netherlands eScience center

Research Software Directory

A content management system tailored to research software

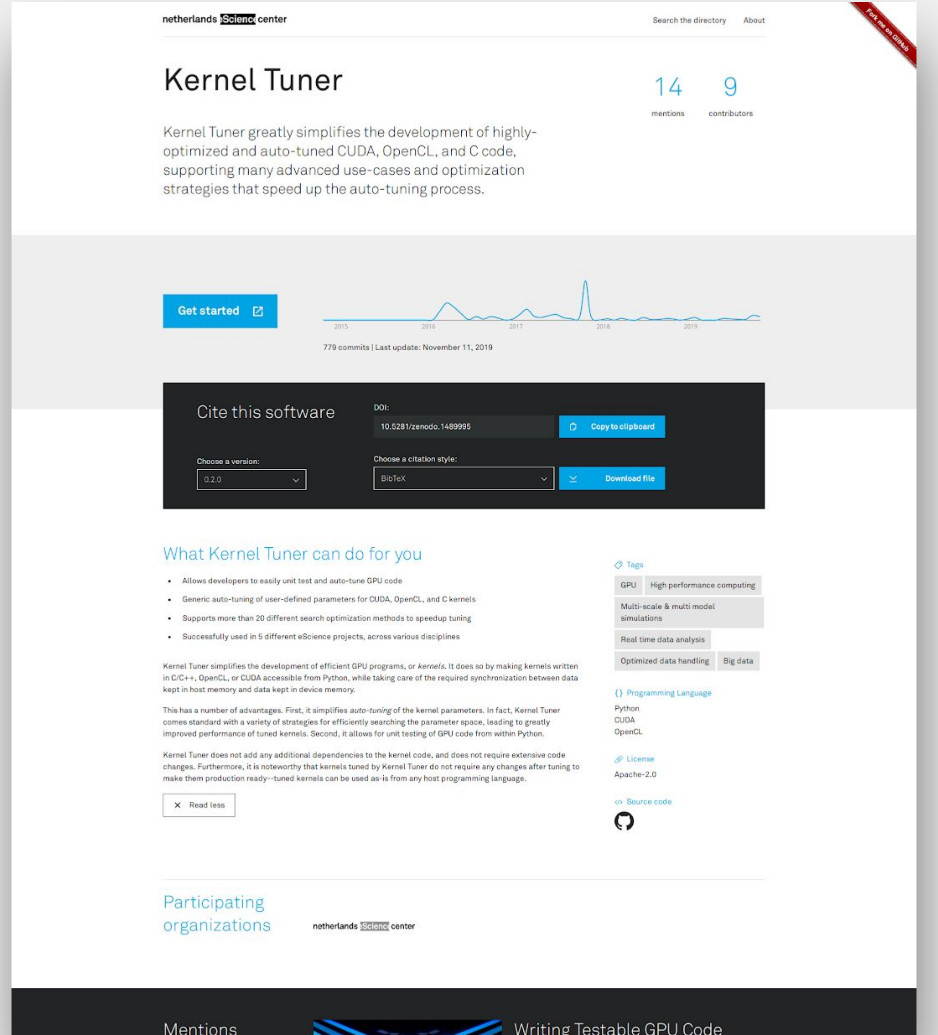
Jurriaan H. Spaaks
Research Software Engineer
Netherlands eScience Center

November 13, 2019
Maryland, USA
Scientific Software Registry Collaboration Workshop

What does the Research Software Directory look like?

Product pages have been designed

- to employ Search Engine Optimization (SEO)
- to be visually attractive
- to be easy to consume for visitors
- to provide context / build trust
- provide a starting point



Kernel Tuner

14 mentions

9 contributors

Kernel Tuner greatly simplifies the development of highly-optimized and auto-tuned CUDA, OpenCL, and C code, supporting many advanced use-cases and optimization strategies that speed up the auto-tuning process.

779 commits | Last update: November 11, 2019

Cite this software

DOI: 10.5281/zenodo.1489995

Choose a version: 0.2.0

Choose a citation style: BibTeX

What Kernel Tuner can do for you

- Allows developers to easily unit test and auto-tune GPU code
- Generic auto-tuning of user-defined parameters for CUDA, OpenCL, and C kernels
- Supports more than 20 different search optimization methods to speedup tuning
- Successfully used in 5 different eScience projects, across various disciplines

Kernel Tuner simplifies the development of efficient GPU programs, or *kernels*. It does so by making kernels written in C/C++, OpenCL, or CUDA accessible from Python, while taking care of the required synchronization between data kept in host memory and data kept in device memory.

This has a number of advantages. First, it simplifies *auto-tuning* of the kernel parameters. In fact, Kernel Tuner comes standard with a variety of strategies for efficiently searching the parameter space, leading to greatly improved performance of tuned kernels. Second, it allows for unit testing of GPU code from within Python.

Kernel Tuner does not add any additional dependencies to the kernel code, and does not require extensive code changes. Furthermore, it is noteworthy that kernels tuned by Kernel Tuner do not require any changes after tuning to make them production ready--tuned kernels can be used as-is from any host programming language.

Tags: GPU, High performance computing, Multi-scale & multi model simulations, Real time data analysis, Optimized data handling, Big data

