

Research Software Directory

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Netherlands eScience Center

netherlands
eScience center

ESCAPE-OSSR Meeting
15/06/2023



netherlands **eScience** center

National center for the development
and application of research software

Founded in 2012 by NWO and SURF

Science Park Amsterdam

~270 projects
(on many different topics)

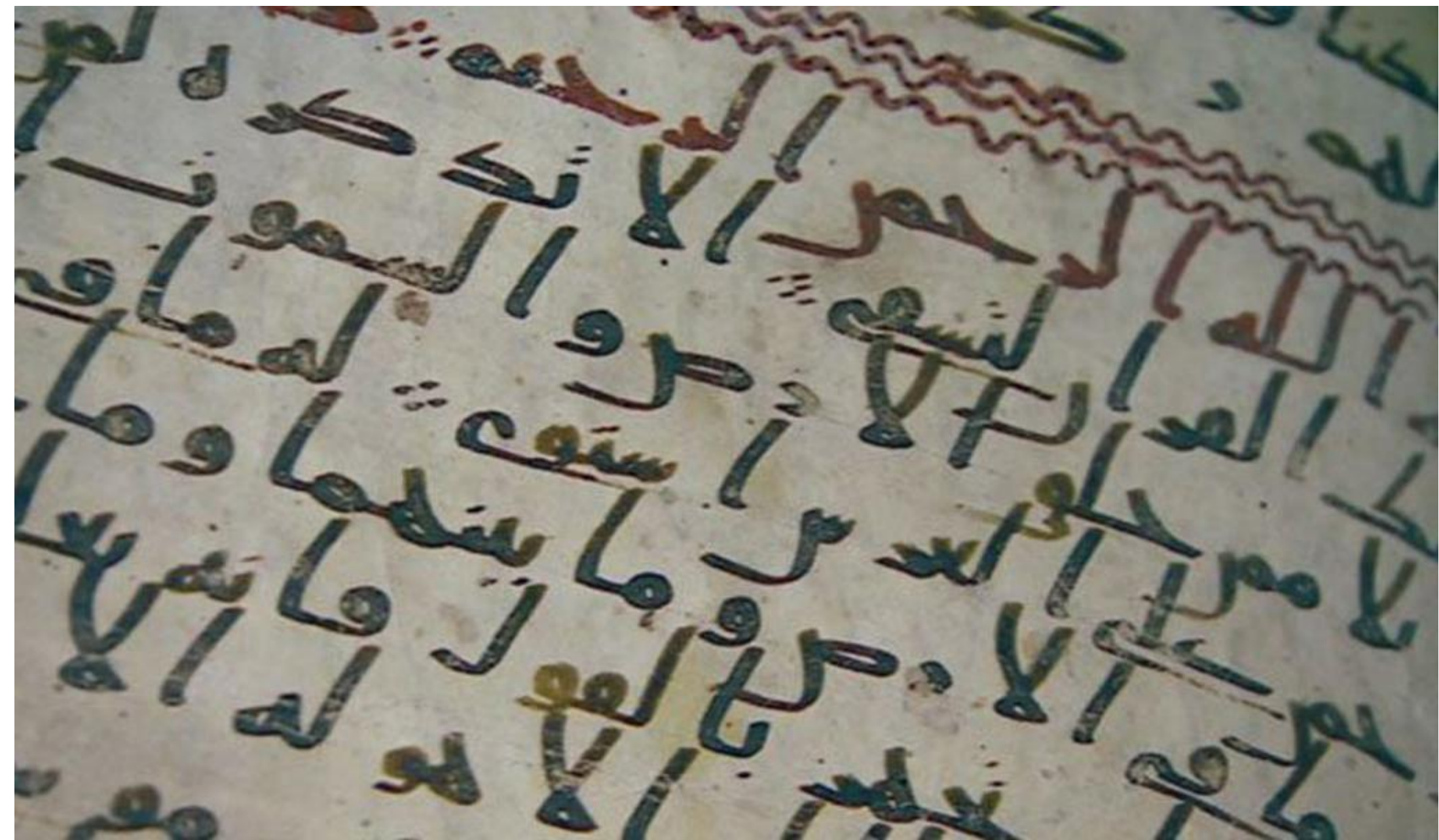
Astronomy: fast radio bursts

In collaboration with ASTRON & UvA



Digital Humanities: Arabic-Islamic corpus

In collaboration with Utrecht University



~270 projects
(on many different topics)

