextension enable nbgitpuller

RUN R -q -e 'remotes::install_version("markdown", version="1.12", repos="cloud.r-project.org")' && \
R -q -e 'remotes::install_version("languageserver", version="0.3.16", repos="cloud.r-project.org")' && \
R -q -e 'remotes::install_version("httpgd", version="2.0.1", repos="cloud.r-project.org")' && \
R -q -e 'remotes::install_github("ManuelHentschel/vscDebugger")' && \
R -q -e 'remotes::install_version("syuzhet", version="1.0.7", repos="cloud.r-project.org")' && \
echo

RUN wget https://github.com/cli/cli/releases/download/v${GITHUB_CLI_VERSION}/gh_${GITHUB_CLI_VERSION}_linux_amd64.tar.gz -O /opt/conda/bin/gh \
tar xvzf - -C /opt/conda/bin gh_${GITHUB_CLI_VERSION}_linux_amd64/bin/gh --strip-components=2

RUN echo "echo \"Jupyter server token: \$(jupyter server list 2>&1 | grep -oP '(?=<token=)[[:alnum:]]*')\" > ${HOME}/.get-jupyter-token" > ${HOME}/.get-jupyter-token
RUN echo "sh ${HOME}/.get-jupyter-token" >> ${HOME}/.bashrc
```

The image

```
1  {
2      "name": "my-awesome-project",
3      "build": {
4          "dockerfile": "Dockerfile",
5          "options": ["--format=docker"]
6      },
7
8      "updateRemoteUserUID": false,
9      "overrideCommand": false,
10     "shutdownAction": "none",
11
12     "workspaceMount": "source=${localWorkspaceFolder},target=/home/jovyan/work,type=bind,z",
13     "workspaceFolder": "/home/jovyan/work",
14
15     "runArgs": [
16         "--name=my-awesome-project", // needs to be unique
17         "--hostname=my-awesome-project_container" // needs to be unique
18     ],
19
20     "forwardPorts": [8888],
21     "portsAttributes": {
22         "8888": {
23             "label": "Jupyterlab",
24             "onAutoForward": "ignore"
25         }
26     },
27
28
29
30
31     "r.rterm.linux": "/opt/conda/bin/radian",
32     "r.bracketedPaste": true,
33     "r.plot.useHttpgd": true
34 },
35
36     "extensions": [
37         "reditorsupport.r",           // for R
38         "RDebugger.r-debugger",       // for R
39         "ms-vscode.live-server",
40         "analytic-signal.preview-pdf"
41     ]
42
43 }
```

System Packages

```
1 FROM quay.io/jupyter/r-notebook:r-4.3.1
2
3 ENV GITHUB_CLI_VERSION 2.30.0
4 ENV R_STUDIO_VERSION 2023.12.1-402
5
6 USER root
7
8 RUN apt-get update && \
9     apt-get install -y --no-install-recommends \
10    lmodern \
11    file \
12    curl \
13    g++ \
14    tmux \
15    psmisc \
16    lsb-release \
17    libssl-dev \
18    libclang-dev \
19    libpq5 \
20    libtiff-dev \
21    && \
22    apt-get clean -y && \
23    rm -rf /var/lib/apt/lists/* /tmp/library-s
24
25 RUN R -e "dotR <- file.path(Sys.getenv('HOME'))"
26 RUN R -e "dotRprofile <- file.path(Sys.getenv(
27
28 RUN wget -q https://download2.rstudio.org/server/
29     apt-get install -yq --no-install-recommend
30     rm -f ./rstudio*.deb && \
31     apt-get clean && \
32     chmod 777 /var/run/rstudio-server && \
33     chmod +t /var/run/rstudio-server
34
35 USER ${NB_USER}
36
37 RUN mamba install -y -c conda-forge --freeze-i
38     jupyter-server-proxy=4.1.0 \
39     jupyter-rsession-proxy=2.2.0 \
40     && \
41     mamba clean --all
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43 RUN pip install \
44     nbgitpuller radian==0.6.11 \
45     && \
46     jupyter labextension enable nbgitpuller
47
48 RUN R -q -e 'remotes::install_version("markdown", version="1.12", repos="cloud.r-project.org")' && \
49     R -q -e 'remotes::install_version("languageserver", version="0.3.16", repos="cloud.r-project.org")' && \
50     R -q -e 'remotes::install_version("httpgd", version="2.0.1", repos="cloud.r-project.org")' && \
51     R -q -e 'remotes::install_github("ManuelHentschel/vscDebugger")' && \
52     R -q -e 'remotes::install_version("syuzhet", version="1.0.7", repos="cloud.r-project.org")' && \
53     echo
54
55 RUN wget https://github.com/cli/cli/releases/download/v${GITHUB_CLI_VERSION}/gh_${GITHUB_CLI_VERSION}_linux_amd64.tar.gz -O - | \
56     tar xvzf - -C /opt/conda/bin gh_${GITHUB_CLI_VERSION}_linux_amd64/bin/gh --strip-components=2
57
58 RUN echo "echo \"Jupyter server token: \$(jupyter server list 2>&1 | grep -oP '(?=<token)=[[:alnum:]]*')\" > ${HOME}/.get-jupyter
59 echo "sh ${HOME}/.get-jupyter-url.sh" >> ${HOME}/.bashrc
```

```
1 {
2     "name": "my-awesome-project",
3     "build": {
4         "dockerfile": "Dockerfile",
5         "options": ["--format=docker"]
6     },
7     "updateRemoteUserUID": false,
8     "overrideCommand": false,
9     "shutdownAction": "none",
10
11     "workspaceMount": "source=${localWorkspaceFolder},target=/home/jovyan/work,type=bind,z",
12     "workspaceFolder": "/home/jovyan/work",
13
14     "runArgs": [
15
16         needs to be unique
17         container" // needs to be unique
18
19         conda/bin/radian",
20         ie,
21         ie
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23         // for R
24         // for R
25         ,
26         w-pdf"
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2 ENV GITHUB_CLI_VERSION 2.30.0
3 ENV R_STUDIO_VERSION 2023.12.1-402
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5 USER root
6
7 RUN apt-get update && \
8     apt-get install -y --no-install-recommends \
9         lmodern \
10        file \
11        curl \
12        g++ \
13        tmux \
14        psmisc \
15        lsb-release \
16        libssl-dev \
17        libclang-dev \
18        libpq5 \
19        libtiff-dev \
20        && \
21    apt-get clean -y && \
22    rm -rf /var/lib/apt/lists/* /tmp/library-scripts
23
24
25 RUN R -e "dotR <- file.path(Sys.getenv('HOME'), '.R'); if(!file.exists(dotR)){ dir.create(dotR) }; Makevars <- file.path(dotR, 'Makevars')"
26 RUN R -e "dotRprofile <- file.path(Sys.getenv('HOME'), '.Rprofile'); if(!file.exists(dotRprofile)){ file.create(dotRprofile) };" > ${HOME}/.Rprofile
27
28 RUN wget -q https://download2.rstudio.org/server/iammv/amd64/rstudio-server-${R_STUDIO_VERSION}-amd64.deb && \
29     RUN R -e "dotR <- file.path(Sys.getenv('HOME'), '.R'); if(!file.exists(dotR)){ dir.create(dotR) }; Makevars <- file.path(dotR, 'Makevars')"
30     RUN R -e "dotRprofile <- file.path(Sys.getenv('HOME'), '.Rprofile'); if(!file.exists(dotRprofile)){ file.create(dotRprofile) };" > ${HOME}/.Rprofile
31
32 chmod +t /var/run/rstudio-server
33
34
35 USER ${NB_USER}
36
37 RUN mamba install -y -c conda-forge --freeze-installed \
38     jupyter-server-proxy=4.1.0 \
39     jupyter-rsession-proxy=2.2.0 \
40     && \
41     mamba clean --all
42
43 RUN pip install \
44     nbgitpuller radian==0.6.11 \
45     && \
46     jupyter labextension enable nbgitpuller
47
48 RUN R -q -e 'remotes::install_version("markdown", version="1.12", repos="cloud.r-project.org")' && \
49     R -q -e 'remotes::install_version("languageserver", version="0.3.16", repos="cloud.r-project.org")' && \
50     R -q -e 'remotes::install_version("httpgd", version="2.0.1", repos="cloud.r-project.org")' && \
51     R -q -e 'remotes::install_github("ManuelHentschel/vscDebugger")' && \
52     R -q -e 'remotes::install_version("syuzhet", version="1.0.7", repos="cloud.r-project.org")' && \
53     echo
54
55 RUN wget https://github.com/cli/cli/releases/download/v${GITHUB_CLI_VERSION}/gh_${GITHUB_CLI_VERSION}_linux_amd64.tar.gz -O - | \
56     tar xvzf - -C /opt/conda/bin gh_${GITHUB_CLI_VERSION}_linux_amd64/bin/gh --strip-components=2
57
58 RUN echo "echo \"Jupyter server token: \$(jupyter server list 2>&1 | grep -oP '(?=<token=)[[:alnum:]]*'\" > ${HOME}/.get-jupyter \
59 echo "sh \${HOME}/.get-jupyter-url.sh" >> ${HOME}/.bashrc

```

R preference files