Programming Language: Python, CUDA, OpenCL

License: Apache-2.0

Source code

Participating organizations: netherlands eScience center

Mentions

Writing Testable GPU Code

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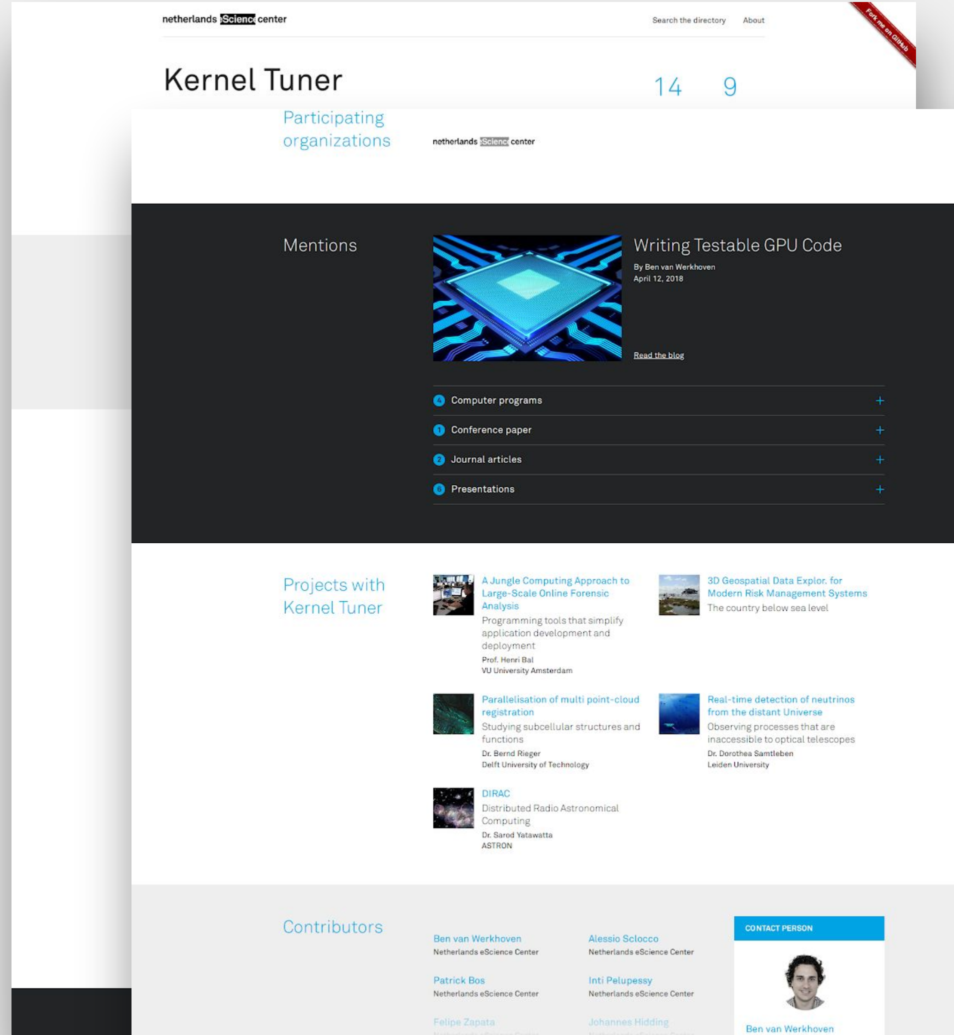

netherlands eScience center

Search the directory About

Kernel Tuner

14 9

Participating organizations

netherlands eScience center

Mentions

Writing Testable GPU Code

By Ben van Werkhoven

April 12, 2018

Read the blog

4 Computer programs +

1 Conference paper +

2 Journal articles +

6 Presentations +

Projects with Kernel Tuner

A Jungle Computing Approach to Large-Scale Online Forensic Analysis

Programming tools that simplify application development and deployment

Prof. Henri Bal

VU University Amsterdam

3D Geospatial Data Explor. for Modern Risk Management Systems

The country below sea level

Parallelisation of multi point-cloud registration

Studying subcellular structures and functions

Dr. Bernd Rieger

Delft University of Technology

Real-time detection of neutrinos from the distant Universe

Observing processes that are inaccessible to optical telescopes

Dr. Dorothea Samtleben

Leiden University

DIRAC

Distributed Radio Astronomical Computing

Dr. Sarod Yatawatta

ASTRON

Contributors

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Patrick Bos

Netherlands eScience Center

Inti Pelupessy

Netherlands eScience Center

Felipe Zapata

Johannes Hidding

CONTACT PERSON

Ben van Werkhoven

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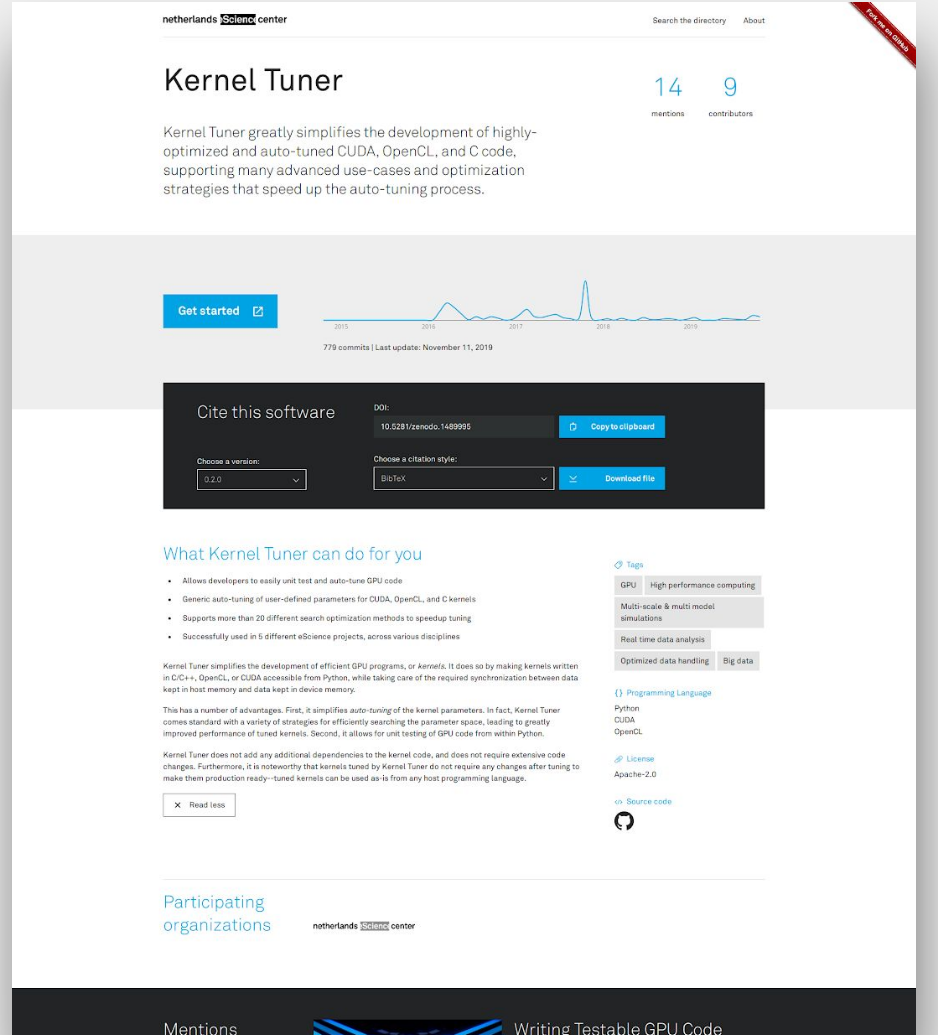

