

---

## **ARC-Finder – A simple, locally-deployed tool to find your peer's research data**

Projektmodul (Modul 9) des Zertifikatskurs FDM (15.07)  
2021 / 2022

Dominik Brilhaus,  
<https://orcid.org/0000-0001-9021-3197>

2022-06-09

## Contents

<b>Introduction</b>	<b>2</b>
Motivation . . . . .	2
DataPLANT and the Annotated Research Context . . . . .	2
<b>Implementation</b>	<b>3</b>
Technical back-end . . . . .	3
The ARC-Finder workflow . . . . .	3
The ARC-Finder GUI . . . . .	5
<b>Discussion</b>	<b>5</b>
<b>Supplemental Material</b>	<b>7</b>
Availability . . . . .	7
Dependencies . . . . .	7
Software . . . . .	7
R libraries . . . . .	7
Platform . . . . .	8
Checks and tests . . . . .	8
Deviation from the original concept . . . . .	8
<b>Scripts</b>	<b>9</b>
arcFinder.sh . . . . .	9
README.md . . . . .	12
ARC-Finder – A simple, locally-deployed tool to find your peer’s research data . . . . .	12
scripts/01_install_dependencies.R . . . . .	13
scripts/01_restore_dependencies.R . . . . .	13
scripts/02_read_from_gitlab.sh . . . . .	13
scripts/03_parse_isaInvxls.R . . . . .	16
scripts/03_pull_together.R . . . . .	19
scripts/05_pull_together_sql.R . . . . .	20
scripts/04_searchApp/app.R . . . . .	20

## Introduction

### Motivation

Research is a highly collaborative endeavor that builds on the synergistic interaction between different stakeholders enabled by efficient knowledge exchange. Gaining a prompt overview of the ongoing research efforts – both pre- and post-publication – is oftentimes hindered for social, legal or technical reasons. This often holds true even between parties of spatially closest and well trusted surroundings of a collaborative consortium such as the Cluster of Excellence on Plant Sciences (CEPLAS<sup>1</sup>). The key to enable discussion on and exchange of research data is *findability*, the first layer of the FAIR principles<sup>2</sup> of data stewardship (Wilkinson *et al.*, 2016<sup>3</sup>). The project presented here aims to address this layer, by making CEPLAS research easily findable and visible amongst CEPLAS researchers and showcase the beauty and ease of data sharing to spike fruitful collaborations with peers.

### DataPLANT and the Annotated Research Context

Research data management (RDM) within CEPLAS is closely aligned with DataPLANT<sup>4</sup>, the NFDI<sup>5</sup> consortium for plant sciences. At the heart of DataPLANT’s RDM strategy lies the Annotated Research Context (ARC<sup>6</sup>), a directory structure that packages research data together with associated metadata and computational workflows into self-sustained research objects. Annotation of research data in the ARC is based on the metadata schema ISA<sup>7</sup> (for investigation – study – assay). Serialized in spread sheet format as *ISA-tab* this enables intuitive, flexible and yet structured and conclusive metadata annotation of the versatile data types produced in plant sciences. ARCs are git<sup>8</sup> repositories that can be shared via DataPLANT’s DataHUB<sup>9</sup>, a customized GitLab<sup>10</sup> instance with a federated authentication interface to allow controlled access across institute borders.

Although the ARC environment is continuously being developed, the choice of these key technical pillars are set: (a) ARC as the structure, (b) ISA as the metadata language, (c) git as version control logic and (d) gitlab for ARC collaboration and user management. This allows to leverage the ARC environment and develop (intermediate) solutions for data findability, knowing that time and efforts are well-invested, since both (meta)data ingest into as well as secondary outputs dependent on the

---

<sup>1</sup>CEPLAS, <https://ceplas.eu>

<sup>2</sup>GO-FAIR, <https://www.go-fair.org/fair-principles/>

<sup>3</sup>Wilkinson, M., Dumontier, M., Aalbersberg, I. et al. The FAIR Guiding Principles for scientific data management and stewardship. *Sci Data* 3, 160018 (2016). <https://doi.org/10.1038/sdata.2016.18>

<sup>4</sup>DataPLANT, <https://nfdi4plants.de>

<sup>5</sup>Nationale Forschungsdaten Infrastruktur, <https://www.nfdi.de/>

<sup>6</sup>ARC specifications, <https://github.com/nfdi4plants/ARC-specification/>

<sup>7</sup>ISA Metadata Schema, <https://isa-tools.org/>

<sup>8</sup>Git, <https://git-scm.com/>

<sup>9</sup>DataPLANT DataHUB, <https://git.nfdi4plants.org>

<sup>10</sup>GitLab, <https://gitlab.com>

ARC will be adoptable and migratable in the future.

While (contents of the) ARCs can be searched via standard GitLab-implemented mechanisms within the DataHUB or via standard routines on a user’s system where the ARCs are locally cloned and stored, a structured and user-friendly search interface tailored to metadata stored in multiple ARCs – including unpublished ARCs – is currently unavailable. With the ARC-Finder presented here, I seek to close this gap with a lightweight quickfix.