```

1 {
2     "name": "my-awesome-project",
3     "build": {
4         "dockerfile": "Dockerfile",
5         "options": ["--format=docker"]
6     },
7     "skipRemoteUserUID": false,
8     "overrideCommand": false,
9     "shutdownAction": "none",
10
11     "workspaceMount": "source=${localWorkspaceFolder},target=/home/jovyan/work,type=bind,z",
12     "workspaceFolder": "/home/jovyan/work",
13
14     "runArgs": [
15         "--name=my-awesome-project", // needs to be unique
16         "--hostname=my-awesome-project_container" // needs to be unique
17     ],
18
19     "forwardPorts": [8888],
20     "portsAttributes": {
21         "8888": {
22             "label": "Jupyterlab",
23             "onAutoForward": "ignore"
24         }
25     },
26
27     "customizations": {
28         "jupyterlab": {
29             "r.plot.useHttpgd": true
30         },
31         "extensions": [
32             "reditorsupport.r", // for R
33             "RDebugger.r-debugger", // for R
34             "ms-vscode.live-server",
35             "analytic-signal.preview-pdf"
36         ]
37     }
38 }
39
40
41
42
43
44

```

```
FROM quay.io/jupyter/r-notebook:r-4.3.1
ENV GITHUB_CLI_VERSION 2.30.0
ENV R_STUDIO_VERSION 2023.12.1-402
USER root
RUN apt-get update && \
    apt-get install -y --no-install-recommends \
        lmodern \
        file \
        curl \
        g++ \
        tmux \
        psmisc \
        lsb-release \
        libssl-dev \
        libclang-dev \
        libpq5 \
        libtiff-dev \
    && \
    apt-get clean -y && \
    rm -rf /var/lib/apt/lists/* /tmp/* /var/tmp/*
RUN R -e 'install.packages("curl")'
RUN wget -q https://download2.rstudio.org/server/jammy/amd64/rstudio-server-2.0.0.1152-amd64.deb
RUN wget -q https://github.com/conda-forge/r-notebook-feedstock/archive/2.30.0.tar.gz
RUN tar xzf 2.30.0.tar.gz -C /opt/conda/lib/R/library/
RUN rm -rf /var/run/rstudio-server
RUN chmod 777 /var/run/rstudio-server && \
    chmod +t /var/run/rstudio-server
RUN mamba install -y -c conda-forge --freeze-installed \
    jupyter-server-proxy=4.1.0 \
    jupyter-rsession-proxy=2.2.0 \
    && \
    mamba clean --all
RUN pip install \
    nbgitpuller radian==0.6.11 \
    && \
    jupyter labextension enable nbgitpuller
RUN R -q -e 'remotes::install_version("markdown", version="1.12", repos="cloud.r-project.org")' && \
    R -q -e 'remotes::install_version("languageserver", version="0.3.16", repos="cloud.r-project.org")' && \
    R -q -e 'remotes::install_version("httpgd", version="2.0.1", repos="cloud.r-project.org")' && \
    R -q -e 'remotes::install_github("ManuelHentschel/vscDebugger")' && \
    R -q -e 'remotes::install_version("syuzhet", version="1.0.7", repos="cloud.r-project.org")' && \
    echo
RUN wget https://github.com/cli/cli/releases/download/v${GITHUB_CLI_VERSION}/gh_${GITHUB_CLI_VERSION}_linux_amd64.tar.gz -O /tmp/gh.tar.gz
RUN tar xzf /tmp/gh.tar.gz -C /opt/conda/bin
RUN echo "echo \"Jupyter server token: \$(jupyter server list 2>&1 | grep -oP '(?=<token=)[[:alnum:]]*')\" > ${HOME}/.get-jupyter-token" > ${HOME}/.bashrc
RUN echo "sh ${HOME}/.get-jupyter-token" >> ${HOME}/.bashrc
```

RStudio

```
1   {
2     "name": "my-awesome-project",
3     "build": {
4       "dockerfile": "Dockerfile",
5       "options": ["--format=docker"]
6     },
7
8     "updateRemoteUserUID": false,
9     "overrideCommand": false,
10    "shutdownAction": "none",
11
12    "workspaceMount": "source=${localWorkspaceFolder},target=/home/jovyan/work,type=bind,z",
13    "workspaceFolder": "/home/jovyan/work",
14
15    "runArgs": [
16      "--name=my-awesome-project", // needs to be unique
17      "--hostname=my-awesome-project_container" // needs to be unique
18    ],
19
20    "forwardPorts": [8888],
21    "portsAttributes": {
22      "8888": {
23        "label": "jupyterlab"
24      }
25    }
26  }
27
28  "extensions": [
29    "reditorsupport.r",           // for R
30    "RDebugger.r-debugger",       // for R
31    "ms-vscode.live-server",
32    "analytic-signal.preview-pdf"
33  ]
34
35  }
36
37  }
38
39  ]
40
41  }
42
43  }
44
```

```

1 FROM quay.io/jupyter/r-notebook:r-4.3.1
2
3 ENV GITHUB_CLI_VERSION 2.30.0
4 ENV R_STUDIO_VERSION 2023.12.1-402
5
6 USER root
7
8 RUN apt-get update && \
9     apt-get install -y --no-install-recommends \
10    lmodern \
11    file \
12    curl \
13    g++ \
14    tmux \
15    psmisc \
16    lsb-release \
17    libssl-dev \
18    libclang-dev \
19    libpq5 \
20    libtiff-dev \
21    && \
22    apt-get clean -y && \
23    rm -rf /var/lib/apt/lists/* /tmp/library-scripts
24
25 RUN R -e "dotR <- file.path(Sys.getenv('HOME'), '.R')"
26 RUN R -e "dotRprofile <- file.path(Sys.getenv('HOME'))
27
28 RUN wget -q https://download2.rstudio.org/server/jamovi \
29     apt-get install -yq --no-install-recommends ./rsync \
30     rm -f ./rstudio*.deb && \
31     apt-get clean && \
32     chmod 777 /var/run/rstudio-server && \
33     chmod +t /var/run/rstudio-server
34
35 USER ${NB_USER}
36
37 RUN mamba install -y -c conda-forge --freeze-installed \
38     jupyter-server-proxy=4.1.0 \
39     jupyter-rsession-proxy=2.2.0 \
40     && \
41     mamba clean --all
42
43 RUN pip install \
44     nbgitpuller radian==0.6.11 \
45     && \
46     jupyter labextension enable nbgitpuller
47
48 RUN R -q -e 'remotes::install_version("markdown", version="1.12", repos="cloud.r-project.org")' && \
49     R -q -e 'remotes::install_version("languageserver", version="0.3.16", repos="cloud.r-project.org")' && \
50     R -q -e 'remotes::install_version("httpgd", version="2.0.1", repos="cloud.r-project.org")' && \
51     R -q -e 'remotes::install_github("ManuelHentschel/vscDebugger")' && \
52     R -q -e 'remotes::install_version("syuzhet", version="1.0.7", repos="cloud.r-project.org")' && \
53     echo
54
55 RUN wget https://github.com/cli/cli/releases/download/v${GITHUB_CLI_VERSION}/gh_${GITHUB_CLI_VERSION}_linux_amd64.tar.gz -O - | \
56     tar xvzf - -C /opt/conda/bin gh_${GITHUB_CLI_VERSION}_linux_amd64/bin/gh --strip-components=2
57
58 RUN echo "echo \"Jupyter server token: \$(jupyter server list 2>&1 | grep -oP '(?=<token)=[[:alnum:]]*')\" > ${HOME}/.get-jupyter-token" > ${HOME}/.bashrc
59

```

Conda/Mamba packages