Astronomy: fast radio bursts

In collaboration with ASTRON & UvA

OXFORD ACADEMIC Journals Books

Monthly Notices

of the Royal Astronomical Society

Volume 499, Issue 4
December 2020

A bright, high rotation-measure FRB that skewers the M33 halo

L Connor, J van Leeuwen, L C Oostrum, E Petroff, Y Maan, E A K Adams, J J Attema, J E Bast, O M Boersma, H Dénes ... Show more

Abstract: We report the detection of a bright fast radio burst, FRB 191108, with Apertif on the Westerbork Synthesis Radio Telescope. The interferometer allows us to localize the FRB to a narrow 5 arcsec x 7 arcmin ellipse by employing both multibeam information within the Apertif phased-array feed beam pattern, and across different tied-array beams. The resulting sightline passes close to Local Group galaxy M33, with an impact parameter of only 18 kpc with respect to the core. It also traverses the much larger circumgalactic medium (CGM) of M31, the Andromeda Galaxy. We find that the shared plasma of the Local Group galaxies could contribute ~10 per cent of its dispersion measure of 588 pc cm⁻³. FRB 191108 has a Faraday rotation measure (RM) of +474 ± 3 rad m⁻², which is too large to be explained by either the Milky Way or the intergalactic medium. Based on the more moderate RMs of other extragalactic sources that traverse the halo of M33, we conclude that the dense magnetized plasma resides in the host galaxy. The FRB exhibits frequency structure on two scales, one that is consistent with quenched Galactic scintillation and broader spectral structure with Δν ≈ 40 MHz. If the latter is due to scattering in the shared M33/M31 CGM, our results constrain the Local Group plasma environment. We found no accompanying persistent radio sources in the Apertif imaging survey data.

Keywords: fast radio bursts
Issue Section: Article

Search or jump to... Pull requests Issues Codespaces Marketplace Explore

dianna-ai/dianna Public

Code Issues 73 Pull requests 6 Actions Projects 1 Security Insights

main 18 branches 7 tags

| | | | |
|--------------------------|---|-------------------|-------------|
| laurasoots | Merge pull request #387 from dianna-ai/352-imaget-model-loa... | 4f2f1bc yesterday | 779 commits |
| .githubhooks | Initialize repo from cookiecutter template | 17 months ago | |
| .github | Run tests also on python 3.10 | 4 months ago | |
| dashboard | fix linting | 5 days ago | |
| dianna | remove redundant comment and refactor | 14 days ago | |
| docs | Bump minor version | 2 months ago | |
| paper | fix more commas | 14 days ago | |
| tests | Merge branch 'main' into 380-bug-p_keep | 21 days ago | |
| tutorials | Make torchtext optional by only requiring it when user explicitly im... | last month | |
| .bumpversion.cfg | Bump minor version | 2 months ago | |
| .gitignore | Ignore file generated by tests | 10 months ago | |
| .prospector.yml | ignore build directory when running prospector | 7 days ago | |
| .readthedocs.yml | Initialize repo from cookiecutter template | 17 months ago | |
| CITATION.cff | Update CITATION.cff | 21 days ago | |
| LICENSE | Initialize repo from cookiecutter template | 17 months ago | |
| MANIFEST.in | remove unused files from cookiecutter template | 10 months ago | |
| README.md | Update README.md | 5 days ago | |
| pyproject.toml | Move testing and coverage to pyproject.toml + add tox config | 12 months ago | |
| setup.cfg | Merge pull request #387 from dianna-ai/352-imaget-model-load-l... | yesterday | |
| setup.py | attempt to fix linting issue | 5 days ago | |
| sonar-project.properties | Fix URL to sonarcloud organization | 17 months ago | |

Releases 6
v0.5.0 (Latest) on Sep 27

Contributors 11

Languages: Jupyter Notebook 78.2%, Python 18.6%, TeX 3.1%, Shell 0.1%

Deep Insight And Neural Network Analysis

DIANNA is a Python package that brings explainable AI (XAI) to your research project. It wraps carefully selected XAI methods in a simple, uniform interface. It's built by, with and for (academic) researchers and research software engineers working on machine learning projects.

Why DIANNA?

