FACILE-RS: archival and long term preservation of research software repositories made easy

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Summary

The FACILE-RS Python package allows to perform tasks pertining to the archival and long term preservation of research software repositories. It consists in a set of Python scripts which facilitate the maintenance of software metadata, by automating its generation in various formats from a unique metadata file that is maintained manually. FACILE-RS also makes it easier to publish and archive software releases according to the Open Science paradigm and the FAIR (Findable, Accessible, Interoperable, Reusable) principles for Research Software, by offering tools to automate the creation of releases and the upload to persistent research data repositories.

In particular, FACILE-RS allows the following:

- Creating a DataCite record based on CodeMeta files present in repositories
- Creating a CFF (Citation File Format) file from CodeMeta files
- Creating archive packages in the BagIt or the BagPack formats
- Creating a release on the GitLab development platform using the GitLab API
- Archiving software releases using the RADAR service
- Using content from markdown files, bibtex files, or python docstrings to create web pages within the Grav CMS

While the scripts can be run manually, they are designed to be used within GitLab CI/CD or another workflow automation system, in order to automate the process of maintaining metadata and creating persistent software releases.

Statement of need

Research software development is a fundamental aspect of academic research (Anzt et al., 2021), and it has now been acknowledged that the FAIR principles (Findable, Accessible, Interoperable, Reusable; (Wilkinson et al., 2016)), historically established to improve the reusability of research data, should also be applied to research software (Chue Hong et al., 2021). In particular, reproducible research requires that software and their associated metadata be easily findable by both machines and humans, and retrievable via standardised protocols. In this context, several metadata standards are widely used across the scientific community:

- The Citation File Format (CFF) (Druskat et al., 2021) is a human- and machine-readable format that indicates how to cite software.
- The DataCite Metadata Schema (DataCite Metadata Working Group, 2021) consists of core metadata properties selected for accurate and consistent identification of research outputs for citation and retrieval purposes, with instructions for recommended use.

- CodeMeta (Jones et al., 2017), an extension of schema.org, is a JSON and XML metadata schema for scientific software that aims to standardize the exchange of software metadata across repositories and organizations.

All of these standards serve specific purposes, and several are required to cover the whole software lifecycle. However, maintaining multiple metadata files in different formats can be a significant burden for research software developers, and an obstacle to the adoption of good software publication practices. In addition, as the content of the different metadata files is largely overlapping, maintaining these files manually can pose a risk to data consistency.

Another requirement for scholarly software to be FAIR is that all software releases are published according to the FAIR principles and assigned a persistent identifier, which can be difficult to implement without an automated process.

FACILE-RS aims to overcome these difficulties by making it easy to create and maintain the metadata associated to research software, as well as to publish software releases according to the FAIR principles on reputable research data repositories.

Functionality

The main prerequisite for using FACILE-RS in a software repository is to create a CodeMeta metadata file, for example using the CodeMeta generator.

The Python scripts that compose FACILE-RS are gathered in Table 1. While each of these scripts can be used individually and executed manually, FACILE-RS was designed to be used within an automated workflow like GitLab CI/CD pipelines, used for automating software development workflow via a continuous and iterative process.

Script	Functionality
create_cff	generates Citation File Format (CFF) metadata file
prepare_release	updates *version* and *dateModified* fields in metadata
create_release	creates release in GitLab
create_datacite	generates DataCite metadata file
create_bag	creates BagIt package
create_bagpack	adds DataCite XML to BagIt package
prepare_radar	reserves DOI on RADAR
create_radar	creates archive and uploads it to RADAR
run_markdown_pipeline	updates Grav CMS website
run_bibtex_pipeline	converts BibTex files and publishes references on Grav CMS website
run_docstring_pipeline	extracts docstrings from Python scripts and publishes them on Grav CMS website

Table 1: Components of FACILE-RS

A typical GitLab CI/CD workflow for FACILE-RS is illustrated on figure Figure 1. In this example, each time a commit is published, the different metadata files are automatically updated from the CodeMeta file.

This workflow also includes an automated process for creating software releases, both on GitLab and on the research repository RADAR, which is triggered by creating a *pre-release* tag (e.g. tag pre-v0.1.0 for creating the release of version v0.1.0). During the *pre-release* phase, a DOI is reserved on RADAR and the software metadata associated with the release is updated. Once this is done, the proper release tag is automatically created, and the GitLab and RADAR releases are created.

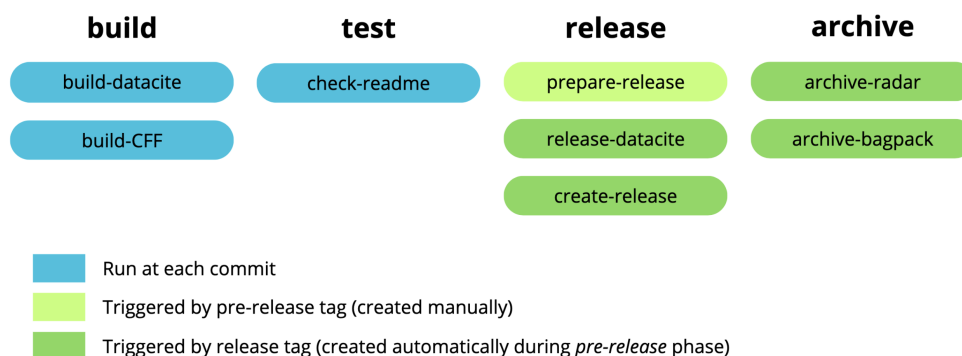Several tutorials for implementing such a workflow are provided within the FACILE-RS repository.

Figure 1: Typical structure of an automated FACILE-RS workflow

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