```

1 {
2     "name": "my-awesome-project",
3     "build": {
4         "dockerfile": "Dockerfile",
5         "options": ["--format=docker"]
6     }
7
8     "updatable": false,
9     "overrideCommand": false,
10    "shutdownAction": "none",
11
12    "workspaceMount": "source=${localWorkspaceFolder},target=/home/jovyan/work,type=bind,z",
13    "workspaceFolder": "/home/jovyan/work",
14
15    "runArgs": [
16        "--name=my-awesome-project", // needs to be unique
17        "--hostname=my-awesome-project_container" // needs to be unique
18    ],
19
20    "forwardPorts": [8888],
21    "portsAttributes": {
22        "8888": {
23            "label": "Jupyterlab",
24            "onAutoForward": "ignore"
25        }
26    }
27
28    "radian": {
29        "path": "/opt/conda/bin/radian",
30        "exec": true,
31        "script": true
32    }
33
34    "extensions": [
35        "reditorsupport.r", // for R
36        "RDebugger.r-debugger", // for R
37        "ms-vscode.live-server",
38        "analytic-signal.preview-pdf"
39    ]
40
41 }
42
43 }
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```

Pip packages

```
1  {
2     "name": "my-awesome-project",
3     "build": {
4         "dockerfile": "Dockerfile",
5         "options": ["--format=docker"]
6     },
7
8     "updateRemoteUserUID": false,
9     "overrideCommand": false,
10    "shutdownAction": "none",
11
12    "workspaceMount": "source=${localWorkspaceFolder},target=/home/jovyan/work,type=bind,z",
13    "workspaceFolder": "/home/jovyan/work",
14
15    "runArgs": [
16        "--name=my-awesome-project", // needs to be unique
17        "--hostname=my-awesome-project_container" // needs to be unique
18    ],
19
20    "forwardPorts": [8888],
21    "portsAttributes": {
22        "8888": {
23            "label": "Jupyterlab",
24            "onAutoForward": "ignore"
25        }
26    }
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```

R packages

```
FROM quay.io/jupyter/r-notebook:r-4.3.1
ENV GITHUB_CLI_VERSION 2.30.0
ENV R_STUDIO_VERSION 2023.12.1-402
USER root
RUN apt-get update && \
    apt-get install -y --no-install-recommends \
        lmodern \
        file \
        curl \
        g++ \
        tmux \
        psmisc \
        lsb-release \
        libssl-dev \
        libclang-dev \
        libpq5 \
        libtiff-dev \
        && \
    apt-get clean -y && \
    rm -rf /var/lib/apt/lists/* /tmp/library-scripts
RUN R -e 'remotes::install_version("markdown", version="1.12", repos="cloud.r-project.org")' && \
RUN R -e 'remotes::install_version("languageserver", version="0.3.16", repos="cloud.r-project.org")' && \
RUN wget \
    apt-get \
    rm -f \
    apt-get \
    chmod \
    chmod \
USER ${NB_USER}
RUN mamba install -y -c conda-forge --freeze-installed \
    jupyter-server-proxy=4.1.0 \
    jupyter-rsession-proxy=2.2.0 \
    && \
    mamba clean --all
RUN pip install \
    nbgitpuller @radian==0.6.11 \
    && \
    jupyter labextension enable nbgitpuller
RUN R -q -e 'remotes::install_version("markdown", version="1.12", repos="cloud.r-project.org")' && \
    R -q -e 'remotes::install_version("languageserver", version="0.3.16", repos="cloud.r-project.org")' && \
    R -q -e 'remotes::install_version("httpgd", version="2.0.1", repos="cloud.r-project.org")' && \
    R -q -e 'remotes::install_github("ManuelHentschel/vscDebugger")' && \
    R -q -e 'remotes::install_version("syuzhet", version="1.0.7", repos="cloud.r-project.org")' && \
    echo
RUN wget https://github.com/cli/cli/releases/download/v${GITHUB_CLI_VERSION}/gh_${GITHUB_CLI_VERSION}_linux_amd64.tar.gz -O - | \
    tar xvzf - -C /opt/conda/bin gh_${GITHUB_CLI_VERSION}_linux_amd64/bin/gh --strip-components=2
RUN echo "echo \"Jupyter server token: \$(jupyter server list 2>&1 | grep -oP '(?=<token)=[[:alnum:]]*')\" > ${HOME}/.get-jupyter" \
    echo "sh ${HOME}/.get-jupyter-url.sh" >> ${HOME}/.bashrc
{
  "name": "my-awesome-project",
  "build": {
    "dockerfile": "Dockerfile",
    "options": ["--format=docker"]
  },
  "updateRemoteUserUID": false,
  "overrideCommand": false,
  "shutdownAction": "none",
  "workspaceMount": "source=${localWorkspaceFolder},target=/home/jovyan/work,type=bind,z",
  "workspaceFolder": "/home/jovyan/work",
  "runArgs": [
    "--name=my-awesome-project", // needs to be unique
    "--hostname=my-awesome-project_container" // needs to be unique
  ],
  "forwardPorts": [8888],
  "portsAttributes": {
    "8888": {
      "label": "Jupyterlab"
    }
  },
  "extensions": [
    "reditorsupport.r", // for R
    "RDebugger.r-debugger", // for R
    "ms-vscode.live-server",
    "analytic-signal.preview-pdf"
  ]
}
```

```

1 FROM quay.io/jupyter/r-notebook:r-4.3.1
2
3 ENV GITHUB_CLI_VERSION 2.30.0
4 ENV R_STUDIO_VERSION 2023.12.1-402
5
6 USER root
7
8 RUN apt-get update && \
9     apt-get install -y --no-install-recommends \
10    lmodern \
11    file \
12    curl \
13    g++ \
14    tmux \
15    psmisc \
16    lsb-release \
17    libssl-dev \
18    libclang-dev \
19    libpq5 \
20    libtiff-dev \
21    && \
22    apt-get clean -y && \
23    rm -rf /var/lib/apt/lists/* /tmp/library-scripts
24
25 RUN R -e "dotR <- file.path(Sys.getenv('HOME'), '.R'); if(!file.exists(dotR)){ dir.create(dotR) }; Makevars <- file.path(dotR, 'Makevars'); if(!file.exists(Makevars)){ file.create(Makevars) };" \
26 RUN R -e "dotRprofile <- file.path(Sys.getenv('HOME'), '.Rprofile'); if(!file.exists(dotRprofile)){ file.create(dotRprofile) };" \
27

```

GitHub CLI

```

55 RUN wget https://github.com/cli/cli/releases/download/v${GITHUB_CLI_VERSION}/gh_${GITHUB_CLI_VERSION}_linux_amd64.tar.gz -O -
56 tar xvzf - -C /opt/conda/bin gh_${GITHUB_CLI_VERSION}_linux_amd64/bin/gh --strip-components=2
57
58 apt-get clean & \
59 chmod 777 /var/run/rstudio-server && \
60 chmod +t /var/run/rstudio-server
61
62 USER ${NB_USER}
63
64 RUN mamba install -y -c conda-forge --freeze-installed \
65     jupyter-server-proxy=4.1.0 \
66     jupyter-rsession-proxy=2.2.0 \
67     && \
68     mamba clean --all
69
70 RUN pip install \
71     nbgitpuller vradian==0.6.11 \
72     && \
73     jupyter labextension enable nbgitpuller
74
75 RUN R -q -e 'remotes::install_version("markdown", version="1.12", repos="cloud.r-project.org")' && \
76     R -q -e 'remotes::install_version("languageserver", version="0.3.16", repos="cloud.r-project.org")' && \
77     R -q -e 'remotes::install_version("httpgd", version="2.0.1", repos="cloud.r-project.org")' && \
78     R -q -e 'remotes::install_github("ManuelHentschel/vscDebugger")' && \
79     R -q -e 'remotes::install_version("syuzhet", version="1.0.7", repos="cloud.r-project.org")' && \
80     echo
81
82 RUN wget https://github.com/cli/cli/releases/download/v${GITHUB_CLI_VERSION}/gh_${GITHUB_CLI_VERSION}_linux_amd64.tar.gz -O - | \
83     tar xvzf - -C /opt/conda/bin gh_${GITHUB_CLI_VERSION}_linux_amd64/bin/gh --strip-components=2
84
85 RUN echo "echo \"Jupyter server token: \$(jupyter server list 2>&1 | grep -oP '(?=<token)=[[:alnum:]]*')\" > ${HOME}/.get-jupyter-token" > ${HOME}/.bashrc
86 echo "sh ${HOME}/.get-jupyter-token" >> ${HOME}/.bashrc

```

