Week 6: Reproducible research with AnVILPublish (Martin Morgan)

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Notes

1. Visit the course schedule for links to the recorded session, and to other workshops in the series.
2. The material below requires a billing account. We provide a billing account during the workshop, but if you're following along on your own see 'Next Steps' for how to create a billing account.
3. Access to the workspaces we use may require registration; please sign up with your AnVIL email address.

Learning Objectives

This week we'll explore elements of reproducible research with the AnVILPublish package. We will illustrate how to make a docker container tailored to a particular purpose (in this case, publishing AnVIL packages!). We'll then emphasize the merits of an R package structure for organizing research activities in a manner that emphasizes provenance and reproducibility. The R package structure coupled with git will form the basis of AnVIL workspace creation, allowing

us to maintain a single, version-controlled source for Jupyter notebook or RStudio-based AnVIL workspaces.

Key Resources

- Visit https://anvil.terra.bio to use the AnVIL platform.
- The directory and text-file structure of R packages make them easy to write, maintain, and validate; the Writing R Extensions vignette that comes with R is the definitive source; an excellent resource is R Packages (e-)book.
- Docker containers form a basis for reproducibility in AnVIL; we make use of custom docker containers extending the terra-jupyter-bioconductor and anvilproject-rstudio-bioconductor images following instructions at Docker tutorial: Custom cloud environments for Jupyter notebooks (terra-docker/README.md is also useful).

Review

Previously…

- The course schedule contains links and videos of previous sessions

Essential steps

- Login
- Workspaces
- Billing accounts
- (R-based) Jupyter notebooks or RStudio for interactive analysis

Cloud computing environment

- Runtime and persistent disk
- Workspace DATA and buckets
- AnVIL package for interaction with workspace components

Workshop Activities

What's the purpose?

- RStudio provides a rich environment for working in R, but Jupyter notebooks are also relevant, e.g., providing a focused analysis for less-experienced collaborators to walk through.

- We'd like to be able to provide users with documentation that is accessible in either environment.
- The documentation should be consistent across environments

Provenance is important

- Who wrote or contributed to the software?
- What does the software do?
- What license is it available under?
- What version of the software is currently in use?