## Implementation

### Technical back-end

The technical back-end of the ARC-Finder is a combination of shell and R scripts. For data retrieval it leverages the GitLab API <sup>11</sup>. The GUI is based on RStudio’s ShinyApp<sup>12</sup>. The design idea was to rely on as few programming language environments as possible. The actual code work is attached in the supplemental materials (see scripts) and available online (see availability). Software dependencies are listed in the supplemental materials (see dependencies).

### The ARC-Finder workflow

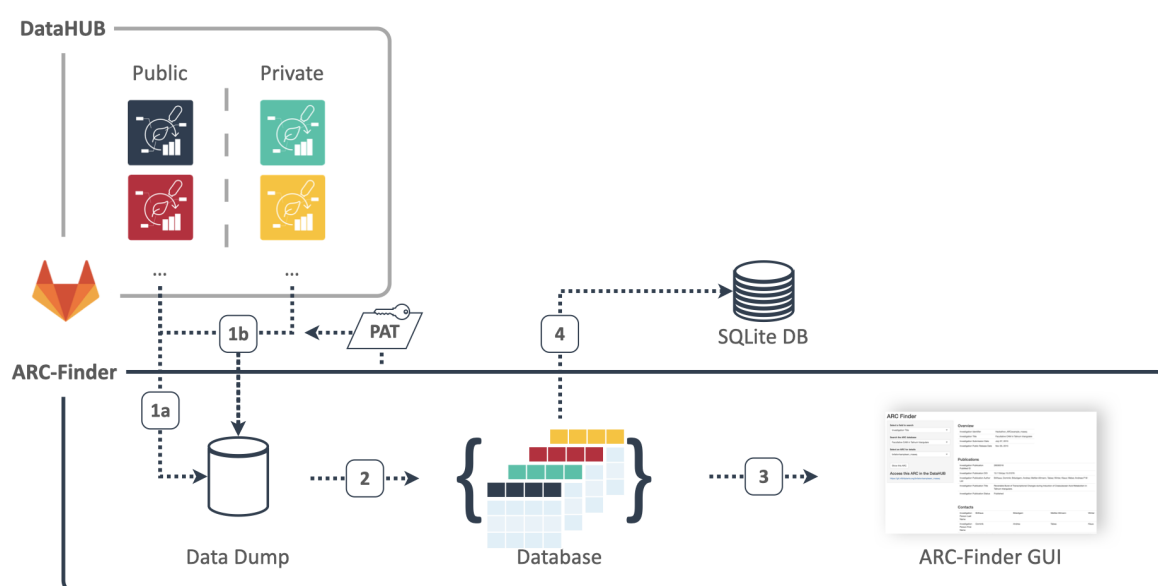
The ARC-Finder employs three concerted, but independent modules of metadata retrieval, restructure, and representation (Fig. 1).

The ARC-Finder can be run in two modes. If the user does not supply a gitlab personal access token (PAT), the ARC-Finder retrieves metadata only from publicly accessible ARCs. If a functional PAT is provided by the registered user, metadata is retrieved from both public and privately shared ARCs. For detailed user instructions see README.md. The ARC-Finder selectively scans all user-accessible ARCs only for the ISA investigation workbooks (`isa.investigation.xlsx`) stored at the root of every ARC. The identified workbooks are downloaded and dumped locally in a temporary folder on the user’s machine. Next, the ARC-Finder restructures the investigation-level metadata into a simple spreadsheet-based database. From the database the metadata is fed into and represented by the ARC-Finder graphical user interface (GUI).

---

<sup>11</sup>GitLab Application Programming Interface (API), <https://docs.gitlab.com/ee/api/>

<sup>12</sup>ShinyApps, <https://www.shinyapps.io/>



**Figure 1: The ARC-Finder Workflow.** Depending whether the user provided a gitlab personal access token (PAT), the ARC-Finder retrieves publicly (1a) or publicly and privately (1b) accessible metadata from the DataHUB and stores it in a local data dump. The metadata is restructured into a searchable database (2) and fed into the ARC-Finder graphical user interface (GUI) for clear representation (3, details see Fig. 2) as well as provided as an SQLite database (DB) (4).

## The ARC-Finder GUI

The ARC-Finder GUI is a responsive ShinyApp running in the user’s default web browser (Fig. 2). Three dropdown search fields build the core of the GUI’s *Query Panel*. The user can select to search any or a specific metadata attribute (Fig. 2 - Field 1) for specific terms provided as free-text or selected from the search field (Fig. 2 - Field 1). Matching ARCs are listed for selection in a dropdown menu (Fig. 2 - Field 3). Once an ARC is selected, a click on the “Show this ARC” button (Fig. 2 - Field 4) reveals the metadata associated with the ARC in the *Result Panel* and provides a link to the respective ARC in the DataHUB (Fig. 2 - Field 5).