```

1 {
2     "name": "my-awesome-project",
3     "build": {
4         "dockerfile": "Dockerfile",
5         "options": ["--format=docker"]
6     },
7
8     "updateRemoteUserUID": false,
9     "overrideCommand": false,
10    "shutdownAction": "none",
11
12    "workspaceMount": "source=${localWorkspaceFolder},target=/home/jovyan/work,type=bind,z",
13    "workspaceFolder": "/home/jovyan/work",
14
15    "runArgs": [
16        "--name=my-awesome-project", // needs to be unique
17        "--hostname=my-awesome-project_container" // needs to be unique
18    ],
19
20    "forwardPorts": [8888],
21    "portsAttributes": {
22        "8888": {
23            "label": "Jupyterlab",
24            "onAutoForward": "ignore"
25        }
26    }
27
28    "extensions": [
29        "r.terminal.terminalIntegration", // optional
30        "r.bracketedPaste": true,
31        "r.plot.useHttpgd": true
32    },
33
34    "extensions": [
35        "reditorsupport.r", // for R
36        "RDebugger.r-debugger", // for R
37        "ms-vscode.live-server",
38        "analytic-signal.preview-pdf"
39    ]
40
41 }
42
43 }
44

```

```
FROM quay.io/jupyter/r-notebook:r-4.3.1
ENV GITHUB_CLI_VERSION 2.30.0
ENV R_STUDIO_VERSION 2023.12.1-402
USER root
RUN apt-get update && \
    apt-get install -y --no-install-recommends \
        lmodern \
        file \
        curl \
        g++ \
        tmux \
        psmisc \
        lsb-release \
        libssl-dev \
        libclang-dev \
        libpq5 \
        libtiff-dev \
        && \
    apt-get clean -y && \
    rm -rf /var/lib/apt/lists/* /tmp/library-scripts
RUN R -e "dotR <- file.path(Sys.getenv('HOME'), '.R'); if(!file.exists(dotR)){ dir.create(dotR) }; Makevars <- file.path(dotR, 'Makevars'); if(!file.exists(Makevars)) file.create(Makevars); Rprofile <- file.path(Sys.getenv('HOME'), '.Rprofile'); if(!file.exists(Rprofile)) file.create(Rprofile)"; dotRprofile <- file.path(Sys.getenv('HOME'), '.Rprofile'); if(!file.exists(dotRprofile)) file.create(dotRprofile)
```

Jupyter Token

```
58 RUN echo "echo \"Jupyter server token: \$(jupyter server list 2>&1 | grep -oP '(?=<token)=[:alnum:]]*')\" > ${HOME}/.get-jupyter
59 echo "sh ${HOME}/.get-jupyter-url.sh" >> ${HOME}/.bashrc
33 chmod +t /var/run/rstudio-server
34
35 USER ${NB_USER}
36
37 RUN mamba install -y -c conda-forge --freeze-installed \
38     jupyter-server-proxy=4.1.0 \
39     jupyter-rsession-proxy=2.2.0 \
40     && \
41     mamba clean --all
42
43 RUN pip install \
44     nbgitpuller radian==0.6.11 \
45     && \
46     jupyter labextension enable nbgitpuller
47
48 RUN R -q -e 'remotes::install_version("markdown", version="1.12", repos="cloud.r-project.org")' && \
49     R -q -e 'remotes::install_version("languageserver", version="0.3.16", repos="cloud.r-project.org")' && \
50     R -q -e 'remotes::install_version("httpgd", version="2.0.11", repos="cloud.r-project.org")' && \
51     R -q -e 'remotes::install_github("ManuelHentschel/vscDebugger")' && \
52     R -q -e 'remotes::install_version("syuzhet", version="1.0.7", repos="cloud.r-project.org")' && \
53     echo
54
55 RUN wget https://github.com/cli/cli/releases/download/v${GITHUB_CLI_VERSION}/gh_${GITHUB_CLI_VERSION}_linux_amd64.tar.gz -O \
56     tar xvzf - -C /opt/conda/bin gh_${GITHUB_CLI_VERSION}_linux_amd64/bin/gh --strip-components=2
57
58 RUN echo "echo \"Jupyter server token: \$(jupyter server list 2>&1 | grep -oP '(?=<token)=[:alnum:]]*')\" > ${HOME}/.get-jupyter
59 echo "sh ${HOME}/.get-jupyter-url.sh" >> ${HOME}/.bashrc
```

```
1  {
2     "name": "my-awesome-project",
3     "build": {
4         "dockerfile": "Dockerfile",
5         "options": ["--format=docker"]
6     },
7     "updateRemoteUserUID": false,
8     "overrideCommand": false,
9     "shutdownAction": "none",
10
11     "workspaceMount": "source=${localWorkspaceFolder},target=/home/jovyan/work,type=bind,z",
12     "workspaceFolder": "/home/jovyan/work",
13
14     "runArgs": [
15         "--name=my-awesome-project", // needs to be unique
16         "--hostname=my-awesome-project_container" // needs to be unique
17     ],
18
19     "forwardPorts": [8888],
20     "portsAttributes": {
21         "8888": {
22             "label": "Jupyterlab",
23             "onAutoForward": "ignore"
24         }
25     }
26 }
```

```
        "r.plot.useHttpgd": true
      },
      "extensions": [
        "reditorsupport.r",
        "RDebugger.r-debugger",
        "ms-vscode.live-server",
        "analytic-signal.preview-pdf"
      ]
    }
  }
}
```

```
FROM quay.io/jupyter/r-notebook:r-4.3.1
```

```
ENV GITHUB_CLI_VERSION 2.30.0  
ENV R_STUDIO_VERSION 2023.12.1-402
```

```
USER root
```

```
RUN apt-get update &&  
    apt-get install -y --no-install-recommends \  
        lmodern \  
        file \  
        curl \  
        g++ \  
        tmux \  
        psmisc \  
        lsb-release \  
        libssl-dev \  
        libclang-dev \  
        libpq5 \  
        libtiff-dev \  
        && \  
    apt-get clean -y && \  
    rm -rf /var/lib/apt/lists/* /tmp/library-scripts  
  
RUN R -e "dotR <- file.path(Sys.getenv('HOME'), '.R'); if(!file.exists(dotR)){ dir.create(dotR) }; Makevars <- file.path(dotR, 'Makevars'); if(!file.exists(Makevars)){ file.create(Makevars) };"  
RUN R -e "dotRprofile <- file.path(Sys.getenv('HOME'), '.Rprofile'); if(!file.exists(dotRprofile)){ file.create(dotRprofile) };"  
  
RUN wget -q https://down...  
12     "workspaceMount": "source=${localWorkspaceFolder},target=/home/jovyan/work,type=bind,z",  
13     "workspaceFolder": "/home/jovyan/work",  
  
USER ${NB_USER}  
  
RUN mamba install -y -c conda-forge --freeze-installed \  
    jupyter-server-proxy=4.1.0 \  
    jupyter-rsession-proxy=2.2.0 \  
    && \  
    mamba clean --all  
  
RUN pip install \  
    nbgitpuller radian==0.6.11 \  
    && \  
    jupyter labextension enable nbgitpuller  
  