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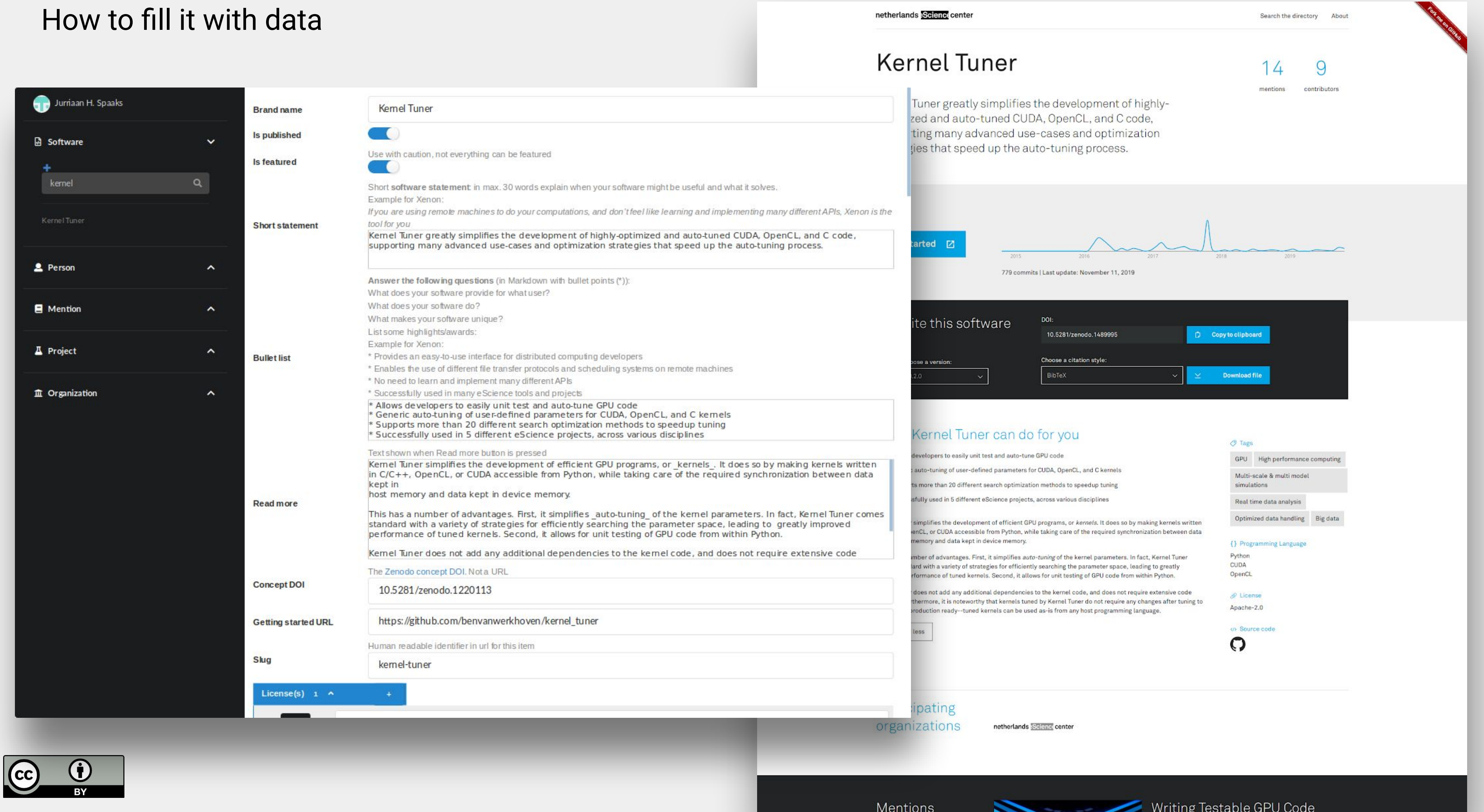
Participating organizations

Mentions

Writing Testable GPU Code

How to fill it with data



Brand name: Kernel Tuner

Is published

Is featured — Use with caution, not everything can be featured

Short **software statement** in max. 30 words explain when your software might be useful and what it solves.
Example for Xenon:
If you are using remote machines to do your computations, and don't feel like learning and implementing many different APIs, Xenon is the tool for you

Short statement: Kernel Tuner greatly simplifies the development of highly-optimized and auto-tuned CUDA, OpenCL, and C code, supporting many advanced use-cases and optimization strategies that speed up the auto-tuning process.

Answer the following questions (in Markdown with bullet points (*)):
What does your software provide for what user?
What does your software do?
What makes your software unique?
List some highlights/awards:
Example for Xenon:
* Provides an easy-to-use interface for distributed computing developers
* Enables the use of different file transfer protocols and scheduling systems on remote machines
* No need to learn and implement many different APIs
* Successfully used in many eScience tools and projects

Bullet list:

```
* Allows developers to easily unit test and auto-tune GPU code
* Generic auto-tuning of user-defined parameters for CUDA, OpenCL, and C kernels
* Supports more than 20 different search optimization methods to speedup tuning
* Successfully used in 5 different eScience projects, across various disciplines
```

Text shown when Read more button is pressed

Read more:

```
Kernel Tuner simplifies the development of efficient GPU programs, or _kernels_. It does so by making kernels written
in C/C++, OpenCL, or CUDA accessible from Python, while taking care of the required synchronization between data
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host memory and data kept in device memory.

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Kernel Tuner does not add any additional dependencies to the kernel code, and does not require extensive code
```

The Zenodo concept DOI. Not a URL

Concept DOI: 10.5281/zenodo.1220113

Getting started URL: https://github.com/benvanwerkhoven/kernel_tuner

Human readable identifier in url for this item

Slug: kernel-tuner

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14 mentions 9 contributors

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Source code

ipating organizations

Mentions

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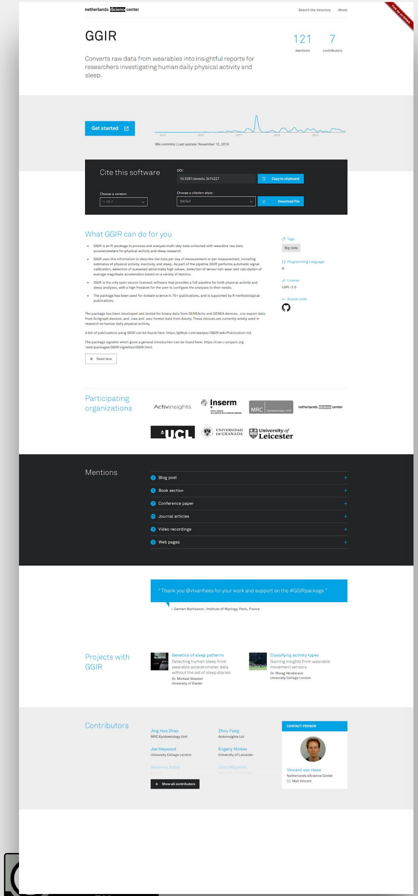
Index page on top of product pages



netherlands eScience center — Search the directory — About

GGIR

121 mentions 7 contributors

Converts raw data from wearables into insightful reports for researchers investigating human daily physical activity and sleep.