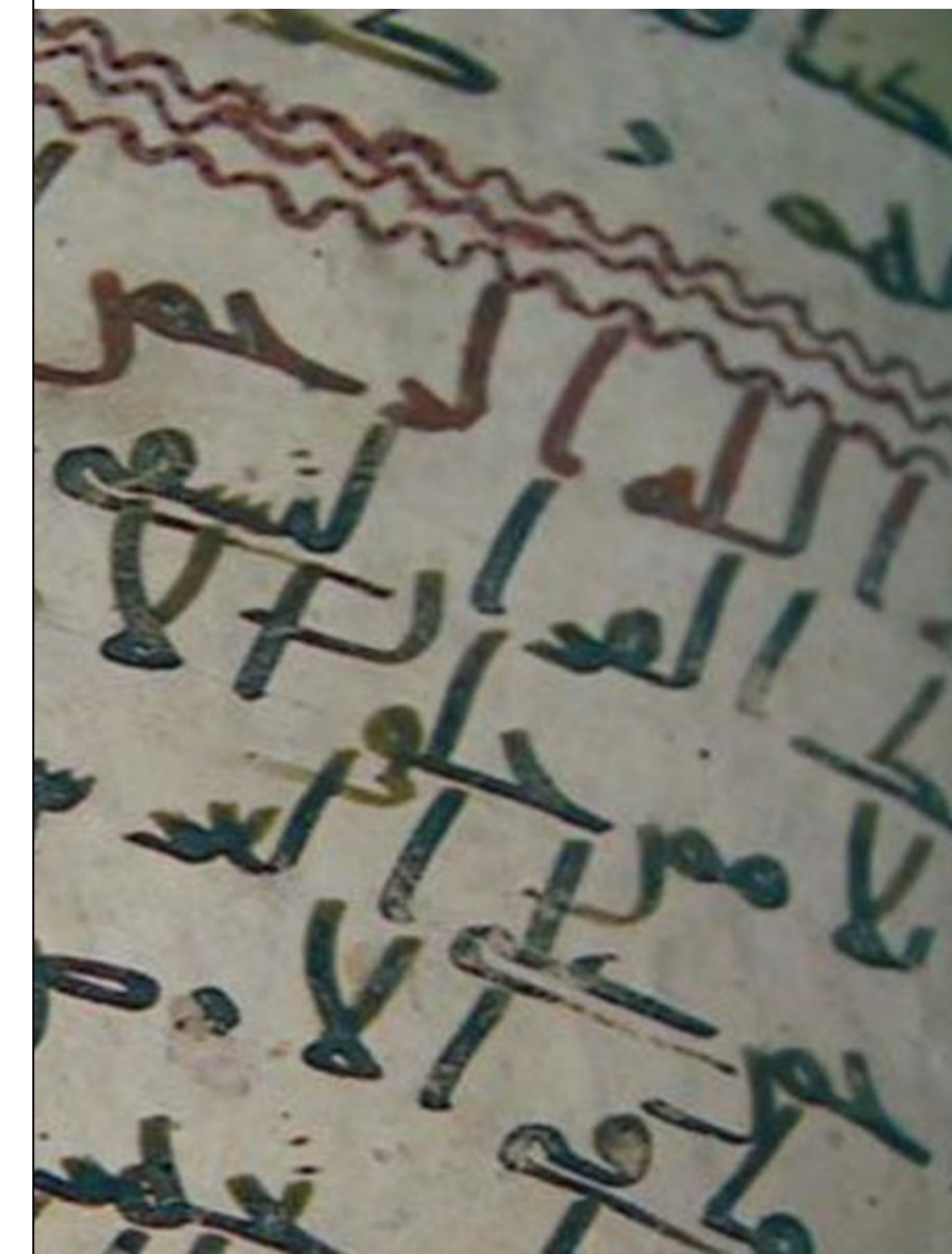
DIANNA software is addressing needs of both (XAI) researchers and mostly the various domains scientists who are using or will use AI models for their research without being experts in (XAI). DIANNA is future-proof: one of the very few XAI library supporting the Open Neural Network Exchange (ONNX) format.