**ARC Finder**

1 Select a field to search  
Investigation Title

2 Search the ARC database  
Facultative CAM in Talinum triangulare

3 Select an ARC for details  
brilator/samplearc\_maseq

4 Show this ARC

5 Access this ARC in the DataHUB  
[https://git.nfdi4plants.org/brilator/samplearc\\_maseq](https://git.nfdi4plants.org/brilator/samplearc_maseq)

**Query Panel**

**Result Panel**

**Overview**

Investigation Identifier	Hackathon_ARCexample_maseq
Investigation Title	Facultative CAM in Talinum triangulare
Investigation Submission Date	July 07, 2015
Investigation Public Release Date	Nov 05, 2015

**Publications**

Investigation Publication PubMed ID	28530316
Investigation Publication DOI	10.1104/pp.15.01076
Investigation Publication Author List	Brilhaus, Dominik; Bräutigam, Andrea; Mettler-Altmann, Tabea; Winter, Klaus; Weber, Andreas P M
Investigation Publication Title	Reversible Burst of Transcriptional Changes during Induction of Crassulacean Acid Metabolism in Talinum triangulare.
Investigation Publication Status	Published

**Contacts**

Investigation Person Last Name	Brilhaus	Bräutigam	Mettler-Altmann	Winter
Investigation Person First Name	Dominik	Andrea	Tabea	Klaus
Investigation Person Email	dominik.brilhaus@nhu.de	NA	NA	NA

**Figure 2: The ARC-Finder GUI** is divided into two panels. The user can search for available ARCs in the *Query Panel* (left, details elaborated in the text). Investigation-level metadata of the selected ARC is presented in the *result panel* (right).

## Discussion

With the ARC-Finder presented here, I tried to tackle a common challenge of RDM within CEPLAS (and likewise many other collaborative research consortia): easy and structured findability of research data of peers, including unpublished datasets that are just in the making. The ARC-Finder is built on the developments within DataPLANT surrounding the ARC environment and especially relies on the ISA metadata model and the GitLab-backed DataHUB.

Leveraging on the ARC environment, the ARC-Finder follows a comparably straight-forward approach and yields an instantaneous benefit to the researcher. Metadata provided by the user to collaboration partners via the DataHUB becomes immediately searchable via the ARC-Finder. While advocating FAIR data stewardship to the users (e.g. plant researchers), one of the major hurdles is the continuously changing plethora of platforms and tools offering one or the other RDM service (supposedly in a better way than competitors). This can range from a variation of electronic lab notebooks, cloud services, wikis, repositories or even chat software, leaving the researcher frustrated and unwilling to use (or adopt to) yet another RDM platform in the future. The ARC-Finder show-cases how the use of established standards, the ISA metadata model and git, facilitates extensibility and boosts sustainable RDM. Even if the tool itself may not see a long-term interest, it serves a quick benefit, while all metadata provided to the DataHUB will be integrable with future developments, including a more sophisticated metadata registry. This avoids user friction and makes the ARC environment more appealing to the researchers. To provide an example for an alternative output, the ARC-Finder stores the structured data as an SQLite database (termed `yourARCs_database.sqlite`) for use in third party applications, Fig. 1 - Field 4).

While the ARC-Finder can list unpublished and thus possibly sensitive data, it does not itself handle any user rights. Data safety and access management depends on the authentication mechanisms provided by the DataHUB. Here, access to the ARCs can be controlled to share them publicly or with invited collaborators. Still, by design the ARC-Finder focuses on metadata at the highest project and least sensitive (i.e. ISA’s “investigation”) level to minimize possible discomfort with data sharing.

The simple design of the ARC-finder comes with a few caveats and leaves room for future improvements. For reasons of simplicity and data safety (see above), the depth of metadata findability is limited to the investigation-level, ignoring the biologically more relevant study and assay levels of the ISA model. Furthermore, only those ARCs shared by individual users (not groups) are included and the ARC-Finder only searches the default `main` branch of the ARCs git backend. Both limitations could be easily extended in future versions of the ARC-Finder.

Several design decisions limit the ARC-finder’s efficiency and scalability. The ARC-Finder is solely deployed locally and does not store any data or interaction on a server-side. Every time the ARC-Finder is run, it removes and overwrites the temporary database from earlier runs rather than updating or appending to it. In the current version, the user cannot make any pre-selection about the scope of ARCs to be searched, e.g. only ARCs associated to a specific user or group. Thus every ARC-Finder run scans and retrieves data from all available ARCs. Two paralleling serializations of ISA metadata exist in the ARC. The user-centered ISA workbooks (e.g. `isa.investigation.xlsx`) allow for intuitive metadata annotation. However, depending on the complexity of the ARC as well as the user input, these files can easily become relatively big adding to the efficiency issue. For programmatic interaction all ISA metadata in the ARC can be exported to the lightweight and less error-prone JSON format (termed `arc.json`). The decision to center the ARC-Finder around the `isa.investigation.xlsx` workbook was made to spare another dependency detour to convert between formats.

## Supplemental Material

### Availability

The ARC-Finder is available for download at <https://github.com/Brilator/arcFinder>.