Get started

984 commits | Last update: November 12, 2019

Cite this software

DOI: 10.5281/zenodo.3474227 — Copy to clipboard

Choose a version: 1.10-7

Choose a citation style: BibTeX — Download file

What GGIR can do for you

- GGIR is an R-package to process and analysis multi-day data collected with wearable raw data accelerometers for physical activity and sleep research.
- GGIR uses this information to describe the data per day of measurement or per measurement, including estimates of physical activity, inactivity, and sleep. As part of the pipeline GGIR performs automatic signal calibration, detection of sustained abnormally high values, detection of sensor non-wear and calculation of

Tags: Big data

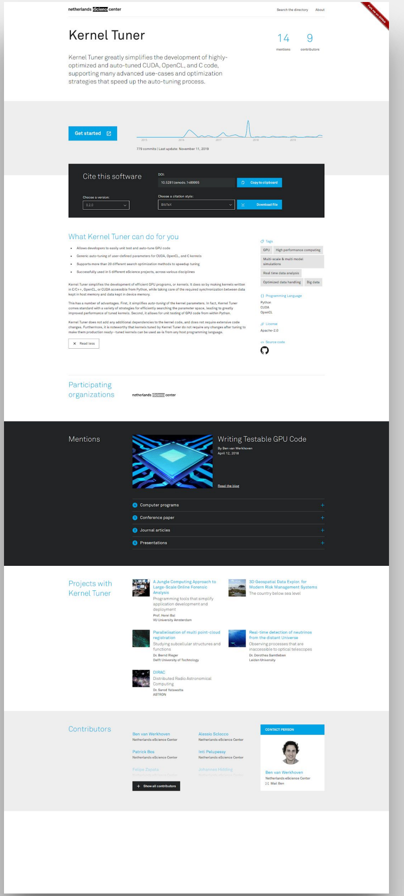
Programming Language: R

Participating organizations

Mentions

Projects with GGIR

Contributors



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779 commits | Last update: November 11, 2019

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Choose a citation style: BibTeX — Download file

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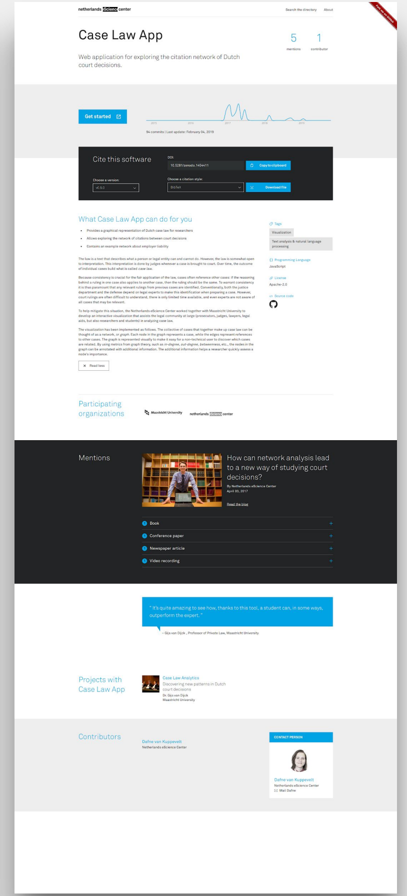


netherlands eScience center — Search the directory — About

Case Law App

5 mentions 1 contributor

Web application for exploring the citation network of Dutch court decisions.

Get started

94 commits | Last update: February 04, 2019

Cite this software

DOI: 10.5281/zenodo.1454411 — Copy to clipboard

Choose a version: v0.5.0

Choose a citation style: BibTeX — Download file

What Case Law App can do for you

- Provides a graphical representation of Dutch case law for researchers
- Allows exploring the network of citations between court decisions
- Contains an example network about employer liability

Tags: Visualization, Text analysis & natural language processing

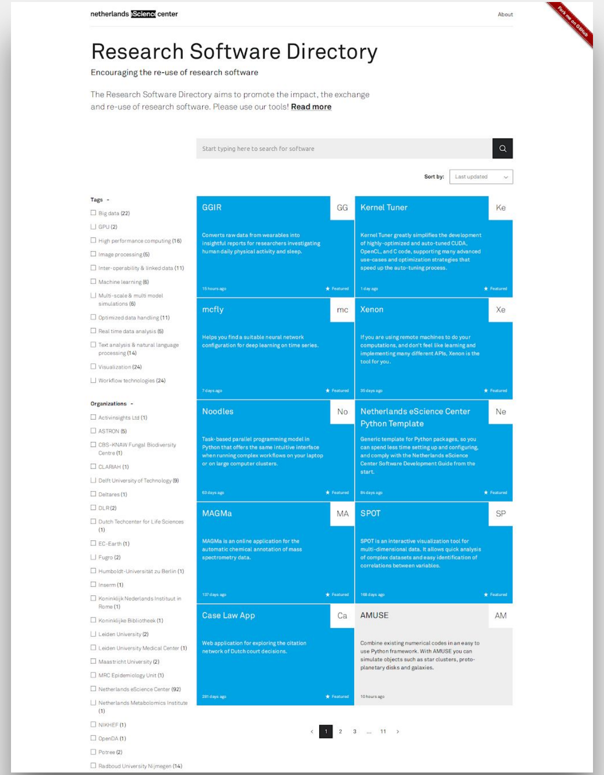
Participating organizations

Mentions

How can network analysis lead to a new way of studying court decisions?