After studying the vast XAI landscape we have made choices in the parts of the XAI Taxonomy on which methods, data modalities and problems types to focus. Our choices, based on the largest usage in scientific literature, are shown graphically in the XAI taxonomy below:

```

graph TD
    Stage --> Ante-hoc
    Stage --> Post-hoc
    Scope --> Global
    Scope --> Local
    Ante-hoc --> Model-agnostic
    Ante-hoc --> Model-specific
    Global --> Classification
    Local --> Regression
  
```

c-Islamic corpus
recht University



Our role in the Research Software landscape

The screenshot shows the GitHub repository for `matchms`. The repository is public and has 15 watchers, 36 forks, and 92 stars. It is a Python library for processing tandem mass spectrometry data and for computing spectral similarities. The repository includes a README, a license (Apache-2.0), and various files such as `.github`, `integration-tests`, `matchms`, `paper`, `readthedocs`, `tests`, `.editorconfig`, `.gitignore`, `.prospector.yml`, `.readthedocs.yml`, `.zenodo.json`, `CHANGELOG.md`, `CITATION.cff`, `CODE_OF_CONDUCT.rst`, `CONTRIBUTING.md`, `LICENSE`, `MANIFEST.in`, `NOTICE`, `README.rst`, `setup.cfg`, `setup.py`, and `sonar-project.properties`. The repository is maintained by Florian Huber and has 3,056 commits. The README describes the package's purpose and provides citation information.

matchms

Matchms is an open-source Python package to import, process, clean, and compare mass spectrometry data (MS/MS). It allows to implement and run an easy-to-follow, easy-to-reproduce workflow from raw mass spectra to pre- and post-processed spectral data. Spectral data can be imported from common formats such as mzML, mzXML, msp, metabolomics-USI, MGF, or json (e.g. GNPS-style json files). Matchms then provides filters for metadata cleaning and checking, as well as for basic peak filtering. Finally, matchms was built to import and apply different similarity measures to compare large amounts of spectra. This includes common Cosine scores, but can also easily be extended by custom measures. Example for spectrum similarity measures that were designed to work in matchms are [Spec2Vec](#) and [MS2DeepScore](#).

If you use matchms in your research, please cite the following software paper:

F. Huber, S. Verhoeven, C. Meijer, H. Spreeuw, E. M. Villanueva Castilla, C. Geng, J.J.J. van der Hooft, S. Rogers, A. Belloum, F. Diblen, J.H. Spaaks, (2020). matchms - processing and similarity evaluation of mass spectrometry data. Journal of Open Source Software, 5(52), 2411, <https://doi.org/10.21105/joss.02411>

| | Badges |
|----------------------------------|--------|
| fair-software.nl recommendations | |
| 1. Code repository | |
| 2. License | |
| 3. Community Registry | |
| 4. Enable Citation | |
| 5. Checklists | |

Our main contribution to research and main output as an institute is **research software**.

Broad impact, re-use, sustainability and proper credit and recognition of research software is very important to us!

Therefore, we are actively involved in:

- Best practices guidelines (Turing way)
- Digital skills training (Software Carpentry)
- FAIR software principles
- Software citation & metadata
- Software Management Plans
- Improving funding of research software
- **Research Software Directory**

FAIR FOR SOFTWARE:
Reproducible Open Science ⑦

Software solution to
their scientific problem.

Research
Software
Users ①

② Search
cite.
Quality + trust.

⑥ Funders
Policy makers

connect
③

RANKING
VITALITY
Open API ④

Research Software Directory
Archive
index
links

Roi
Statistics.
Impact.