RUN R -q -e 'remotes::install_version("markdown", version="1.12", repos="cloud.r-project.org")' && \  
    R -q -e 'remotes::install_version("languageserver", version="0.3.16", repos="cloud.r-project.org")' && \  
    R -q -e 'remotes::install_version("httpgd", version="2.0.1", repos="cloud.r-project.org")' && \  
    R -q -e 'remotes::install_github("ManuelHentschel/vscDebugger")' && \  
    R -q -e 'remotes::install_version("syuzhet", version="1.0.7", repos="cloud.r-project.org")' && \  
    echo  
  
RUN wget https://github.com/cli/cli/releases/download/v${GITHUB_CLI_VERSION}/gh_${GITHUB_CLI_VERSION}_linux_amd64.tar.gz -O - | \  
    tar xvzf - -C /opt/conda/bin gh_${GITHUB_CLI_VERSION}_linux_amd64/bin/gh --strip-components=2  
  
RUN echo "echo \"Jupyter server token: \$(jupyter server list 2>&1 | grep -oP '(?=<token=)[[:alnum:]]*\')\" > ${HOME}/.get-jupyter" > ${HOME}/.bashrc  
echo "sh ${HOME}/.get-jupyter-url.sh" >> ${HOME}/.bashrc
```

```
1 {  
2     "name": "my-awesome-project",  
3     "build": {  
4         "dockerfile": "Dockerfile",  
5         "options": ["--format=docker"]  
6     },  
7     "updateContainerImage": false,  
8     "overrideCommand": false,  
9     "shutdownAction": "none",  
10    "workspaceMount": "source=${localWorkspaceFolder},target=/home/jovyan/work,type=bind,z",  
11    "workspaceFolder": "/home/jovyan/work",  
12  
13    "runArgs": [  
14        "--name=my-awesome-project", // needs to be unique  
15        "--hostname=my-awesome-project_container" // needs to be unique  
16    ],  
17  
18    "forwardPorts": [8888],  
19    "portsAttributes": {  
20        "8888": {  
21            "label": "Jupyterlab",  
22            "onAutoForward": "ignore"  
23        }  
24    },  
25  
26    "rterm": {  
27        "rtermLinux": "rterm/conda/bin/rterm",  
28        "r.bracketedPaste": true,  
29        "r.plot.useHttpgd": true  
30    },  
31  
32    "extensions": [  
33        "reditorsupport.r", // for R  
34        "RDebugger.r-debugger", // for R  
35        "ms-vscode.live-server",  
36        "analytic-signal.preview-pdf"  
37    ]  
38},  
39  
40},  
41  
42},  
43  
44}
```

```

1 FROM quay.io/jupyter/r-notebook:r-4.3.1
2 ENV GITHUB_CLI_VERSION 2.30.0
3 ENV R_STUDIO_VERSION 2023.12.1-402
4
5 USER root
6
7 RUN apt-get update &gt;
8     apt-get install -y --no-install-recommends \
9         lmodern \
10        file \
11        curl \
12        g++ \
13        tmux \
14        psmisc \
15        lsb-release \
16        libssl-dev \
17        libclang-dev \
18        libpq5 \
19        libtiff-dev \
20        && \
21    apt-get clean -y && \
22    rm -rf /var/lib/apt/lists/* /tmp/library-scripts
23
24
25 RUN R -e "dotR <- file.path(Sys.getenv('HOME')[[1]]).R); if(!file.exists(dotR)) dir.create(dotR); Makevars <- file.path(dotR, 'Makevars')"
26 RUN R -e "dotRprofile <- file.path(Sys.
27
28 RUN wget -q https://download2.rstudio.o
29     apt-get install -yq --no-install-re
30     rm -f ./rstudio*.deb && \
31     apt-get clean && \
32     chmod 777 /var/run/rstudio-server &
33     chmod +t /var/run/rstudio-server
34
35 USER ${NB_USER}
36
37 RUN mamba install -y -c conda-forge --freeze-installed \
38     jupyter-server-proxy=4.1.0 \
39     jupyter-rsession-proxy=2.2.0 \
40     && \
41     mamba clean --all
42
43 RUN pip install \
44     nbgitpuller radian==0.6.11 \
45     && \
46     jupyter labextension enable nbgitpuller
47
48 RUN R -q -e 'remotes::install_version("markdown", version="1.12", repos="cloud.r-project.org")' && \
49     R -q -e 'remotes::install_version("languageserver", version="0.3.16", repos="cloud.r-project.org")' && \
50     R -q -e 'remotes::install_version("httpgd", version="2.0.1", repos="cloud.r-project.org")' && \
51     R -q -e 'remotes::install_github("ManuelHentschel/vscDebugger")' && \
52     R -q -e 'remotes::install_version("syuzhet", version="1.0.7", repos="cloud.r-project.org")' && \
53     echo
54
55 RUN wget https://github.com/cli/cli/releases/download/v${GITHUB_CLI_VERSION}/gh_${GITHUB_CLI_VERSION}_linux_amd64.tar.gz -O - | \
56     tar xvzf - -C /opt/conda/bin gh_${GITHUB_CLI_VERSION}_linux_amd64/bin/gh --strip-components=2
57
58 RUN echo "echo \"Jupyter server token: \$(jupyter server list 2>&1 | grep -oP '(?=<token)=[[:alnum:]]*')\" > ${HOME}/.get-jupyter" > ${HOME}/.bashrc
59

```

```

1 {
2     "name": "my-awesome-project",
3     "build": {
4         "dockerfile": "Dockerfile",
5         "options": ["--format=docker"]
6     }
7
8     "skipRemoteUserUID": false,
9     "overrideCommand": false,
10    "shutdownAction": "none",
11
12    "workspaceMount": "source=${localWorkspaceFolder},target=/home/jovyan/work,type=bind,z",
13    "workspaceFolder": "/home/jovyan/work",
14
15    "runArgs": [
16        "--name=my-awesome-project", // needs to be unique
17        "--hostname=my-awesome-project_container" // needs to be unique
18    ]
19
20    "forwardPorts": [8888],
21    "portsAttributes": {
22        "8888": {
23            "label": "Jupyterlab",
24            "onAutoForward": "ignore"
25        }
26    }
27
28
29    "r.plot.useTango": true
30
31    "extensions": [
32        "reditorsupport.r", // for R
33        "RDebugger.r-debugger", // for R
34        "ms-vscode.live-server",
35        "analytic-signal.preview-pdf"
36    ]
37
38
39
40
41
42
43
44

```

15 "runArgs": [
16 "--name=my-awesome-project", // needs to be unique
17 "--hostname=my-awesome-project_container" // needs to be unique
18],

```
FROM quay.io/jupyter/r-notebook:r-4.3.1
ENV GITHUB_CLI_VERSION 2.30.0
ENV R_STUDIO_VERSION 2023.12.1-402
USER root
RUN apt-get update && \
    apt-get install -y --no-install-recommends \
        lmodern \
        file \
        curl \
        g++ \
        tmux \
        psmisc \
        lsb-release \
        libssl-dev \
        libclang-dev \
        libpq5 \
        libtiff-dev \
        && \
    apt-get clean -y && \
    rm -rf /var/lib/apt/lists/* /tmp/library-scripts
RUN R -e "dotR <- file.path(Sys.getenv('HOME'), '.R'); if(!file.exists(.R))" \
    RUN R -e "dotRprofile <- file.path(Sys.getenv('HOME'), '.Rprofile'); if(!file.exists(.Rprofile))" \
    RUN wget -q https://download2.rstudio.org/server/jammy/amd64/rstudio-server.deb \
        apt-get install -yq --no-install-recommends ./rstudio*.deb && \
        rm -f ./rstudio*.deb && \
        apt-get clean && \
        chmod 777 /var/run/rstudio-server && \
        chmod +t /var/run/rstudio-server
USER ${NB_USER}
RUN mamba install -y -c conda-forge --freeze-installed \
    jupyter-server-proxy=4.1.0 \
    jupyter-rsession-proxy=2.2.0 \
    && \
    mamba clean --all
RUN pip install \
    nbgitpuller radian==0.6.11 \
    && \
    jupyter labextension enable nbgitpuller
RUN R -q -e 'remotes::install_version("markdown", version="1.12", repos="cloud.r-project.org")' && \
    R -q -e 'remotes::install_version("languageserver", version="0.3.16", repos="cloud.r-project.org")' && \
    R -q -e 'remotes::install_version("httpgd", version="2.0.1", repos="cloud.r-project.org")' && \
    R -q -e 'remotes::install_github("ManuelHentschel/vscDebugger")' && \
    R -q -e 'remotes::install_version("syuzhet", version="1.0.7", repos="cloud.r-project.org")' && \
    echo
RUN wget https://github.com/cli/cli/releases/download/v${GITHUB_CLI_VERSION}/gh_${GITHUB_CLI_VERSION}_linux_amd64.tar.gz -O \
    tar xvzf - -C /opt/conda/bin gh_${GITHUB_CLI_VERSION}_linux_amd64/bin/gh --strip-components=2
RUN echo "echo \"Jupyter server token: \$(jupyter server list 2>&1 | grep -oP '(?=<token=)[[:alnum:]]*')\" > ${HOME}/.get-jupyter-token" > ${HOME}/.bashrc
RUN echo "sh \$({HOME}/.get-jupyter-token)" >> ${HOME}/.bashrc
RUN echo "forwardPorts": [8888],  
"portsAttributes": {  
    "8888": {  
        "label": "Jupyter",  
        "onAutoForward": true  
    }  
},
```