Projects with Case Law App

Contributors



netherlands eScience center — About

Research Software Directory

Encouraging the re-use of research software

The Research Software Directory aims to promote the impact, the exchange and re-use of research software. Please use our tools! **Read more**

Start typing here to search for software

Sort by: Last updated

Tags -

- □ Big data (22)
- □ GPU (2)
- □ High performance computing (16)
- □ Image processing (5)
- □ Inter-operability & linked data (11)
- □ Machine learning (6)
- □ Multi-scale & multi model simulations (6)
- □ Optimized data handling (11)
- □ Real time data analysis (5)
- □ Text analysis & natural language processing (14)
- □ Visualization (24)
- □ Workflow technologies (24)

Organizations -

- □ Activinsights Ltd (1)
- □ ASTRON (5)
- □ CBS-KNAW Fungal Biodiversity Centre (1)
- □ CLARIAH (1)
- □ Delft University of Technology (9)
- □ Deltares (1)
- □ DLR (2)
- □ Dutch Techcenter for Life Sciences (1)
- □ EC-Earth (1)
- □ Fugro (2)
- □ Humboldt-Universität zu Berlin (1)
- □ Inserm (1)
- □ Koninklijk Nederlands Instituut in Rome (1)
- □ Koninklijke Bibliotheek (1)
- □ Leiden University (2)
- □ Leiden University Medical Center (1)
- □ Maastricht University (2)
- □ MRC Epidemiology Unit (1)
- □ Netherlands eScience Center (92)
- □ Netherlands Metabolomics Institute (1)
- □ NIKHEF (1)
- □ OpenDA (1)
- □ Potree (2)
- □ Radboud University Nijmegen (14)

GGIR (GG)
Converts raw data from wearables into insightful reports for researchers investigating human daily physical activity and sleep.
15 hours ago — ★ Featured

Kernel Tuner (Ke)
Kernel Tuner greatly simplifies the development of highly-optimized and auto-tuned CUDA, OpenCL, and C code, supporting many advanced use-cases and optimization strategies that speed up the auto-tuning process.
1 day ago — ★ Featured

mcfly (mc)
Helps you find a suitable neural network configuration for deep learning on time series.
7 days ago — ★ Featured

Xenon (Xe)
If you are using remote machines to do your computations, and don't feel like learning and implementing many different APIs, Xenon is the tool for you.
35 days ago — ★ Featured

Noodles (No)
Task-based parallel programming model in Python that offers the same intuitive interface when running complex workflows on your laptop or on large computer clusters.
63 days ago — ★ Featured

Netherlands eScience Center Python Template (Ne)
Generic template for Python packages, so you can spend less time setting up and configuring, and comply with the Netherlands eScience Center Software Development Guide from the start.
84 days ago — ★ Featured

MAGMa (MA)
MAGMa is an online application for the automatic chemical annotation of mass spectrometry data.
137 days ago — ★ Featured

SPOT (SP)
SPOT is an interactive visualization tool for multi-dimensional data. It allows quick analysis of complex datasets and easy identification of correlations between variables.
168 days ago — ★ Featured

Case Law App (Ca)
Web application for exploring the citation network of Dutch court decisions.
281 days ago — ★ Featured

AMUSE (AM)
Combine existing numerical codes in an easy to use Python framework. With AMUSE you can simulate objects such as star clusters, proto-planetary disks and galaxies.
10 hours ago

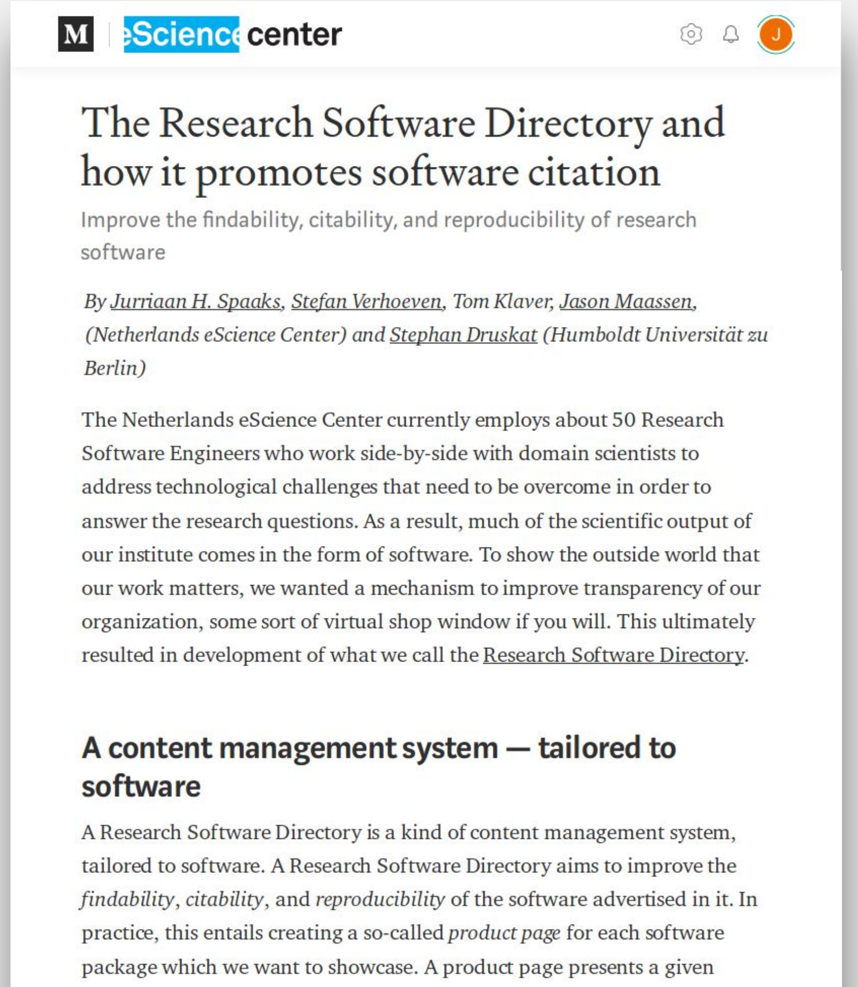
Resources

Research Software Directory

- bit.ly/rsd-blog
- bit.ly/rsdpromo
- research-software.nl
- github.com/research-software-directory
- free service to help you get started
- bit.ly/citable-software

Other

- bit.ly/awesome-registries



The Research Software Directory and how it promotes software citation

Improve the findability, citability, and reproducibility of research software

By Jurriaan H. Spaaks, Stefan Verhoeven, Tom Klaver, Jason Maassen, (Netherlands eScience Center) and Stephan Druskat (Humboldt Universität zu Berlin)

The Netherlands eScience Center currently employs about 50 Research Software Engineers who work side-by-side with domain scientists to address technological challenges that need to be overcome in order to answer the research questions. As a result, much of the scientific output of our institute comes in the form of software. To show the outside world that our work matters, we wanted a mechanism to improve transparency of our organization, some sort of virtual shop window if you will. This ultimately resulted in development of what we call the Research Software Directory.