⑤ Research Groups /
Institutes / projects

Research
Software
Developers

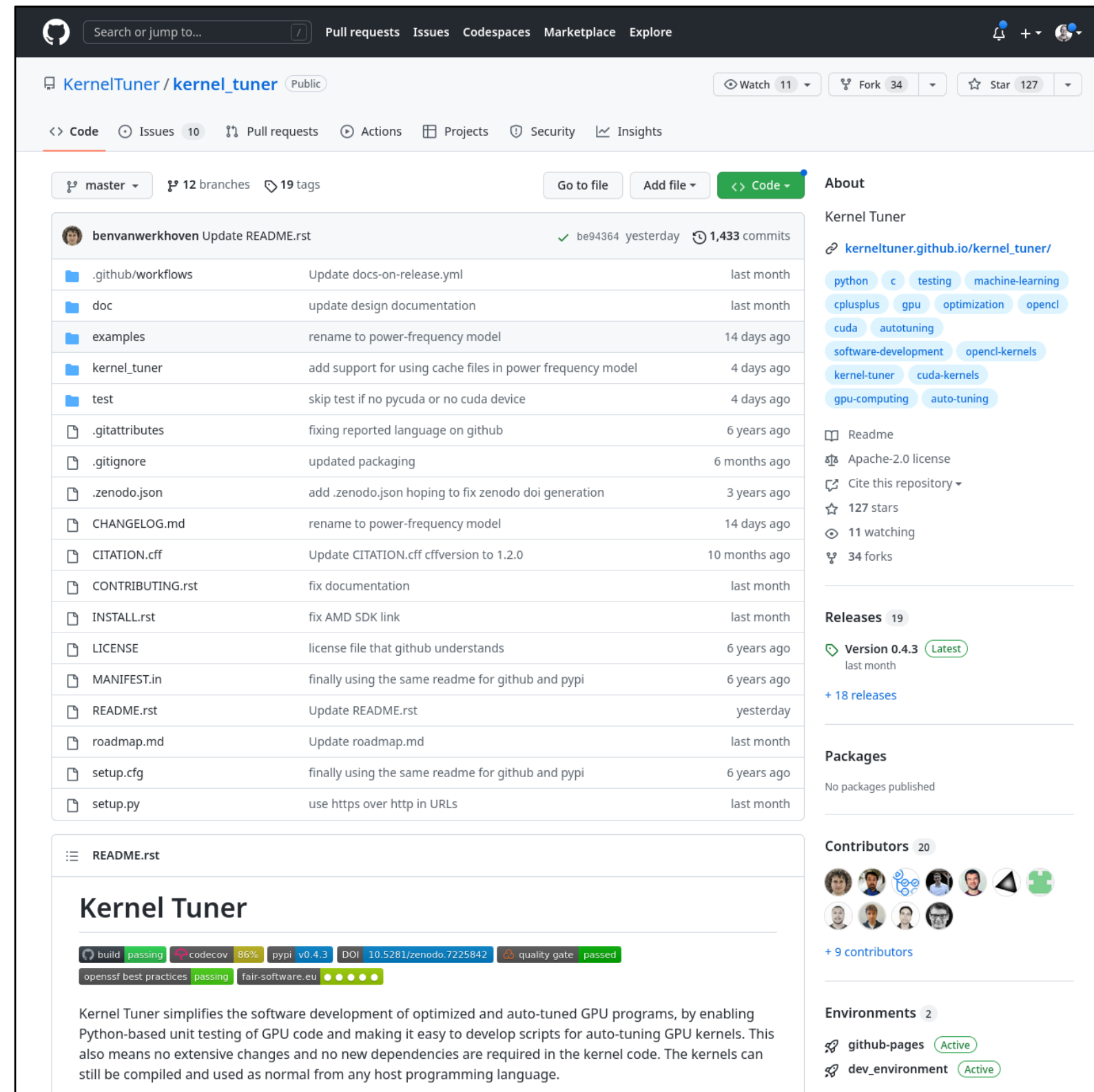
Software
+ metadata
⑧

Citable
visibility
re-use ⑨

Credits / impact / community building.

Research Software Directory?

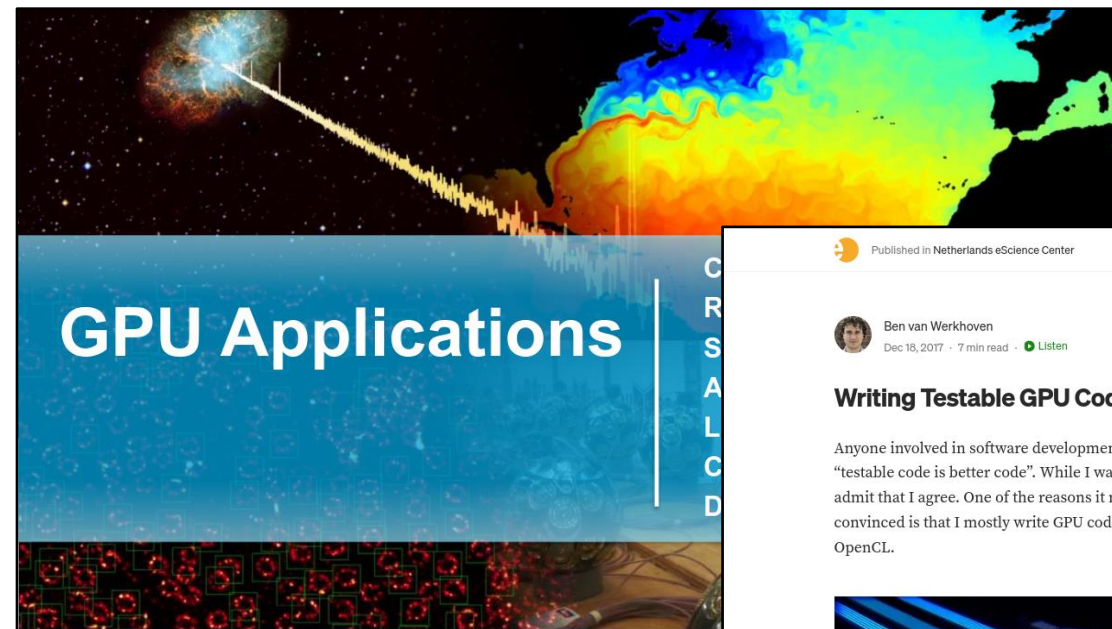
Research software is an essential output of research projects