```
1  {
2     "name": "my-awesome-project",
3     "build": {
4         "dockerfile": "Dockerfile",
5         "options": ["--format=docker"]
6     },
7     "updateNotebookDocker": false,
8     "overrideCommand": false,
9     "shutdownAction": "none",
10
11    "workspaceMount": "source=${localWorkspaceFolder},target=/home/jovyan/work,type=bind,z",
12    "workspaceFolder": "/home/jovyan/work",
13
14    "runArgs": [
15        "--name=my-awesome-project", // needs to be unique
16        "--hostname=my-awesome-project_container" // needs to be unique
17    ],
18
19    "forwardPorts": [8888],
20    "portsAttributes": {
21        "8888": {
22            "label": "Jupyterlab",
23            "AutoForward": "ignore"
24        }
25    }
26
27    "options": {
28        "": {
29            "settings": {
30                "r.rterm.linux": "/opt/conda/bin/radian",
31                "r.bracketedPaste": true,
32                "r.plot.useHttpgd": true
33            }
34        }
35    }
36
37    "extensions": [
38        "reditorsupport.r",           // for R
39        "RDebugger.r-debugger",       // for R
40        "ms-vscode.live-server",
41        "analytic-signal.preview-pdf"
42    ]
43 }
```

```
FROM quay.io/jupyter/r-notebook:r-4.3.1

ENV GITHUB_CLI_VERSION 2.30.0
ENV R_STUDIO_VERSION 2023.12.1-402

USER root
RUN apt-get update &&
    apt-get install -y --no-install-recommends \
        lmodern \
        file \
        curl \
        g++ \
        tmux \
        psmisc \
        lsb-release \
        libssl-dev \
        libclang-dev \
        libpq5 \
        libtiff-dev \
        && \
    apt-get clean -y && \
    rm -rf /var/lib/apt/lists/* /tmp/*
RUN R -e "dotR <- file.path(Sys.getenv('R_HOME'))"
RUN R -e "dotRprofile <- file.path(Sys.getenv('R_PROFILE'))"

RUN wget -q https://download2.rstudio.org/debian/rstudio-1.5.3-1_all.deb
apt-get install -yq --no-install-recommends ./rstudio*.deb && \
    apt-get clean && \
    chmod 777 /var/run/rstudio-server & \
    chmod +t /var/run/rstudio-server

USER ${NB_USER}

RUN mamba install -y -c conda-forge --force \
    jupyter-server-proxy=4.1.0 \
    jupyter-rsession-proxy=2.2.0 \
    && \
    mamba clean --all

RUN pip install \
    nbgrader > radian==0.6.11 \
    && \
jupyter labextension enable nbgrader

RUN R -q -e 'remotes::install_version("markdown", version="1.12", repos="cloud.r-project.org")' && \
    R -q -e 'remotes::install_version("languageserver", version="0.3.16", repos="cloud.r-project.org")' && \
    R -q -e 'remotes::install_version("httpgd", version="2.0.1", repos="cloud.r-project.org")' && \
    R -q -e 'remotes::install_github("ManuelHentschel/vscDebugger")' && \
    R -q -e 'remotes::install_version("syuzhet", version="1.0.7", repos="cloud.r-project.org")' && \
    echo

RUN wget https://github.com/cli/cli/releases/download/v${GITHUB_CLI_VERSION}/gh_${GITHUB_CLI_VERSION}_linux_amd64.tar.gz -O /tmp/gh.tar.gz
tar xzvf /tmp/gh.tar.gz -C /opt/conda/bin gh_${GITHUB_CLI_VERSION}_linux_amd64/bin/gh --strip-components=2