### Dependencies

#### Software

**Table 1:** Software used during development, testing and writing.

Software	Version	Platform
GNU bash	3.2.57(1)-release	x86_64-apple-darwin21
curl	7.79.1	x86_64-apple-darwin21.0
R	4.2.0	x86_64-apple-darwin17.0
RStudio	2022.02.2 Build 485	-
Visual Studio Code	1.67.2	-
Codes Spell Checker (VS Code Extension)	2.03	-
pandoc	2.18	-
TeX Live 2022	MacTeX-2022	-

#### R libraries

To provide best reproducibility, R package dependencies are handled via [renv](#)<sup>13</sup> (version 0.15.3) and stored in the root file “renv.lock”. In the first step of [arcFinder](#), the virtual environment is automatically restored, including installation of all required dependencies. Depending on the local setup (installation of R and packages), this may take some time. However, [renv](#) prevents interference with the local setup, thus keeping the system intact.

**Table 2:** R packages specifically loaded for individual R scripts

Package (version)	Main purpose	Used in script(s)
renv_0.15.4	Manage R package dependencies	01_install_dependencies.R 01_restore_dependencies.R

<sup>13</sup>R package “renv”, <https://rstudio.github.io/renv/>



**Table 2:** R packages specifically loaded for individual R scripts

Package (version)	Main purpose	Used in script(s)
readxl_1.4.0 (part of ‘tidyverse’)	Read data from Microsoft Excel workbooks	03_parse_isaInvxlsx.R
tidyverse_1.3.1	Tidy data into a useful format	04_searchApp/app.R
shiny_1.7.1	Prepare and launch a shiny app	04_searchApp/app.R
DBI_1.1.2	Write data to an ‘*.sqlite’ object	05_pull_together_sql.R

## Platform

The DataPLANT’s DataHUB<sup>14</sup> is a customized instance of GitLab<sup>15</sup>, currently running under version 14.10.2, hosted and maintained by the DataPLANT node at Albert-Ludwigs-University Freiburg. Data is retrieved from the DataHUB via GitLab API version 4.

After registration<sup>16</sup> with DataPLANT, users can share and access non-public ARCs via the DataHUB. As explained in the [arcFinder](#)’s README, a GitLab private access token (PAT) needs to be generated within the DataHUB and provided to [arcFinder](#).

## Checks and tests

Currently tested only under macOS Monterey 12.3.1 (x86\_64-apple-darwin17.0, 64-bit) with software versions specified under Dependencies.

## Deviation from the original concept

The originally proposed concept targeted an automated workflow for easier metadata-ingestion from previously published manuscripts into an the ISA model of an ARC. As this workflow (a) targets a completely other “side” of the ARC and DataHUB environment and thus (b) comes with multiple additional and more complicated dependencies, it was omitted from the ARC-Finder presented here.

<sup>14</sup>DataPLANT DataHUB, <https://git.nfdi4plants.org>

<sup>15</sup>GitLab, <https://gitlab.com>

<sup>16</sup>DataPLANT registration, <https://register.nfdi4plants.org/>

## Scripts

### arcFinder.sh

```

1 #####
2 ### Create root folder for temporary data
3 #####
4
5 ### If exists, remove and create fresh.
6 ### This is to prevent data piling.
7 ### TODO Should probably be replaced with safer / better logic for
  debugging. TODO
8
9 if [ -d ".tmp/" ]; then
10     rm -r .tmp/
11     mkdir .tmp/
12 else
13     mkdir .tmp/
14 fi
15
16 #####
17 ### Restore env session
18 #####
19
20 echo "### Restore virtual environment"
21 echo "-----"
22
23 Rscript ./scripts/01_restore_dependencies.R 2>&1 >> .tmp/01.log
24
25 #####
26 ### Read GitLab personal access token (PAT)
27 #####
28
29 ### Read GitLab PAT from -p flag
30
31 while getopts p: flag
32 do
33     case "${flag}" in
34         p) gitlab_pat=${OPTARG};;
35     esac
36 done
37
38 ### Check if argument supplied with `-p` is a file.
39 ### If yes, read that file.
40 ### If not, use the input (PAT as a string) directly
41
42 if [ -f "$gitlab_pat" ]; then
43     echo "Using GitLab token stored in '$gitlab_pat'."
44     gitlab_pat=$(< $gitlab_pat)
45 fi

```

```

46
47 ### check if string is empty
48
49 [ -z "$gitlab_pat" ] && printf "No GitLab token supplied or GitLab
    token is empty. \nReading from public ARCs only.\n"
50
51 #####
52 ### Run gitlab reader
53 #####
54
55 echo "-----"
56 echo "### Step 01: Downloading metadata of available ARCs from the
    DataHUB."
57 echo "-----"
58
59 echo "log of 02_read_from_gitlab.sh" > .tmp/02.log
60 bash ./scripts/02_read_from_gitlab.sh -p "${gitlab_pat}" 2>&1 >> .tmp
    /02.log
61
62 #####
63 ### Run xlsx parser
64 #####
65
66 ## store paths of isa.investigation.xlsx files into variable
67 ## while loop
68 ## - extract arc id from part of path
69 ## - run script with arc id and path
70
71 echo "### Step 02: Structuring ARC metadata."
72 echo "-----"
73 echo "log of 03_parse_isaInvxlsx.R" > .tmp/03.log
74
75 invs=$(find .tmp/02_investigations -name '*.xlsx' | sort -n)
76 echo "$invs" | while IFS= read -r current_inv_path;
77 do
78     arc_id=$(echo $current_inv_path | cut -d/ -f3 | cut -d"_" -f1)
79
80     Rscript ./scripts/03_parse_isaInvxlsx.R "$arc_id" $current_inv_path
        2>&1 >> .tmp/03.log
81
82 done
83
84
85 #####
86 ### Pull together data
87 #####
88
89 echo "### Step 03: Building a searchable database of ARC metadata"
90 echo "-----"
91
92 Rscript ./scripts/03_pull_together.R 2>&1 >> .tmp/03.log