A content management system — tailored to software

A Research Software Directory is a kind of content management system, tailored to software. A Research Software Directory aims to improve the *findability*, *citability*, and *reproducibility* of the software advertised in it. In practice, this entails creating a so-called *product page* for each software package which we want to showcase. A product page presents a given

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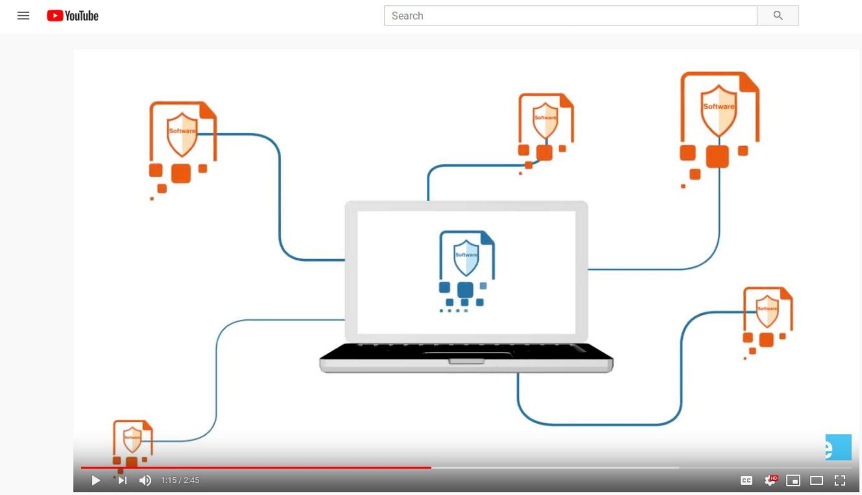

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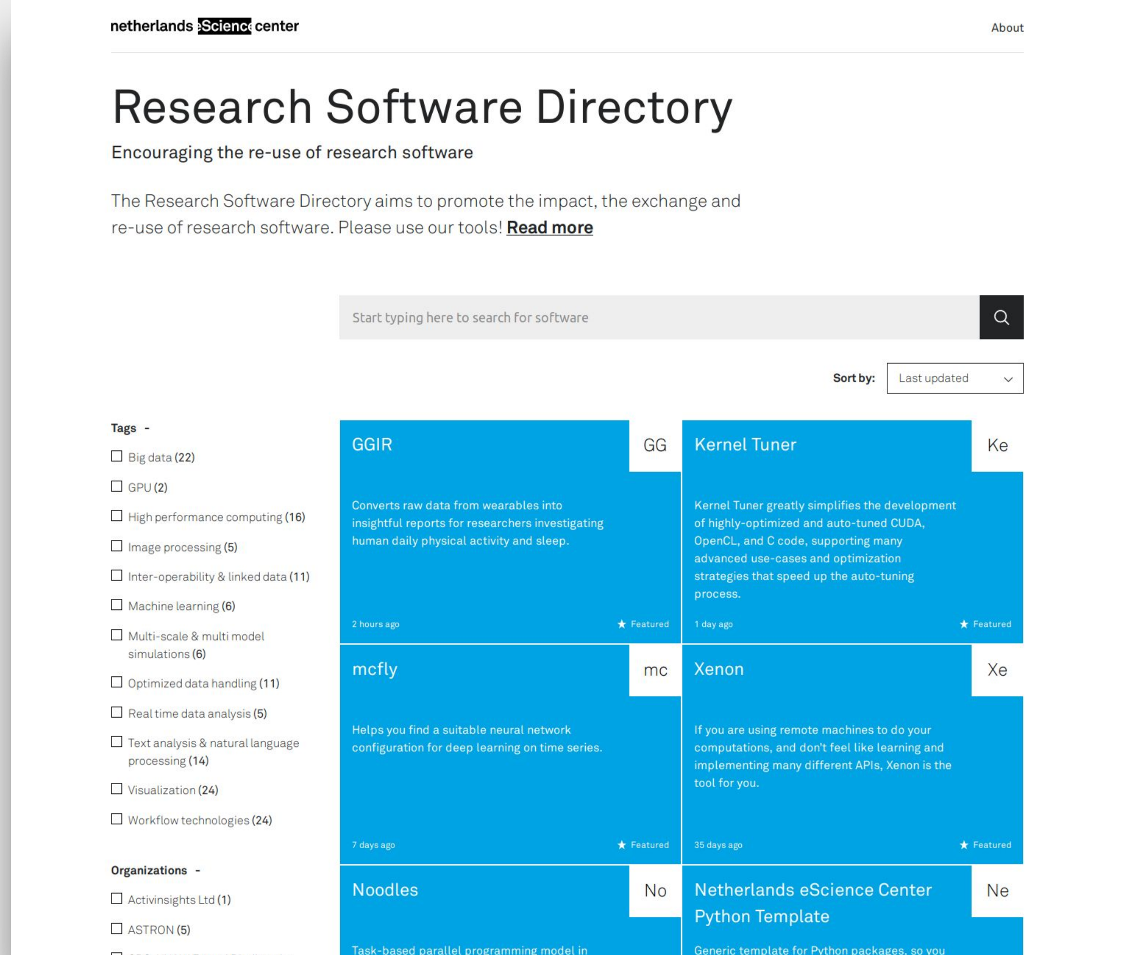

