

Package ‘FAIRmaterials’

June 24, 2024

Title Ontology Tools with Data FAIRification in Development

Version 0.4.2

Description Translates several CSV files with ontological terms and corresponding data into RDF triples. These RDF triples are stored in OWL and JSON-LD files, facilitating data accessibility, interoperability, and knowledge unification. The triples are also visualized in a graph saved as an SVG. The input CSVs must be formatted with a template from a public Google Sheet; see README or vignette for more information. This is a tool is used by the SDLE Research Center at Case Western Reserve University to create and visualize material science ontologies, and it includes example ontologies to demonstrate its capabilities. This work was supported by the U.S. Department of Energy’s Office of Energy Efficiency and Renewable Energy (EERE) under Solar Energy Technologies Office (SETO) Agreement Numbers E-EE0009353 and DE-EE0009347, Department of Energy (National Nuclear Security Administration) under Award Number DE-NA0004104 and Contract number B647887, and U.S. National Science Foundation Award under Award Number 2133576.

License BSD_3_clause + file LICENSE

Encoding UTF-8

Imports dplyr, rdflib, jsonld, httr, utils, DiagrammeR, DiagrammeRsvg, stringr, xml2, tidyr, readr

RoxygenNote 7.3.1

Depends R (>= 3.1.1)

Suggests knitr, rmarkdown, testthat (>= 3.0.0)

Config/testthat/edition 3

VignetteBuilder knitr

SystemRequirements macOS: redland (>= 1.0.14); Linux: librdf0 (>= 1.0.14), librdf0-dev (>= 1.0.14)

NeedsCompilation no

Author Jonathan E Gordon [aut] (<<https://orcid.org/0009-0007-5958-7386>>),
Alexander Harding Bradley [aut]
(<<https://orcid.org/0009-0000-2917-773X>>),
Priyan Rajamohan [aut] (<<https://orcid.org/0009-0003-5326-1706>>),

Nathaniel Hahn [aut],
Kiefer Lin [aut],
Arafath Nihar [aut] (<<https://orcid.org/0000-0003-4826-290X>>),
Hayden Cadwell [aut],
Jiana Kambo [aut],
Jayvic Jimenez [aut] (<<https://orcid.org/0000-0002-2342-5648>>),
Kristen J Hernandez [aut] (<<https://orcid.org/0000-0001-6139-1218>>),
Hein Htet-Aung [aut] (<<https://orcid.org/0000-0002-8191-8213>>),
Brian Giera [aut] (<<https://orcid.org/0000-0001-6543-7498>>),
Weiqi Yue [aut] (<<https://orcid.org/0000-0002-3253-7991>>),
Mohammad Redad Mehdi [aut] (<<https://orcid.org/0000-0002-0593-5222>>),
Finley Holt [aut],
Quynh Tran [aut] (<<https://orcid.org/0009-0006-4025-1834>>),
Gabriel Ponon [aut] (<<https://orcid.org/0000-0002-9366-6199>>),
Daniel Savage [aut] (<<https://orcid.org/0000-0001-9973-2030>>),
Donald Brown [aut],
Jarod Kaltenbaugh [aut] (<<https://orcid.org/0009-0007-4576-7714>>),
Kush Havinal [aut],
Nicholas Gray [aut],
Max Liggett [aut],
Benjamin G Pierce [aut] (<<https://orcid.org/0000-0002-9080-4584>>),
Raymond Wieser [aut] (<<https://orcid.org/0000-0003-1531-6430>>),
Yangxin Fan [aut] (<<https://orcid.org/0000-0003-1728-9560>>),
Tommy Ciardi [aut],
Olatunde J Akanbi [aut] (<<https://orcid.org/0000-0001-7719-2619>>),
Hadiza Iawal [aut] (<<https://orcid.org/0000-0001-5086-2344>>),
Will Oltjen [aut] (<<https://orcid.org/0000-0003-0380-1033>>),
Maliesha Kalutotage [aut] (<<https://orcid.org/0009-0009-6440-8180>>),
Antony Lino [aut],
Van Tran [aut] (<<https://orcid.org/0009-0008-4355-0543>>),
Mingjian Lu [aut],
Xuanji Yu [aut] (<<https://orcid.org/0000-0003-1967-3769>>),
Liangyi Huang [aut] (<<https://orcid.org/0000-0003-0845-3293>>),
Zelin Li [aut] (<<https://orcid.org/0000-0002-6287-3697>>),
Abhishek Daundkar [aut],
Hope Omodolor [aut] (<<https://orcid.org/0009-0005-7842-406X>>),
Deepa Bhuvanagiri [aut] (<<https://orcid.org/0000-0002-5896-545X>>),
Mirra Rasmussen [aut],
Sameera Nalin-Venkat [aut] (<<https://orcid.org/0000-0002-9114-4602>>),
Tian Wang [aut] (<<https://orcid.org/0000-0002-6088-4405>>),
Rounak Chawla [aut],
Leean Jo [aut] (<<https://orcid.org/0000-0001-7026-3779>>),
Jeffrey M Yarus [aut] (<<https://orcid.org/0000-0002-9331-9568>>),
Kristopher O Davis [aut] (<<https://orcid.org/0000-0002-5772-6254>>),
Mengjie Li [aut] (<<https://orcid.org/0000-0002-9531-2474>>),
Yinghui Wu [aut] (<<https://orcid.org/0000-0003-3991-5155>>),
Pawan K Tripathi [aut] (<<https://orcid.org/0000-0002-8604-7744>>),
Laura S Bruckman [aut] (<<https://orcid.org/0000-0003-1271-1072>>),