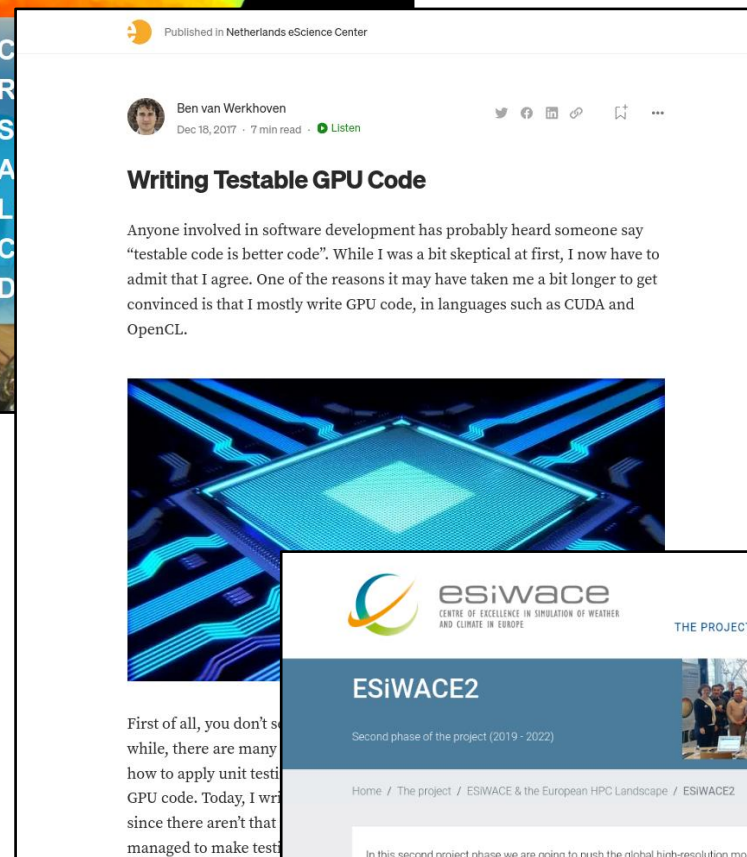
The screenshot shows the GitHub repository page for `KernelTuner/kernel_tuner`. The repository is public and has 11 watchers, 34 forks, and 127 stars. The main content area displays a list of files and folders, including `.github/workflows`, `doc`, `examples`, `kernel_tuner`, `test`, `.gitattributes`, `.gitignore`, `.zenodo.json`, `CHANGELOG.md`, `CITATION.cff`, `CONTRIBUTING.rst`, `INSTALL.rst`, `LICENSE`, `MANIFEST.in`, `README.rst`, `roadmap.md`, `setup.cfg`, and `setup.py`. The `README.rst` file is selected, showing the title "Kernel Tuner" and a description: "Kernel Tuner simplifies the software development of optimized and auto-tuned GPU programs, by enabling Python-based unit testing of GPU code and making it easy to develop scripts for auto-tuning GPU kernels. This also means no extensive changes and no new dependencies are required in the kernel code. The kernels can still be compiled and used as normal from any host programming language." The page also features a sidebar with "About" information, including the repository URL, tags like `python`, `c`, `testing`, `machine-learning`, `cplusplus`, `gpu`, `optimization`, `opengl`, `cuda`, `autotuning`, `software-development`, `opengl-kernels`, `kernel-tuner`, `cuda-kernels`, `gpu-computing`, and `auto-tuning`, and a "Releases" section showing the latest version 0.4.3.