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- ☐ ASTRON **(5)**

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2 hours ago ★ Featured

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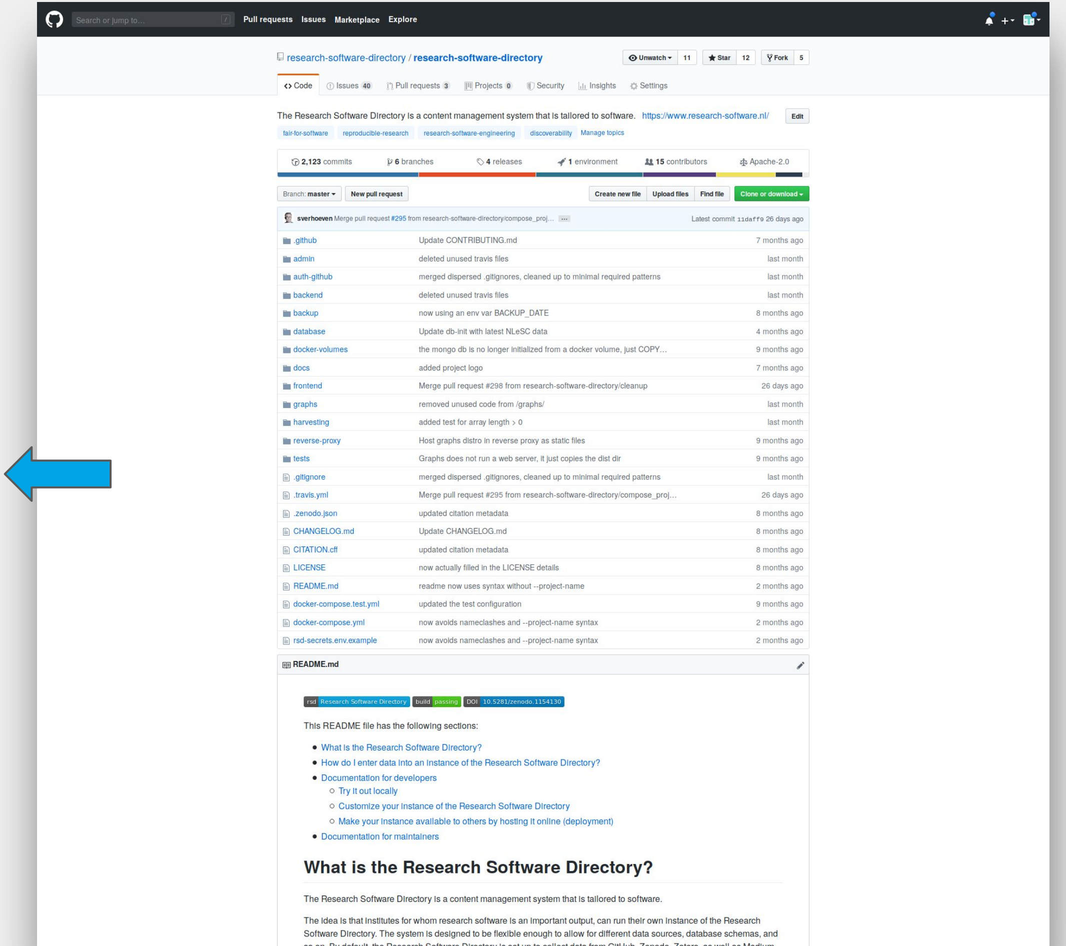

The Research Software Directory is a content management system that is tailored to software. https://www.research-software.nl/

sverhoeven Merge pull request #295 from research-software-directory/compose_proj... … Latest commit 11daff9 26 days ago

.github	Update CONTRIBUTING.md	7 months ago
admin	deleted unused travis files	last month
auth-github	merged dispersed .gitignores, cleaned up to minimal required patterns	last month
backend	deleted unused travis files	last month
backup	now using an env var BACKUP_DATE	8 months ago
database	Update db-init with latest NLeSC data	4 months ago
docker-volumes	the mongo db is no longer initialized from a docker volume, just COPY…	9 months ago
docs	added project logo	7 months ago
frontend	Merge pull request #298 from research-software-directory/cleanup	26 days ago
graphs	removed unused code from /graphs/	last month
harvesting	added test for array length > 0	last month
reverse-proxy	Host graphs distro in reverse proxy as static files	9 months ago
tests	Graphs does not run a web server, it just copies the dist dir	9 months ago
.gitignore	merged dispersed .gitignores, cleaned up to minimal required patterns	last month
.travis.yml	Merge pull request #295 from research-software-directory/compose_proj…	26 days ago
.zenodo.json	updated citation metadata	8 months ago
CHANGELOG.md	Update CHANGELOG.md	8 months ago
CITATION.cff	updated citation metadata	8 months ago
LICENSE	now actually filled in the LICENSE details	8 months ago
README.md	readme now uses syntax without --project-name	2 months ago
docker-compose.test.yml	updated the test configuration	9 months ago
docker-compose.yml	now avoids nameclashes and --project-name syntax	2 months ago
rsd-secrets.env.example	now avoids nameclashes and --project-name syntax	2 months ago

This README file has the following sections:

- What is the Research Software Directory?
- How do I enter data into an instance of the Research Software Directory?
- Documentation for developers
  - Try it out locally
  - Customize your instance of the Research Software Directory
  - Make your instance available to others by hosting it online (deployment)
- Documentation for maintainers

What is the Research Software Directory?

The Research Software Directory is a content management system that is tailored to software.

The idea is that institutes for whom research software is an important output, can run their own instance of the Research Software Directory. The system is designed to be flexible enough to allow for different data sources, database schemas, and so on. By default, the Research Software Directory is set up to collect data from GitHub, Zenodo, Zotero, as well as Medium

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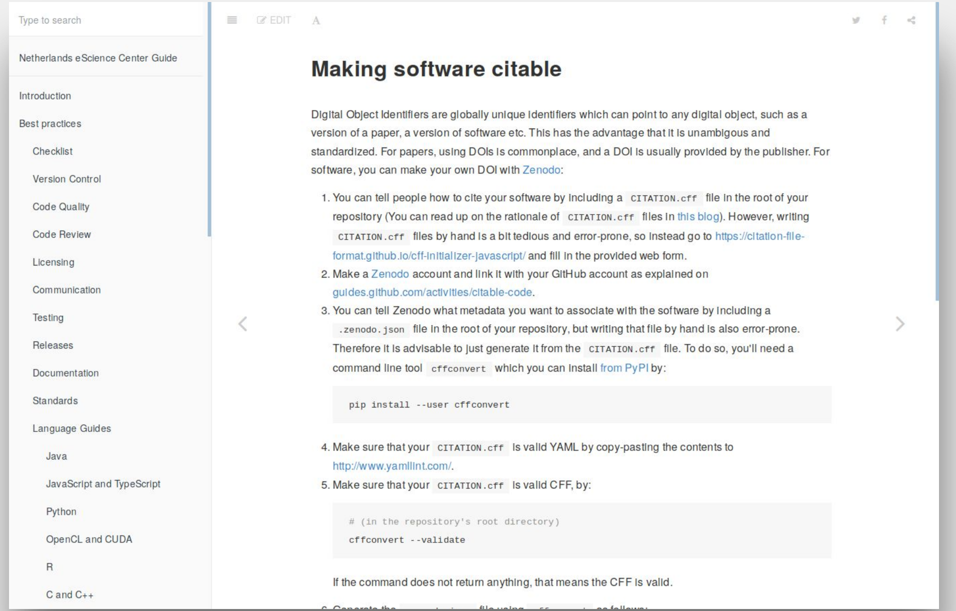