```

```
93
94 #####
95 ### Optional: Prepare SQLite database
96 #####
97
98 Rscript ./scripts/05_pull_together_sql.R 2>&1 >> .tmp/05.log
99
100 #####
101 ### Run the search APP
102 #####
103
104 echo "### Voila: The ARC Finder is running in your default browser."
105 echo "### Close the browser window or tab to shut down the app."
106
107 Rscript -e 'load(".tmp/03_allARCs.RData"); shiny::runApp("./scripts/04
    _searchApp/app.R", launch.browser = TRUE)' 2>&1 >> .tmp/04.log
```

## README.md

### ARC-Finder – A simple, locally-deployed tool to find your peer’s research data

This is a tool to help you find metadata about ARCs stored in the DataPLANT DataHUB. Visit the DataPLANT website for more information about ARCs (annotated research contexts).

### Usage

- Git clone or download this repository.
- Open a command line or terminal and navigate to the `arcFinder` directory.
- Run one of the following two options:

#### Option 1: Search public ARCs only

```
1 ./arcFinder.sh
```

#### Option 2: Search Public + privately shared ARCs

Note: Replace `<gitlab pat>` with the path pointing to a file which stores a GitLab personal access token (PAT).

```
1 ./arcFinder.sh -p <gitlab pat>
```

**Registration with DataPLANT** In order to use the `<gitlab pat>` option, please follow these steps:

1. Sign up with DataPLANT.
2. Generate a personal access token in the DataHUB PAT settings
  - Provide a “Token name”, e.g. `arcFinder`
  - Select either option “api” or “read\_api” and click “Create personal access token”
  - Copy the generated token on top of the page.
3. Paste the bare token into a text file and save it (e.g. `gitlab_token` stored in the root of this directory)
4. Supply the file path to `arcFinder`, e.g.:

```
1 ./arcFinder.sh -p gitlab_token
```

**scripts/01\_install\_dependencies.R**

```
1 #####
2 ### Script to install all R dependencies
3 #####
4
5
6 if(!require(tidyverse, quietly = TRUE)){install.packages("tidyverse")}
7 if(!require(DBI, quietly = TRUE)){install.packages("DBI")}
8 if(!require(shiny, quietly = TRUE)){install.packages("shiny")}
9 if(!require(renv, quietly = TRUE)){install.packages("renv")}
10
11 renv::init(bare = T)
12
13 # save library state to lockfile
14 renv::snapshot()
15
16 renv::status()
```

**scripts/01\_restore\_dependencies.R**

```
1
2 #####
3 ### Restore R virtual environment via renv
4 #####
5
6 # restore lockfile, thereby installing dependencies from renv.lock
7
8 renv::restore()
```