https://github.com/KernelTuner/kernel_tuner

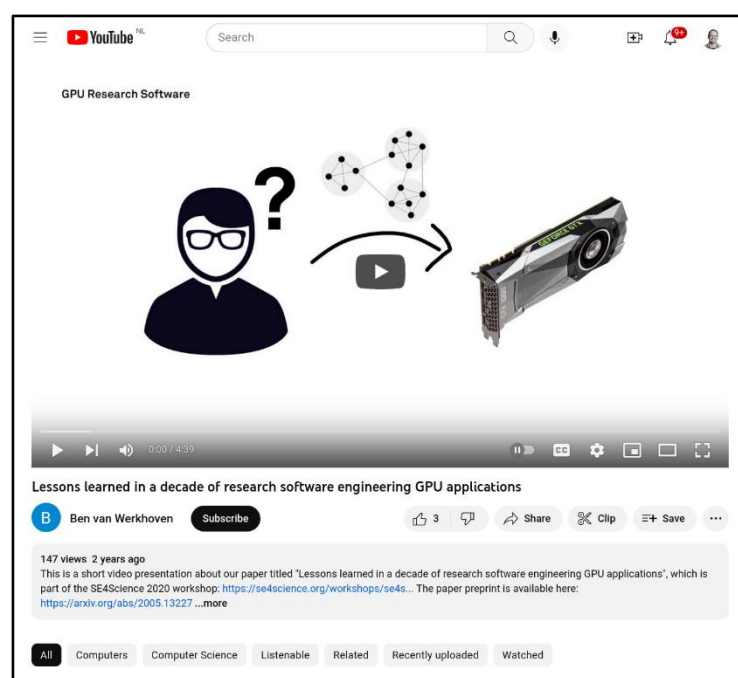
Research software has context