RUN echo "echo \"Jupyter server token: \$(jupyter server list 2>&1 | grep -oP '(?=<token=)[[:alnum:]]*'\" > ${HOME}/.get-jupyter-token
RUN echo "sh ${HOME}/.get-jupyter-url.sh" >> ${HOME}/.bashrc
```

Additional VS Code preferences



So how does this all come together?

The screenshot shows a Visual Studio Code interface for a LaTeX project named "paper-containers".

File Explorer: Shows the project structure under "WORK [DEV CONTAINER: PAPER-CONTAINERS]". Key files include ".devcontainer", "devcontainer.json", "Dockerfile", ".vscode", "imgs", "src" (containing "_extensions", "containers_files", ".gitignore", "bibliography.bib", "code-listing.tex", "containers.pdf", "containers.qmd", "sn-apacite bst", "sn-aps bst", "sn-basic bst", "sn-chicago bst", "sn-jnl.cls", "sn-mathphys bst", "sn-nature bst").

Editor: Three tabs are open: "containers.qmd", "devcontainer.json 1, M", and "bibliography.bib".

- containers.qmd:** Contains a section titled "# Portability" explaining the portability of containers across different environments, mentioning Apptainer and Docker.
- devcontainer.json:** Configuration for the development container, showing a single port mapping from Jupyterlab (8888) to localhost:8888.
- bibliography.bib:** BibTeX bibliography file listing entries for "Meurer2017" and "Microsoft2024".

Bottom Status Bar: Shows the current file is "Dev Container: paper-containers", has 1 edit, 0 errors, 1 warning, and is using Quarto 1.4.549. It also displays the current line (Ln 6249, Col 16), character count (9 selected), and encoding (UTF-8 LF). Other icons include BibTeX, off/on status, and a gear icon with a '1'.

[PROBLEMS](#)[OUTPUT](#)[DEBUG CONSOLE](#)[TERMINAL](#)[PORTS](#)

1

Port**Forwarded Add...** **Running Process****Origin**

- Jupyterlab (8888) [localhost:8888](#) /opt/conda/bin/python3.11 /opt/con... Dev Containers

[Add Port](#)

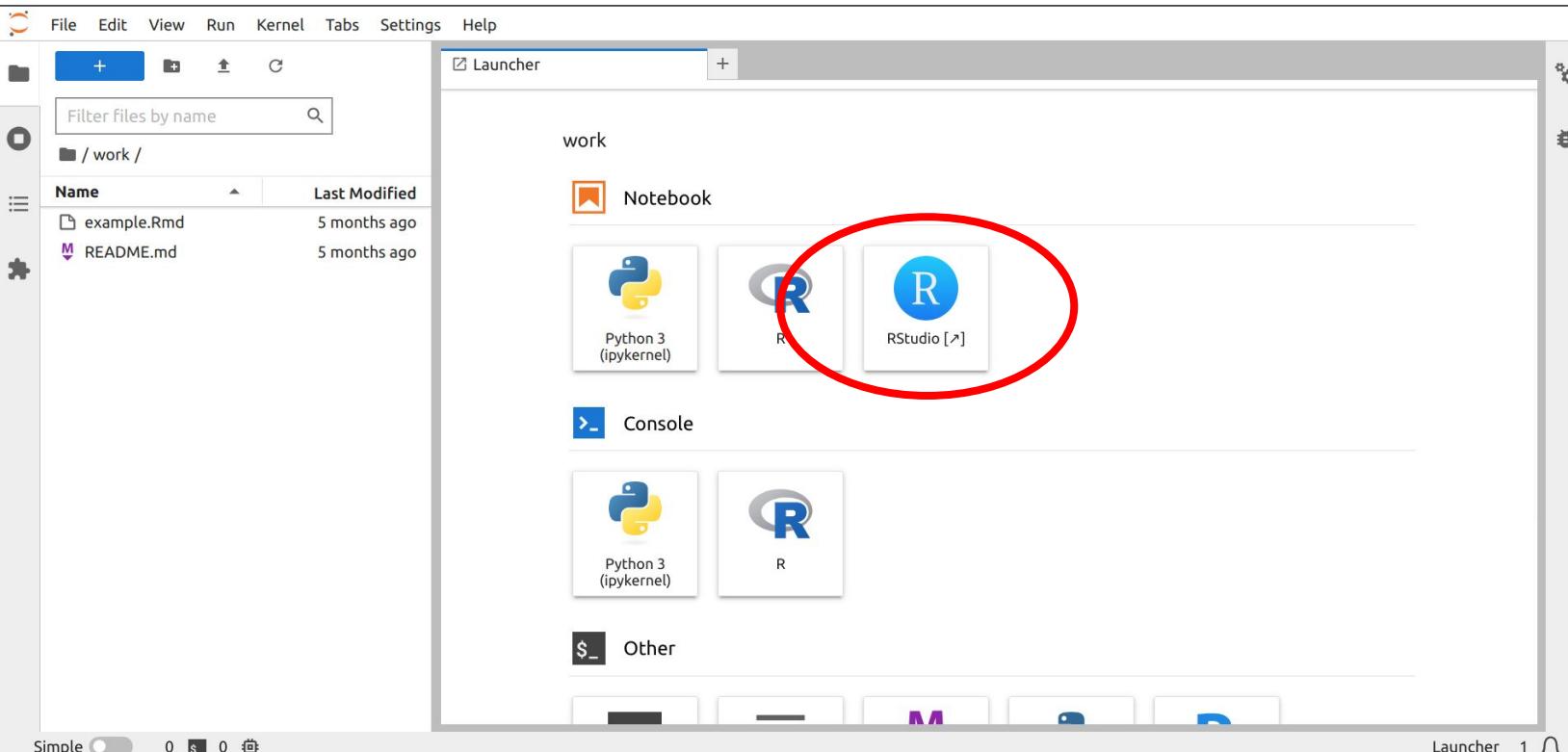
Port

Forwarded Add... Running Process

Origin

- Jupyterlab (8888) localhost:8888 /opt/conda/bin/python3.11 /opt/con... Dev Containers

Add Port



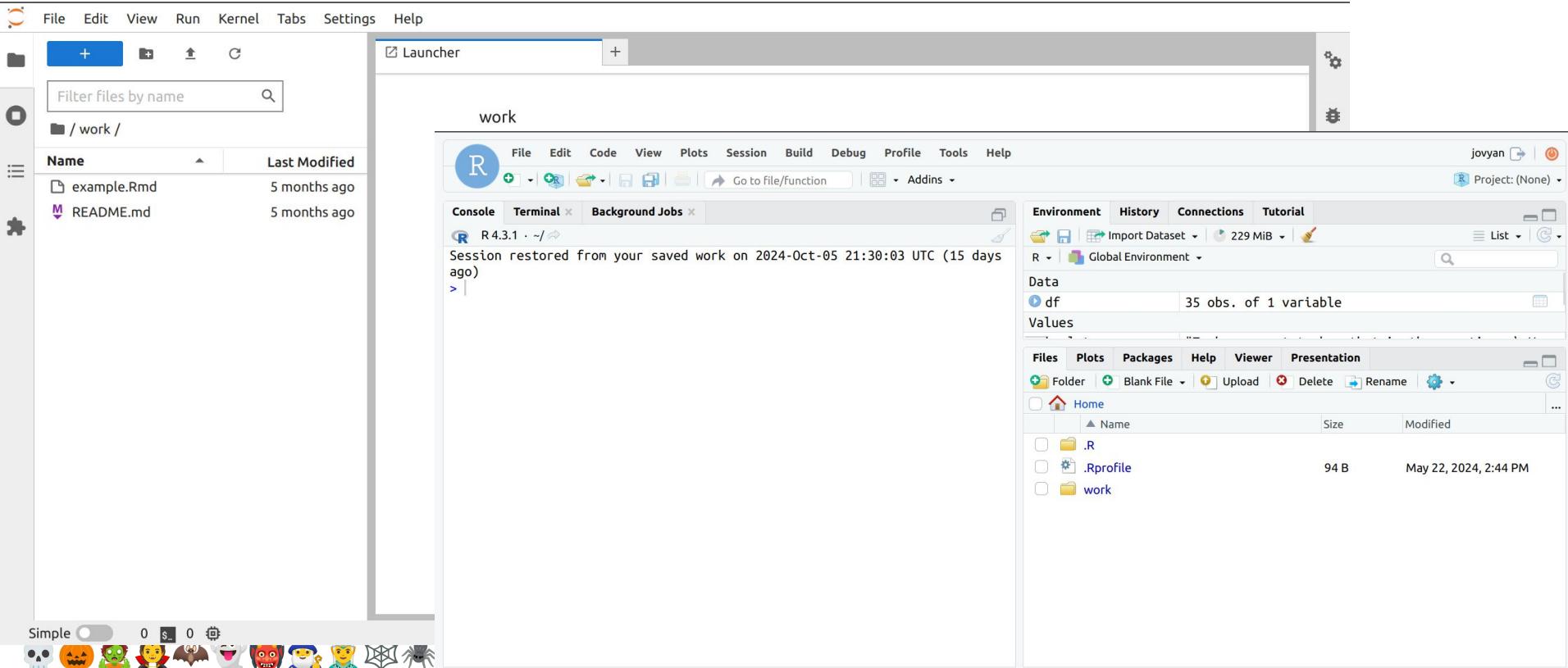
Port

Forwarded Add... Running Process

Origin

- Jupyterlab (8888) localhost:8888 /opt/conda/bin/python3.11 /opt/con... Dev Containers

Add Port





← →



Search

