Save your tears for the data: A touch of Docker in a Data Scientist's workflow

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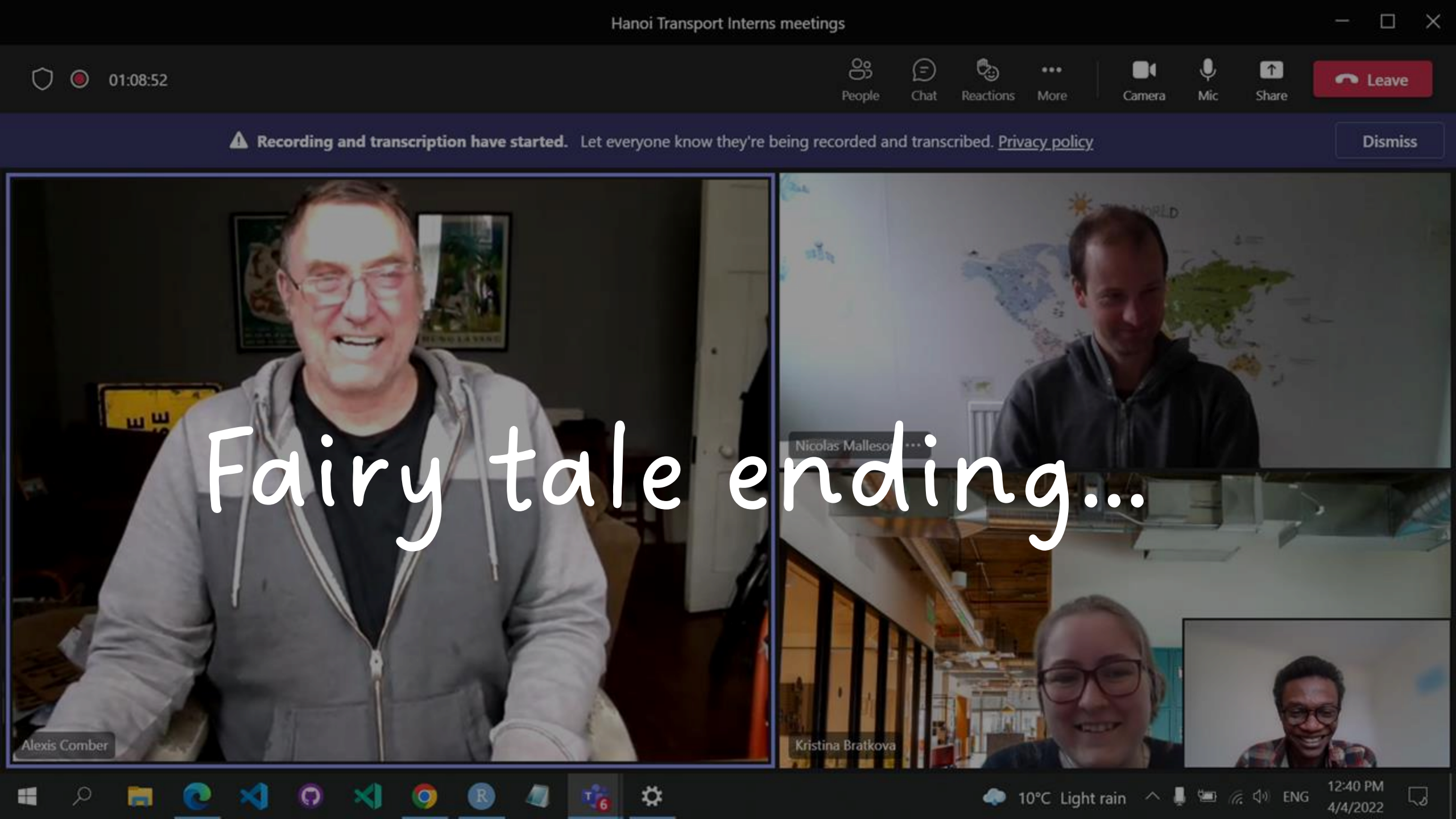
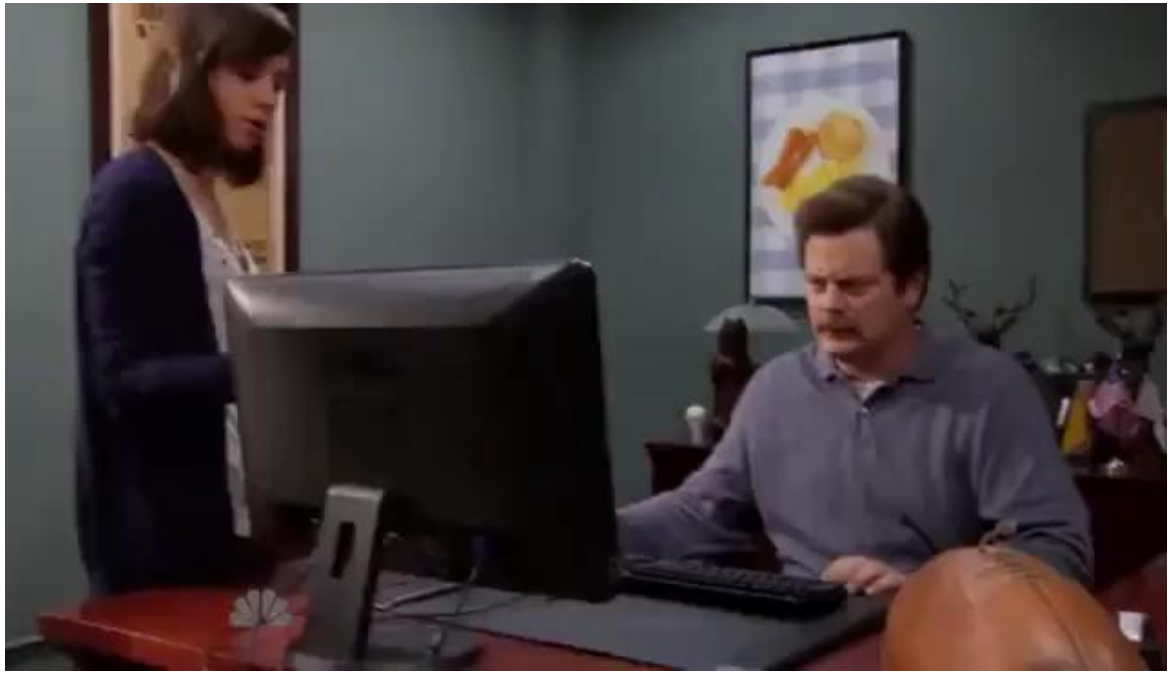
Eric Wanjau, Data Scientist - LIDA