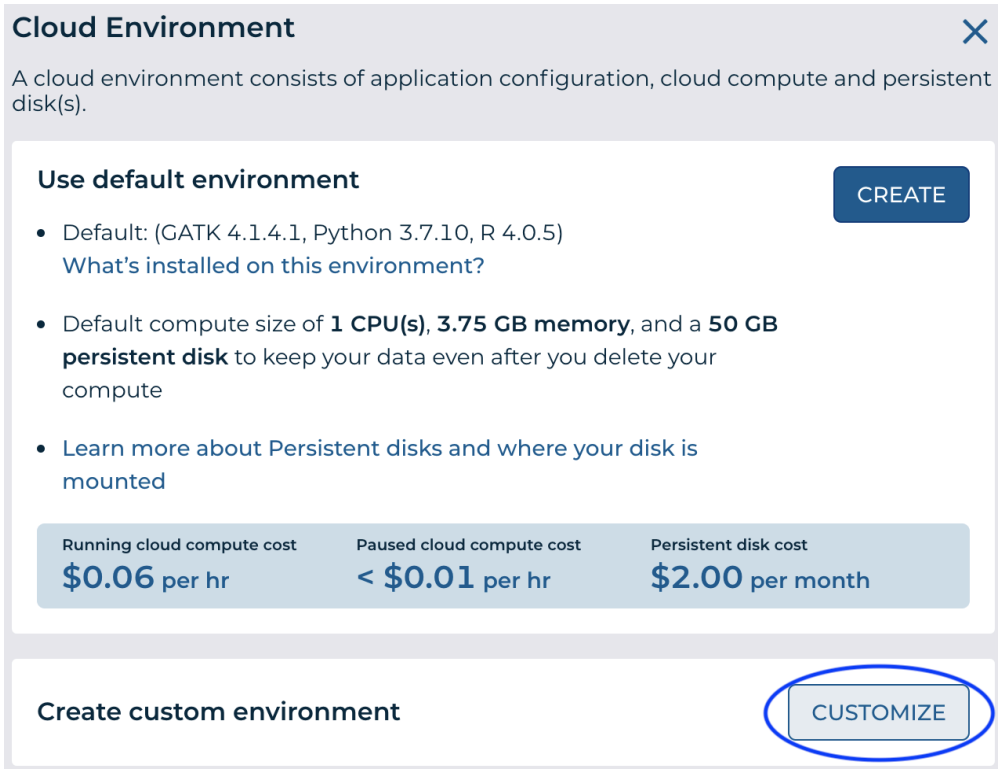
Setup

Setup

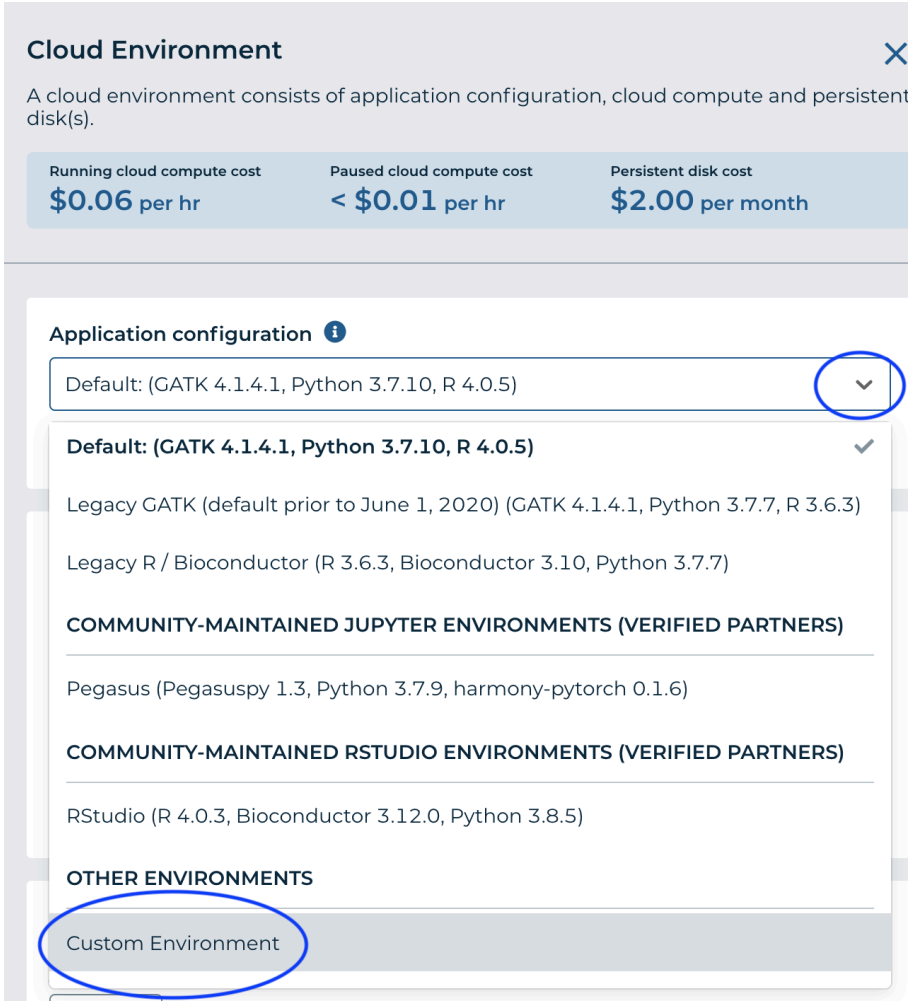
- Log in to AnVIL using the email address you used to register for the course, and navigate (via the HAMBURGER) to Workspaces.
- Clone the Bioconductor-Workshop-AnVILPublish workspace
    - Unique workspace name
    - Billing project: deeppilots-bioconductor-jun7

Start a CUSTOM CLOUD ENVIRONMENT

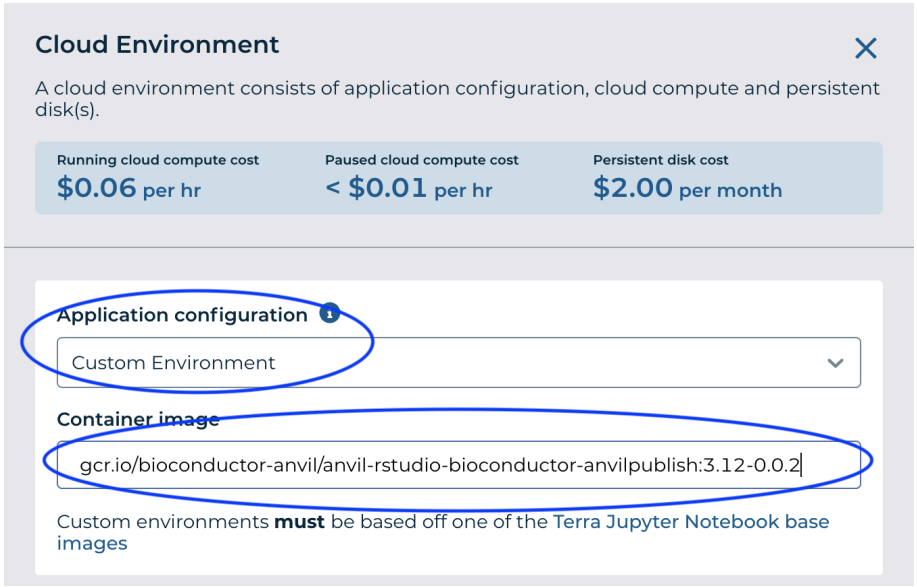
- 'Cloud Environment' in the top right of the workspace, choose 'Customize'