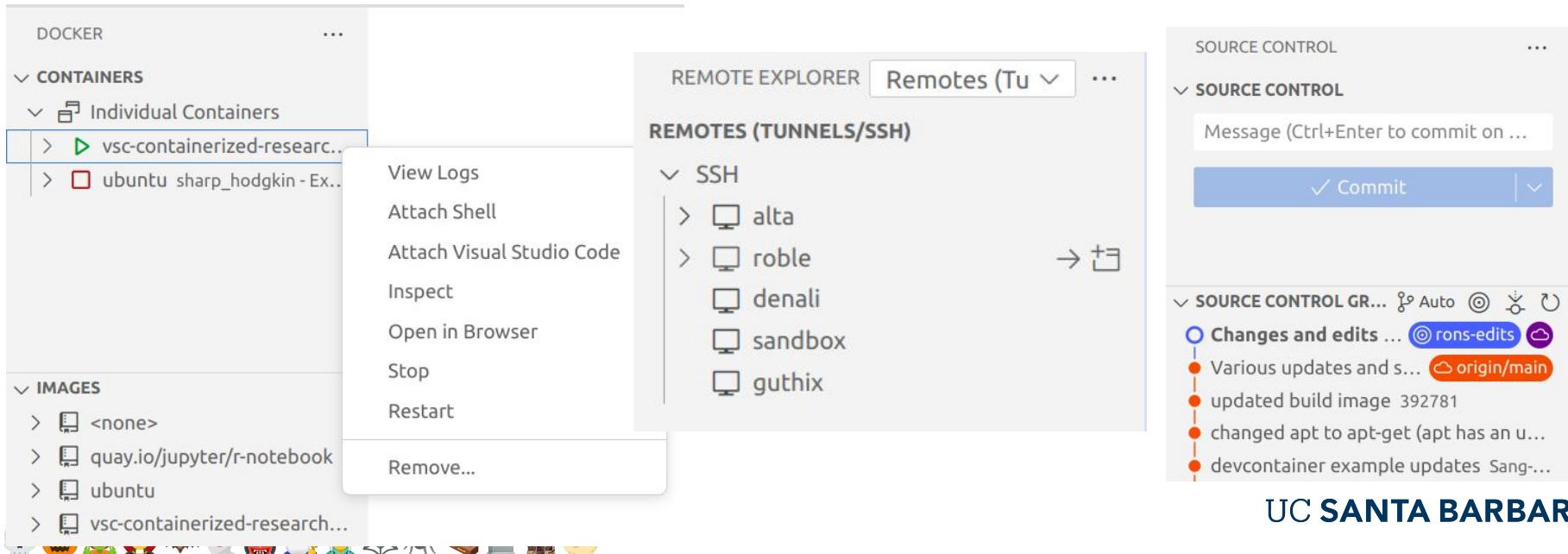


⊗ 0 △ 0 ⚡ 0



💪 Further Extending Usability

- With additional extensions we can build and manage our containers (and images) interactively
- This simplifies the overall management process of your project (and more)





Real World Usage - Our Department

- Want to revamp department server...
 - Original server was centrally managed
 - Languages, packages, software were all shared by users
 - Tools like RStudio were only accessible via a specific server
- Needless to say this limited users...
 - Locked users to specific software versions
 - New packages needed to be requested
 - Dependency conflicts everywhere
 - Access limited to terminal interaction
- Solution?: Devcontainers





Some Requirements

- Ability to reproduce and share work
- Work on a multiuser system in isolation
 - Something that is possible to configure for containers but somewhat nontrivial
- Ease of use
 - As seen previously, creating more complex Dockerfiles can be, again, a nontrivial task
 - Researchers should be able to spin up a custom image with ease
 - More than that, they should be able to have a starting point for configuration
 - Should also be able to easily connect to and manage remote servers!





Dev Container Template

- Because writing container files can be a difficult process...

...we created an extendable template!



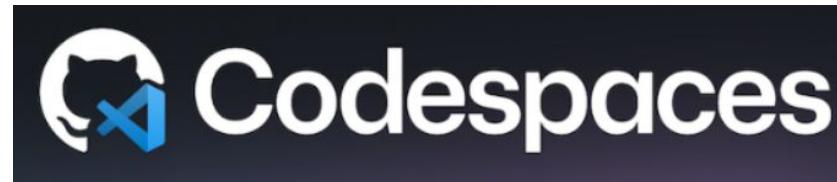
```
○ [ronaldas@alta ~]$ █
```

✨ Beyond...

- We include our template tooling with an image on Jetstream2
- Usage is exactly the same between different systems



- Additionally, devcontainer files can be run without any additional tooling once uploaded on GitHub via a feature called CodeSpaces
- This is a feature that is available with GitHub Pro (which is free for all academics)





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4

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main ▾

2 Branches

Tags

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Code ▾



392781 Changed navigation order of new-devices and basic-usage

.devcontainer

devcontainer for b

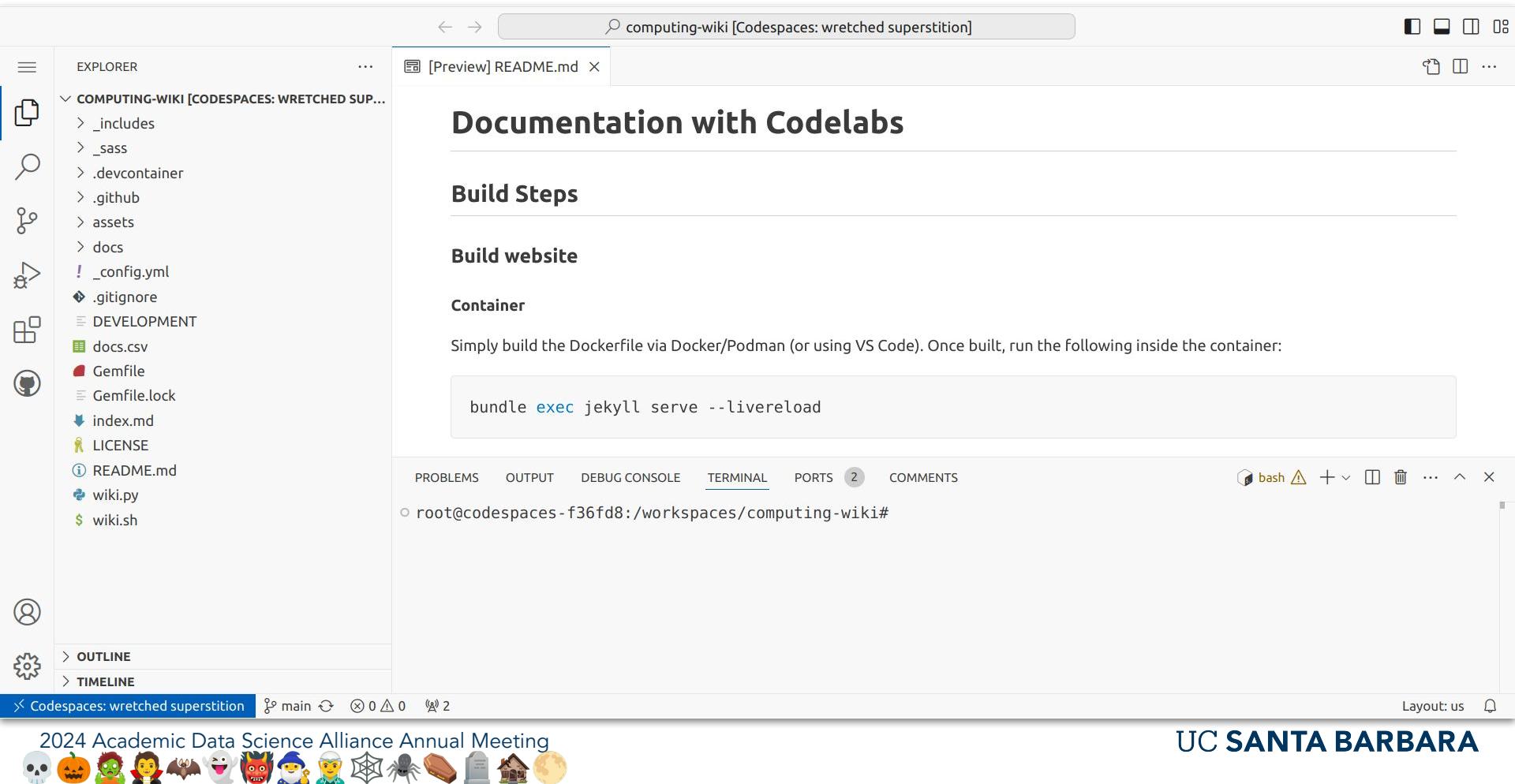
Local

Codespaces

Codespaces

Your workspaces in the cloud

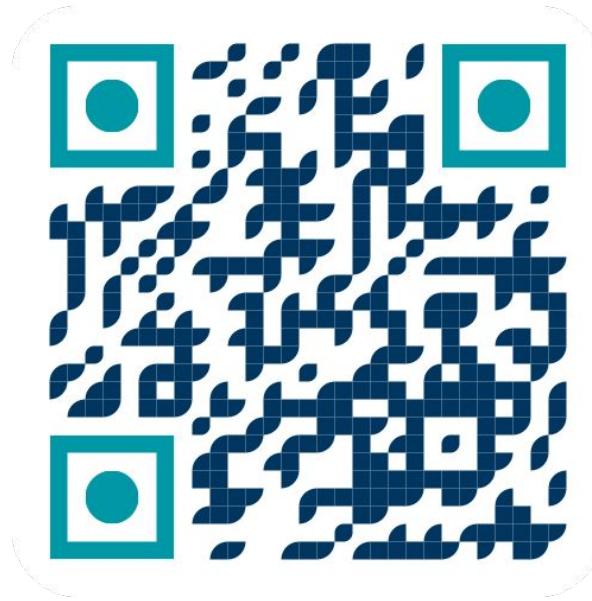






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