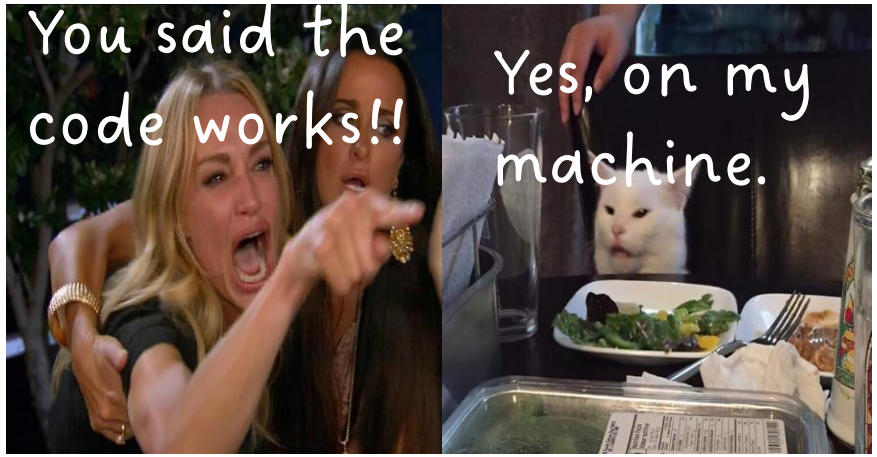
github.com/R-icntay/res_comp_leeds_2022

@ericntay at #ResCompLeedsCon2022


Hanoi Transport Interns meetings
01:08:52
People
Chat
Reactions
More
Camera
Mic
Share
Leave
Recording and transcription have started. Let everyone know they're being recorded and transcribed. Privacy policy
Dismiss
Fairy tale ending...
Alexis Comber
Nicolas Malleson
Kristina Bratkova
10°C Light rain
ENG
12:40 PM
4/4/2022

But somewhere along the line, it felt like ...





I am running on xxx OS

The model could make the dashboard lag

Reproducibility

Isolation

Portability

To the rescue: Dev containers - Docker containers configured to provide a full-featured development environment

- Tailored environment with all the tools and runtimes e.g R, Python, Julia
- IDE of choice e.g VS Code, RStudio
- Portable i.e GitHub Codespaces, local machine, container hosts e.g Azure, AWS, GCP
- Same experience for every user

Let's set one up: R + Python + VS Code + Rstudio

Container Config: Dockerfile

```
# R version: 4, 4.1, 4.0
ARG VARIANT="4.2"
FROM rocker/tidyverse:${VARIANT}
```

FROM command describes a base environment, so we don't need to start from scratch

```
# Install Python and some packages
RUN apt-get -y install \
        python3-pip \
&& pip --disable-pip-version-check --no-cache-dir install pandas \
&& pip --disable-pip-version-check --no-cache-dir install seaborn \
```

```
# Install R packages
&& install2.r --error --skipinstalled --ncpus -1 \
        palmerpenguins \
        tidymodels \
        languageserver \
```

RUN changes the base environment e.g. installing additional packages

Customizing dev environment: devcontainer.json -- VS Code

```
"name": "res_comp_leeds22",
    "build": {
        "dockerfile": "Dockerfile",
         "args": { "VARIANT": "4.2" }
    },
```

Specifies the name of dev container and references the Dockerfile we defined earlier

```
"settings": {
        "r.rpath.linux": "/usr/local/lib/R/bin/R",
},

"extensions": [
        // R extensions
        "ikuyadeu.r",
        "rdebugger.r-debugger",
        "reditorsupport.r",

        // Add Jupyter and Python  vs code extensions
        "ms-toolsai.jupyter",
        "ms-python.python"
],
```

Standard elements everyone working in the dev env would need

But, what if I really really really love the RStudio IDE?

Customizing dev environment: devcontainer.json -- RStudio

```
    "forwardPorts": [8787],
    "portsAttributes": {
        "8787": {
            "label": "RStudio",
            "requireLocalPort": true,
            "onAutoForward": "ignore"
        }
},
```

forwardPorts: makes a list of ports inside the container available locally.

portsAttributes: specifies the properties of the ports

```
    "onCreateCommand": "sudo rstudio-server start"
```

onCreateCommand: finalizes setup by specifying what to execute immediately after container is created

Python Demo: VS Code / Docker

github.com/R-icntay/res_comp_leeds_2022

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R Demo: Rstudio/ GithubCodespaces

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Wrapping up:

Reproducible and customizable development environments

Isolated environments that won't change pre-existing setups

Portable: MacOS, Linux, or Windows

Great for workshops!

Tears of joy ...

Thank you!

Slides, links, resources and Dev Container:

github.com/R-icntay/res_comp_leeds_2022

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