**scripts/02\_read\_from\_gitlab.sh**

```
1 #!/usr/bin/env bash
2
3 #####
4 ### Script to skim GitLab for accessible ARCs and
5 ### retrieve their isa.investigation.xlsx's
6 #####
7
8 ### Goal
9 # 1. read gitlab pat
10 # 2. Store a list of all available projects (e.g. tab)
11 # 3. Iterate over project trees
12 #   - check for isa.investigation file
13 #   - present: download raw and dump to temp
14 #   - absent: leave loop
```

```
15
16 #####
17 ### Read GitLab token (PAT)
18 #####
19
20 ### Read GitLab PAT from -p flag
21
22 while getopts p: flag
23 do
24     case "${flag}" in
25         p) gitlab_pat=${OPTARG};;
26     esac
27 done
28
29 # ### Check if argument supplied with `-p` is a file.
30 # ### If yes, read that file.
31 # ### If not, use the input (PAT as a string) directly
32
33 # if [ -f "$gitlab_pat" ]; then
34 #     echo "Using GitLab token stored in '$gitlab_pat'."
35 #     gitlab_pat=$(< $gitlab_pat)
36 # else
37 #     echo "Using supplied GitLab token"
38 #     # This would be gitlab_pat=$gitlab_pat    ### TODO: probably safer
39 #     # to change this
40 # fi
41
42 # ### check if string is empty
43 # [ -z "$gitlab_pat" ] && printf "No GitLab token supplied or GitLab
44 # token is empty. \nReading from public ARCs only.\n"
45
46 #####
47 ### List available ARCs
48 #####
49
50 # Writing to json first
51 curl --silent --request GET --header "PRIVATE-TOKEN: $gitlab_pat" "
52     https://git.nfdi4plants.org/api/v4/projects/" > .tmp/02
53     _arcs_available.json
54
55 # grepping project IDs
56 grep -oE '"id": [0-9]{1,}, "description"' .tmp/02_arcs_available.json |
57     grep -oE '[0-9]{1,}' > .tmp/02_arcs_ids
58
59 # Could be piped directly (without the temporary .json)
60 # But will keep the json, for trouble-shooting
61 # curl --request GET --header "PRIVATE-TOKEN: $gitlab_pat" "https://git
62 # .nfdi4plants.org/api/v4/projects/" | grep -oE '"id": [0-9]{1,}, "
63 # description"' | grep -oE '[0-9]{1,}' > projects_list
```

```
59
60
61 #####
62 ### Iterate over ARCS
63 #####
64
65 ### create a dump directory for the isa.investigation.xlsx files
66 if ! [ -d ".tmp/02_investigations" ]; then mkdir ".tmp/02
    _investigations"; fi
67
68 ### write a table to collect ARC id and path with namespace
69 printf "ARC id\tARC path\tcomment" > .tmp/02_investigations/arc_list.
    tsv
70
71 all_arc_IDs=$(< .tmp/02_arcs_ids)
72 echo "$all_arc_IDs" | while IFS= read -r arc_id;
73 do
74     # echo $arc_id
75
76     ### get project info
77     curl --silent --header "PRIVATE-TOKEN: $gitlab_pat" "https://git.
        nfdi4plants.org/api/v4/projects/$arc_id" > .tmp/02
        _current_arc_info.json
78
79     ### extract git path with namespace
80     arc_path=$(grep -oE '"path_with_namespace": ".*", "created_at' .tmp/02
        _current_arc_info.json | cut -d'"' -f 4)
81
82     echo $arc_path
83
84     ### get project tree
85     curl --silent --header "PRIVATE-TOKEN: $gitlab_pat" "https://git.
        nfdi4plants.org/api/v4/projects/$arc_id/repository/tree" > .tmp/02
        _current_arc_tree.json
86
87     ### check that file `isa.investigation.xlsx` exists at ARC root
88     ### if yes: download and dump
89     ### if no: error message
90
91     inv_path=$(grep -oE '"path": "isa.investigation.xlsx",' .tmp/02
        _current_arc_tree.json)
92
93     ### check if variable is empty
94     if [ -z "$inv_path" ]
95     then
96         printf "Missing 'isa.investigation.xlsx' at the root of $arc_path\n
            "
97         printf "\n$arc_id\t$arc_path\tisa.investigation.xlsx missing" >> .
            tmp/02_investigations/arc_list.tsv
98     else
```



```

99     curl -L --silent --request GET --header "PRIVATE-TOKEN: $gitlab_pat
      " "https://git.nfdi4plants.org/api/v4/projects/$arc_id/
      repository/files/isa%2Einvestigation%2Exlsx/raw?ref=main" -o .
      tmp/02_investigations/$arc_id'_isa.inv.xlsx'
100     printf "\n$arc_id\t$arc_path\tisa.investigation.xlsx detected" >> .
      tmp/02_investigations/arc_list.tsv
101     fi
102
103     rm .tmp/02_current_arc*
104
105 done

```

### scripts/03\_parse\_isaInvxlsx.R

```

1
2 #####
3 ### Script to read metadata from an isa.investigation.xlsx
4 #####
5
6 ## rough idea:
7
8 # 0. Takes two arguments as CLI input: <ARC id> and <isa.investigation.
   xlsx>
9 # 1. Check whether its an investigation sheet or loop over sheets
10 # 2. focus on investigation only
11 # 3. subset into investigation sections
12 # 4. Store JSON-like as (nested) lists
13 #   - column 1 = keys
14 #   - column(s) 2:n = values as a list
15 # 5. put out as RData for further processing
16
17
18 #####
19 ### Setup
20 #####
21
22 ### If package "readxl" is not installed, install it.
23 # if(!require("readxl", quietly = TRUE)){install.packages("readxl")}
24
25 ### load the package
26 library(readxl)
27
28
29 #####
30 ### Inputs
31 #####
32
33 args = commandArgs(trailingOnly=TRUE)
34