Making software citable

Digital Object Identifiers are globally unique identifiers which can point to any digital object, such as a version of a paper, a version of software etc. This has the advantage that it is unambigous and standardized. For papers, using DOIs is commonplace, and a DOI is usually provided by the publisher. For software, you can make your own DOI with Zenodo:

1. You can tell people how to cite your software by including a `CITATION.cff` file in the root of your repository (You can read up on the rationale of `CITATION.cff` files in this blog). However, writing `CITATION.cff` files by hand is a bit tedious and error-prone, so instead go to https://citation-file-format.github.io/cff-initializer-javascript/ and fill in the provided web form.
2. Make a Zenodo account and link it with your GitHub account as explained on guides.github.com/activities/citable-code.
3. You can tell Zenodo what metadata you want to associate with the software by including a `.zenodo.json` file in the root of your repository, but writing that file by hand is also error-prone. Therefore it is advisable to just generate it from the `CITATION.cff` file. To do so, you'll need a command line tool `cffconvert` which you can install from PyPI by:

   ```
   pip install --user cffconvert
   ```

4. Make sure that your `CITATION.cff` is valid YAML by copy-pasting the contents to http://www.yamllint.com/.
5. Make sure that your `CITATION.cff` is valid CFF, by:

   ```
   # (in the repository's root directory)
   cffconvert --validate
   ```

   If the command does not return anything, that means the CFF is valid.

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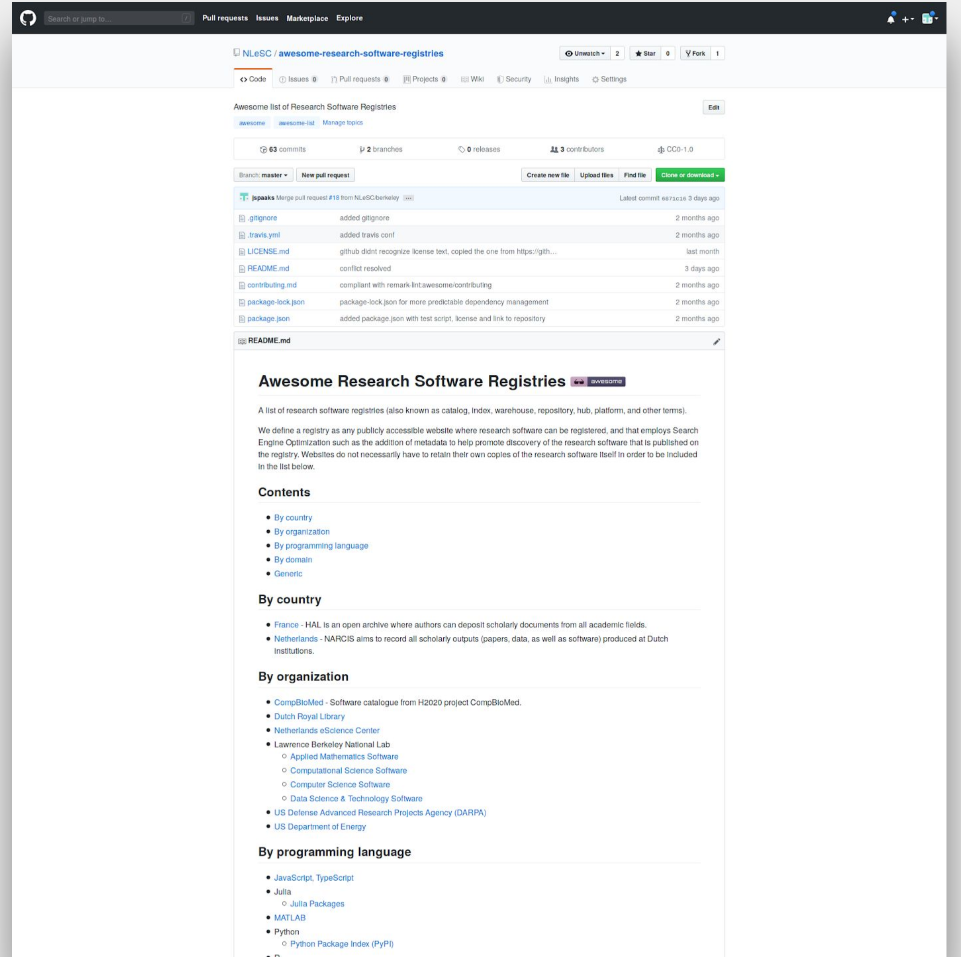
- bit.ly/citable-software

Other

- bit.ly/awesome-registries



NLeSC / awesome-research-software-registries

Awesome list of Research Software Registries

63 commits · 2 branches · 0 releases · 3 contributors · CC0-1.0

jspaaks Merge pull request #18 from NLeSC/berkeley ... Latest commit 6871c16 3 days ago

.gitignore	added gitignore	2 months ago
.travis.yml	added travis conf	2 months ago
LICENSE.md	github didnt recognize license text, copied the one from https://gith...	last month
README.md	conflict resolved	3 days ago
contributing.md	compliant with remark-lint:awesome/contributing	2 months ago
package-lock.json	package-lock.json for more predictable dependency management	2 months ago
package.json	added package.json with test script, license and link to repository	2 months ago

README.md

Awesome Research Software Registries

A list of research software registries (also known as catalog, index, warehouse, repository, hub, platform, and other terms).

We define a registry as any publicly accessible website where research software can be registered, and that employs Search Engine Optimization such as the addition of metadata to help promote discovery of the research software that is published on the registry. Websites do not necessarily have to retain their own copies of the research software itself in order to be included in the list below.

Contents

- By country
- By organization
- By programming language
- By domain
- Generic

By country

- France - HAL is an open archive where authors can deposit scholarly documents from all academic fields.
- Netherlands - NARCIS aims to record all scholarly outputs (papers, data, as well as software) produced at Dutch institutions.

By organization

- CompBioMed - Software catalogue from H2020 project CompBioMed.
- Dutch Royal Library
- Netherlands eScience Center
- Lawrence Berkeley National Lab
  - Applied Mathematics Software
  - Computational Science Software
  - Computer Science Software
  - Data Science & Technology Software
- US Defense Advanced Research Projects Agency (DARPA)
- US Department of Energy

By programming language

- JavaScript, TypeScript
- Julia
  - Julia Packages
- MATLAB
- Python
  - Python Package Index (PyPI)