- From the 'Application Configuration' dropdown, choose 'Custom Environment'



- For 'Container Image' enter gcr.io/bioconductor-anvil/anvil-rstudio-bioconductor-anvilpublish:3.12-0.0.2



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R Packages

Create local git clones of the source code of two packages

```
system2("git", c("clone", "https://github.com/Bioconductor/AnVILPublish"))
system2("git", c("clone", "https://github.com/mtmorgan/AnVILPublishDemo"))
```

Simple text-based files organize R code, help pages, vignettes and metadata.

```
AnVILPublishDemo$ tree
.
├── DESCRIPTION
├── NAMESPACE
├── R
│   └── utilities.R
├── README.md
├── man
│   └── utilities.Rd
└── vignettes
    └── A_Introduction.Rmd
```

Packages are extensible, e.g., all files under an 'inst/' directory are installed with the package

```
├── inst
│   ├── docker
│   │   ├── anvil-rstudio-bioconductor-anvilpublish
│   │   │   └── Dockerfile
│   │   └── terra-juptyer-bioconductor-anvilpublish
│   │       └── Dockerfile
│   ├── tables
│   │   └── participants.csv
│   └── workflows
│       └── coming_soon.wdl
```

The DESCRIPTION file provides provenance, including title, version, description, author(s) & their contributions, licensing, as well as system dependencies.

```
Package: AnVILPublishDemo
Title: Simple Demonstration of AnVILPublish Functionality
Version: 0.0.1
Authors@R:
    c(person(
        given = "Martin",
        family = "Morgan",
```

```
        role = c("aut", "cre"),
        email = "mtmorgan.bioc@gmail.com",
        comment = c(ORCID = "0000-0002-5874-8148")
    ))
Description: AnVILPublish is a way to transform R / Bioconductor
    packages, especially vignettes, in Jupyter notebooks for use in
    the AnVIL computational environment. The AnVILPublishDemo package
    illustrates some of this functionality.
License: Artistic-2.0
Encoding: UTF-8
LazyData: true
Roxygen: list(markdown = TRUE)
RoxygenNote: 7.1.1
Suggests:
    knitr,
    rmarkdown
VignetteBuilder: knitr
```

Vignettes

- A natural place to document what the package does in a narrative 'literate programming' manner. If the code in the vignette does not work, then the package does not build and check successfully.
- Vignettes may also contain metadata, e.g., the author and date last revised.

From R Package to AnVIL Workspace

Easy!

```
AnVILPublish::as_workspace(
    "~/AnVILPublishDemo",
    "deeppilots-bioconductor-jun7",
    "AnVILPublishDemo-YOUR_NAME_HERE",
    create = TRUE
)
```

What do we get?

- DASHBOARD: Provenance -- title, authors, description, version, license
- NOTEBOOKS: ready to evaluate under an R kernel
- DATA: tables from packages added. Interpolation of google bucket possible
- All described in the AnVILPublish vignette

Maybe a little surprising…

- The package can be developed on your own computer (for instance), and published from there, provided gcloud software is installed.

A Little Under the Hood: Custom Docker Files

Summary

What You've Accomplished

Appreciated R package structure

- Organizing components of analysis
- Literate programming
- Provenance

Transforming packages to notebooks and workspaces

- Metadata as DASHBOARD entries, including provenance
- Vignettes as Jupyter notebooks
- DATA tables populated from the package
- Coming soon: addition of workflows; creating workspaces for RStudio

Next Steps

- Follow instructions at Set up billing with $300 Google credits to explore Terra to enable billing for your own projects.

Frequently Asked Question

- What docker images can be used as base images for customization? The main images derive from terra-jupyter-bioconductor (for Jupyter-based images) and anvil-rstudio-bioconductor (for RStudio-based images). Any container can be used in a workflow.
- Can you specify the runtime environment as part of the workspace? This does not seem to be possible at the moment. One could include a notebook or other code that checked the runtime to see that it meets particular conditions, but this would rely on the user running the code.
- Enhance reproducibility by 'fixing' package versions, e.g., using packr? Instead, specify precise package versions in a customized Dockerfile.