```

```
35 # test if arguments are supplied: if not, return an error
36 if (length(args)!=2) {
37
38     stop("<ARC id> and <isa.investigation.xlsx> must be supplied as
        arguments", call.=FALSE)
39
40 } else if (length(args)==2) {
41
42     # default output file
43     isa_inv_wb <- args[2]
44     print(paste("Reading file", isa_inv_wb))
45     arc_id <- args[1]
46 }
47
48 #####
49 ### read data from excel
50 #####
51
52 ### loop over sheets of workbook
53 for(sheet in excel_sheets(isa_inv_wb)){
54
55     ### read sheet
56     current_sheet <- as.data.frame(read_xlsx(isa_inv_wb, col_names = F,
        sheet = sheet, .name_repair = "minimal"))
57
58     ### Simple sanity check for ISA investigation format
59
60     if(current_sheet[1, 1] == "ONTOLOGY SOURCE REFERENCE" & current_sheet
        [2, 1] == "Term Source Name"){
61
62         print(paste("Reading from excel sheet", sheet))
63         invdata <- current_sheet
64
65     }else{
66         print(paste("Excel sheet", sheet, "is not in ISA investigation
            format"))
67         invdata <- NULL
68     }
69
70 }
71
72 ### Stop if no proper ISA sheet detected
73 if(is.null(invdata)){stop(simpleError("No valid ISA investigation sheet
        detected"))}
74
75
76 #####
77 ### wrangle / extract only relevant data
78 #####
79
80
```

```

81 ### subset to investigation only (excluding study, assay layers)
82 investigation_data <- invdata[grepl("^investigation", invdata[, 1],
83   ignore.case = T), ]
84
85 ### first column as row names
86 rownames(investigation_data) <- investigation_data[,1]
87 investigation_data2 <- investigation_data[,-1, drop = F]
88
89 ### extract investigation subsections (some redundancy with above)
90 inv_sections <- which(grepl("^INVESTIGATION", row.names(investigation_
91   data2), ignore.case = F))
92
93 investigation_list <- list()
94 for(i in 1:length(inv_sections))
95 {
96   if(i == length(inv_sections))
97   {
98     section_range <- (inv_sections[i] + 1):nrow(investigation_data2)
99   }else{
100     section_range <- (inv_sections[i] + 1):(inv_sections[i+1] - 1)
101   }
102
103   current_section <- investigation_data2[section_range, , drop =F]
104
105   ### remove columns that are only NA
106   current_section <- current_section[, apply(current_section, 2,
107     function(x){sum(is.na(x)) != nrow(current_section)}), drop = F]
108
109   ### transpose / pivot data to transform into list
110   current_section_transposed <- as.data.frame(t(current_section))
111   rownames(current_section_transposed) <- NULL
112
113   # TODO stupid work-around to circumvent the bug with a section having
114   # only NAs
115   if(nrow(current_section_transposed) == 0){current_section_transposed
116     [1, ] = NA}
117
118   current_section_transposed$arc_id <- arc_id
119
120   ### extract current section name
121   current_section_name <- row.names(investigation_data2)[inv_sections[i]]
122
123   # ### transform to named list, omitting NAs
124   # investigation_list[[current_section_name]] <- lapply(current_
125     section_transposed, function(v){v[!is.na(v)]})
126
127   #
128   # stack(current_section_transposed)

```

```

124   investigation_list[[current_section_name]] <- current_section_
      transposed
125
126 }
127
128 #####
129 ### output to .RData
130 #####
131
132 if(!dir.exists(".tmp/03_rdata_dumps/")){dir.create(".tmp/03_rdata_dumps
      /")}
133
134 print(paste0("Storing outputs in: .tmp/03_rdata_dumps/", arc_id, ".
      Rdata"))
135
136 save(investigation_list, isa_inv_wb, arc_id, file = paste0(".tmp/03_
      rdata_dumps/", arc_id, ".RData"))

```

### scripts/03\_pull\_together.R

```

1 #####
2 ### Script to pull together output of previous scripts
3 #####
4
5 ### for loop over available RData dumps from 03_parse_isaInvxlsx.R
6
7 all_arcs <- list()
8
9 for(i in dir(".tmp/03_rdata_dumps/", full.names = T, pattern = ".RData"
      ))
10 {
11   ### load the data
12   load(i)
13
14   ### store in named list
15
16   all_arcs[[arc_id]] <- investigation_list
17 }
18
19
20 ### row-bind the second-level (i.e. INVESTIGATION "sections") of the
      lists, respectively
21
22 all_arcs_db <- do.call(Map, c(f = rbind, all_arcs))
23
24 ### read the arc_list (translating the ARC id to the ARC path) produced
      by 02_read_from_gitlab.sh
25 ### and append to above list
26

```

```
27 arc_list <- read.table(".tmp/02_investigations/arc_list.tsv", sep = "\t", header = T)
28 colnames(arc_list)[1] <- "arc_id"
29
30 # all_arcs_db[["arc_list"]] <- arc_list
31
32 ### store the output as RData
33
34 save(all_arcs, all_arcs_db, arc_list, file = ".tmp/03_allARCs.RData")
```

### scripts/05\_pull\_together\_sql.R

```
1 #####
2 ### Convert data into SQLite database
3 #####
4
5 # if(!require("DBI", quietly = TRUE)){install.packages("DBI")}
6 library(DBI)
7
8 load(".tmp/03_allARCs.RData")
9
10 ### Write into an SQLite DB file
11
12 mydb <- dbConnect(RSQLite::SQLite(), "yourARCs_database.sqlite")
13
14 for(i in names(all_arcs_db))
15 {
16   dbWriteTable(mydb, i, all_arcs_db[[i]], overwrite = T)
17 }
18
19 dbWriteTable(mydb, "ARC list", arc_list, overwrite = T)
20
21 dbListTables(mydb)
22 dbDisconnect(mydb)
```