Erika I Barcelos [aut] (<<https://orcid.org/0000-0002-9273-8488>>),
 Roger H French [aut, cre, cph]
 (<<https://orcid.org/0000-0002-6162-0532>>)

Maintainer Roger H French <roger.french@case.edu>

Repository CRAN

Date/Publication 2024-06-24 14:40:07 UTC

Contents

process_ontology_files	3
Index	6

process_ontology_files
Process Ontology CSV Files

Description

This function reads, processes, and combines ontology CSV files from a specified folder. These CSV files must be formatted with template from:

<https://docs.google.com/spreadsheets/d/1k7gFRc1Ys1c-m65aWfFCxqk5UtrKZ19c3GyEFQvLSFU/edit?usp=sharing>

It can handle subdirectories by producing separate unmerged outputs for each subdirectory. The function generates an ontology tree plot, saves it as SVG, and serializes the RDF object to Turtle and JSON-LD formats in the specified folder. Additionally, it allows for the merging of multiple ontologies, with options to customize the merged RDF dataset's metadata.

Usage

```
process_ontology_files(
  folder_path,
  add_external_onto_info = FALSE,
  include_graph_valuetype = TRUE,
  merge_base_uri = NULL,
  merge_title = NULL,
  merge_author = NULL,
  merge_version = NULL,
  merge_description = NULL
)
```

Arguments

folder_path	Path to the folder containing ontology CSV files.
add_external_onto_info	Logical indicating whether to update information in RDF.
include_graph_valuetype	Logical indicating whether to include value types in the graph.
merge_base_uri	String containing base URI for the merged ontology. Defaults to NULL but is required for merging ontologies. Leave as default when only processing one ontology.
merge_title	String containing title for the merged ontology.. Defaults to NULL will concatenate titles of all merged ontologies. Leave as default when only processing one ontology.
merge_author	One String containing authors for the merged ontology. Defaults to NULL will concatenate all unique Author names of merged ontologies. Leave as default when only processing one ontology.
merge_version	String containing version for the merged ontology.. Defaults to NULL will leave version blank. Leave as default when only processing one ontology.
merge_description	String containing description for the merged ontology. Defaults to NULL will concatenate descriptions of all merged ontologies with relative titles as prefixes. Leave as default when only processing one ontology.

Details

This function processes ontology CSV files in a specified folder and its subdirectories. For each subdirectory, it creates separate unmerged outputs named with the folder name prefix. The merged output is generated in the main folder path.

If you have a single ontology, place all CSV files in the specified folder and run the function with default parameters. The function will generate outputs for this single ontology, including an ontology tree plot and serialized RDF formats.

For multiple ontologies across different subdirectories, the function will process each subdirectory separately. Each subdirectories ontology will have its own set of outputs. Additionally the function will merge the ontologies from all subdirectories. This merged output can have customized metadata such as title, authors, version, URL, and description. If no metadata is specified the merging process concatenates titles, authors, and descriptions from all included ontologies. Note that specifying a base uri is required for merging ontologies.

Examples

```
# Process the CSV files in the XRay folder
example_folder1 <- system.file("extdata", "XRay", package = "FAIRmaterials")
process_ontology_files(example_folder1, add_external_onto_info = FALSE)

## Not run:
# Process the CSV files in the PV folder
example_folder2 <- system.file("extdata", "PV", package = "FAIRmaterials")
process_ontology_files(example_folder2, add_external_onto_info = FALSE)
```

End(Not run)

Index

`process_ontology_files`, 3