### scripts/04\_searchApp/app.R

```
1 #####
2 ### The ARC-Finder GUI Shiny App
3 #####
4
5 suppressMessages(library(tidyverse))
6 suppressMessages(library(shiny))
7
8 # load(".tmp/03_allARCs.RData")
9
```

```

10  ### Flatten ALL values into a 3-column (arc_id | key | value) df to
    provide search across "any field"
11
12  all_values <- do.call(
13    rbind.data.frame, lapply(all_arcs_db, function(x){
14      pivot_longer(x, cols = setdiff(colnames(x), "arc_id"), values_drop_na
        = T)}))
15
16  all_values <- as.data.frame(all_values)
17
18  arc_list <- unique(arc_list)
19
20  shinyApp(
21    ui = pageWithSidebar(
22      headerPanel("ARC Finder"),
23      sidebarPanel(
24        selectizeInput('search_key', 'Select a field to search',
25          choices = c("Any field", unique(all_values$name))),
26        uiOutput("search_field"),
27        selectInput(inputId = "arc_path", label = "Select an ARC
28          for details", choices = NULL),
29        br(),
30        actionButton("go", "Show this ARC"),
31        h3("Access this ARC in the DataHUB"),
32        uiOutput("arc_gitlab"),
33      ),
34    mainPanel(
35      h3("Overview"),
36      tableOutput("table_INV"),
37      br(),
38      h3("Publications"),
39      tableOutput("table_INV_PUBS"),
40      br(),
41      h3("Contacts"),
42      tableOutput("table_INV_Contacts")
43    )
44  ),
45  server = function(input, output, session) {
46
47    ##### reactive input field for text-search
48
49
50
51
52    output$search_field <- renderUI({
53
54      # check whether user wants to filter by cyl;
55      # if not, then filter by selection
56      if ('Any field' %in% input$search_key) {

```

```
57     df <- all_values
58   } else {
59     df <- subset(all_values, name == input$search_key)
60   }
61
62
63   selectizeInput('search_value', 'Search the ARC database', choices
64     = c("", sort(unique(df$value))))
65 })
66
67 ##### ARC choices (arc_id) matching user-input
68
69   arc_choices_id <- reactive({
70
71     if ('Any field' %in% input$search_key) {
72
73       subset(all_values, value == input$search_value, arc_id, drop
74         = T)
75
76     } else {
77
78       subset(all_values, name == input$search_key & value == input$
79         search_value, arc_id, drop = T)
80
81     }
82   })
83
84   ### retrieve path for matching ARCs from arc list
85
86   arc_choices_path <- reactive({
87
88     subset(arc_list, arc_id %in% arc_choices_id(), ARC.path, drop =
89       T)
90
91   })
92
93   ##### reactive ARC selection: updated Input to let user pick from
94
95   observe({
96     updateSelectInput(session = session, inputId = "arc_path",
97       choices = arc_choices_path())
98   })
99
100   ##### User's ARC choice
101
102   selected_arc <- eventReactive(input$go, {
```

```

103
104     all_arcs[[as.character(subset(arc_list, ARC.path %in% input$arc
105                                _path, arc_id, drop = T))]]
106   })
107
108
109   ##### render table INVESTIGATION
110
111   output$table_INV <- renderTable(colnames = F, rownames = F, {
112
113     selected_table <- selected_arc()$INVESTIGATION
114     selected_table <- selected_table[, -which(colnames(selected_
115                                                table) == "arc_id")]
116
117     selected_table$pivot_col <- row.names(selected_table)
118     long <- pivot_longer(selected_table, setdiff(colnames(
119         selected_table), "pivot_col"), values_drop_na = T)
120
121     pivot_wider(long, names_from = pivot_col)
122   })
123
124   ##### render table INVESTIGATION PUBLICATIONS
125
126   output$table_INV_PUBS <- renderTable(colnames = F, rownames = F
127     , {
128
129     selected_table <- selected_arc()$`INVESTIGATION PUBLICATIONS`
130     selected_table <- selected_table[, -which(colnames(selected_
131                                                table) == "arc_id")]
132
133     selected_table$pivot_col <- row.names(selected_table)
134     long <- pivot_longer(selected_table, setdiff(colnames(
135         selected_table), "pivot_col"), values_drop_na = T)
136
137     pivot_wider(long, names_from = pivot_col)
138   })
139
140   ##### render table INVESTIGATION CONTACTS
141
142   output$table_INV_Contacts <- renderTable(colnames = F, rownames
143     = F, {
144
145     selected_table <- selected_arc()$`INVESTIGATION CONTACTS`
146     selected_table <- selected_table[, -which(colnames(selected_
147                                                table) == "arc_id")]

```



```
146     selected_table$pivot_col <- row.names(selected_table)
147     long <- pivot_longer(selected_table, setdiff(colnames(
148         selected_table), "pivot_col"), values_drop_na = T)
149     pivot_wider(long, names_from = pivot_col)
150
151   })
152
153   ##### render link to gitlab
154
155     output$arc_gitlab <- renderUI(a(href = paste0('https://git.
156         nfdi4plants.org/', input$arc_path),
157         paste0('https://git.nfdi4plants
158             .org/', input$arc_path) ,
159         target="_blank"))
160
161     session$onSessionEnded(function() {
162         stopApp()
163     })
164 }
```