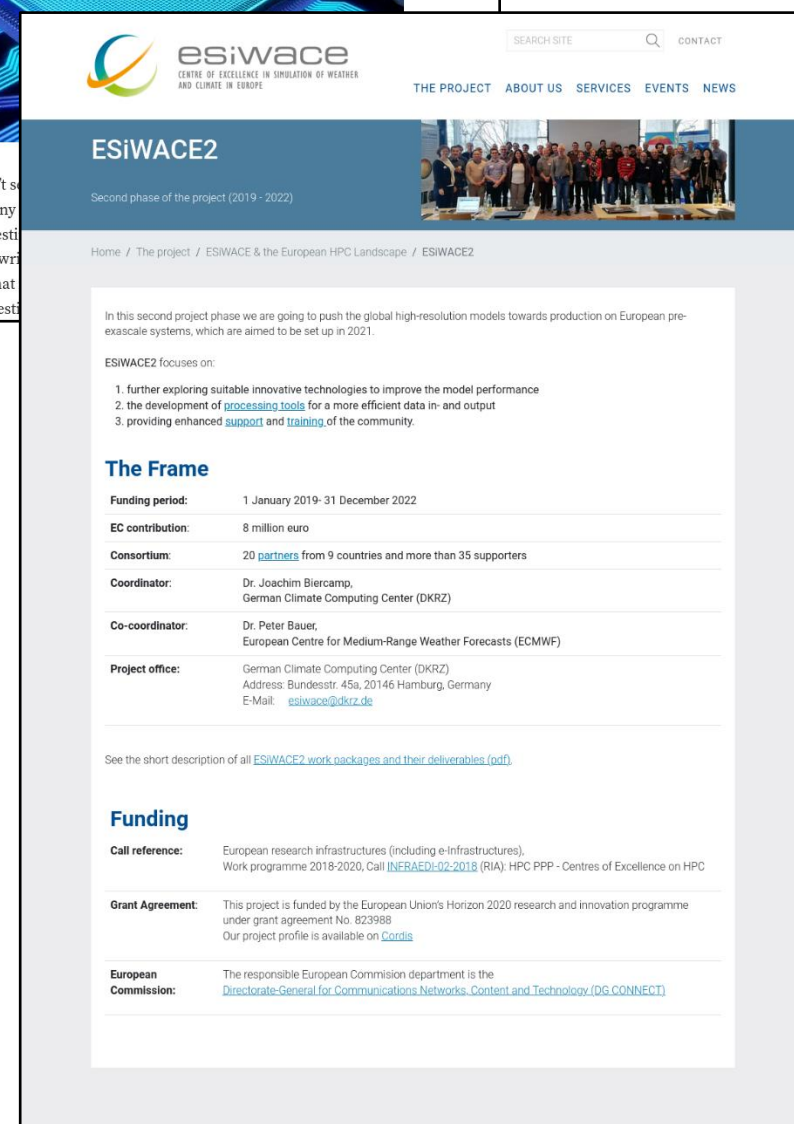
presentations



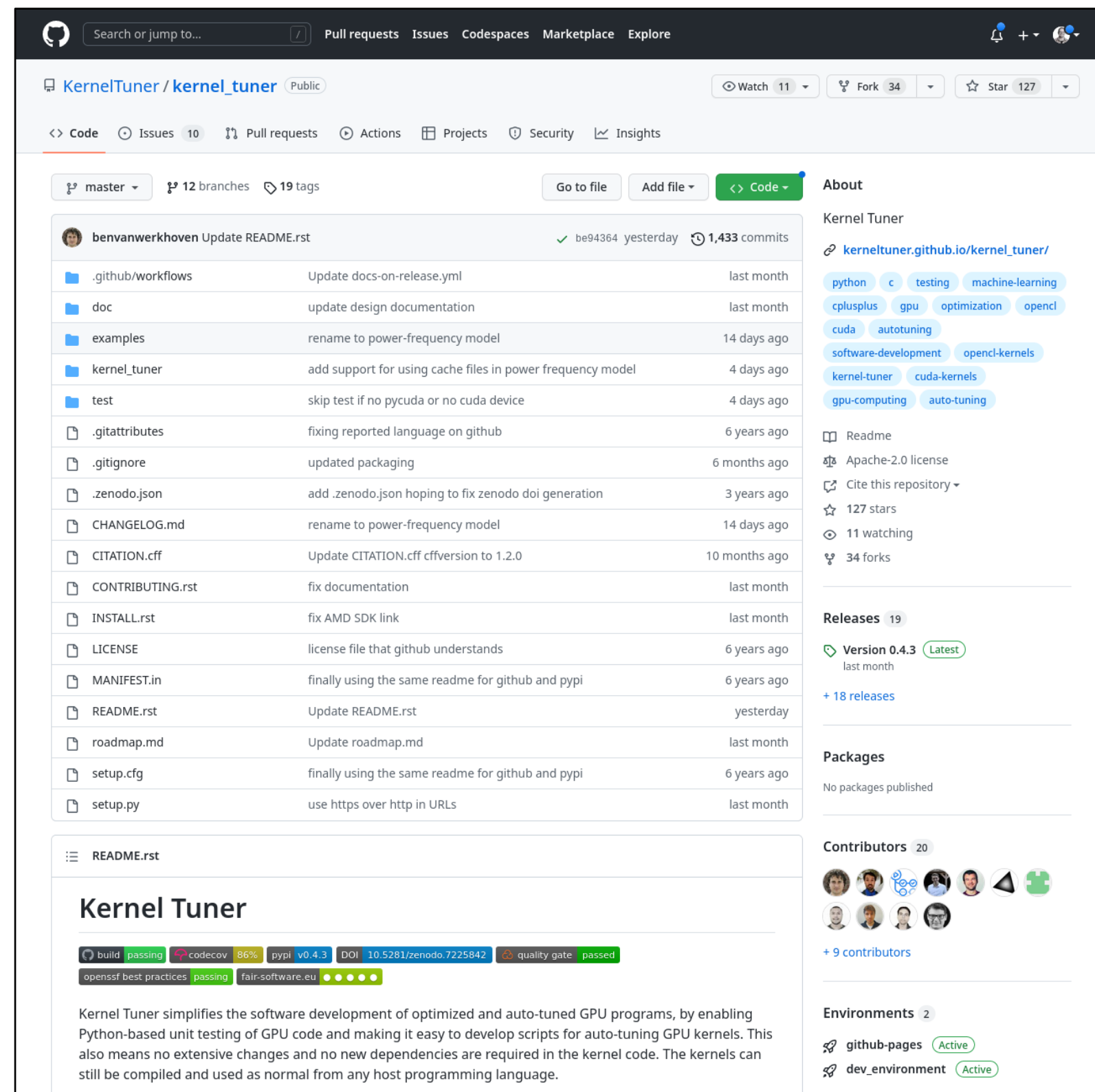
blogs



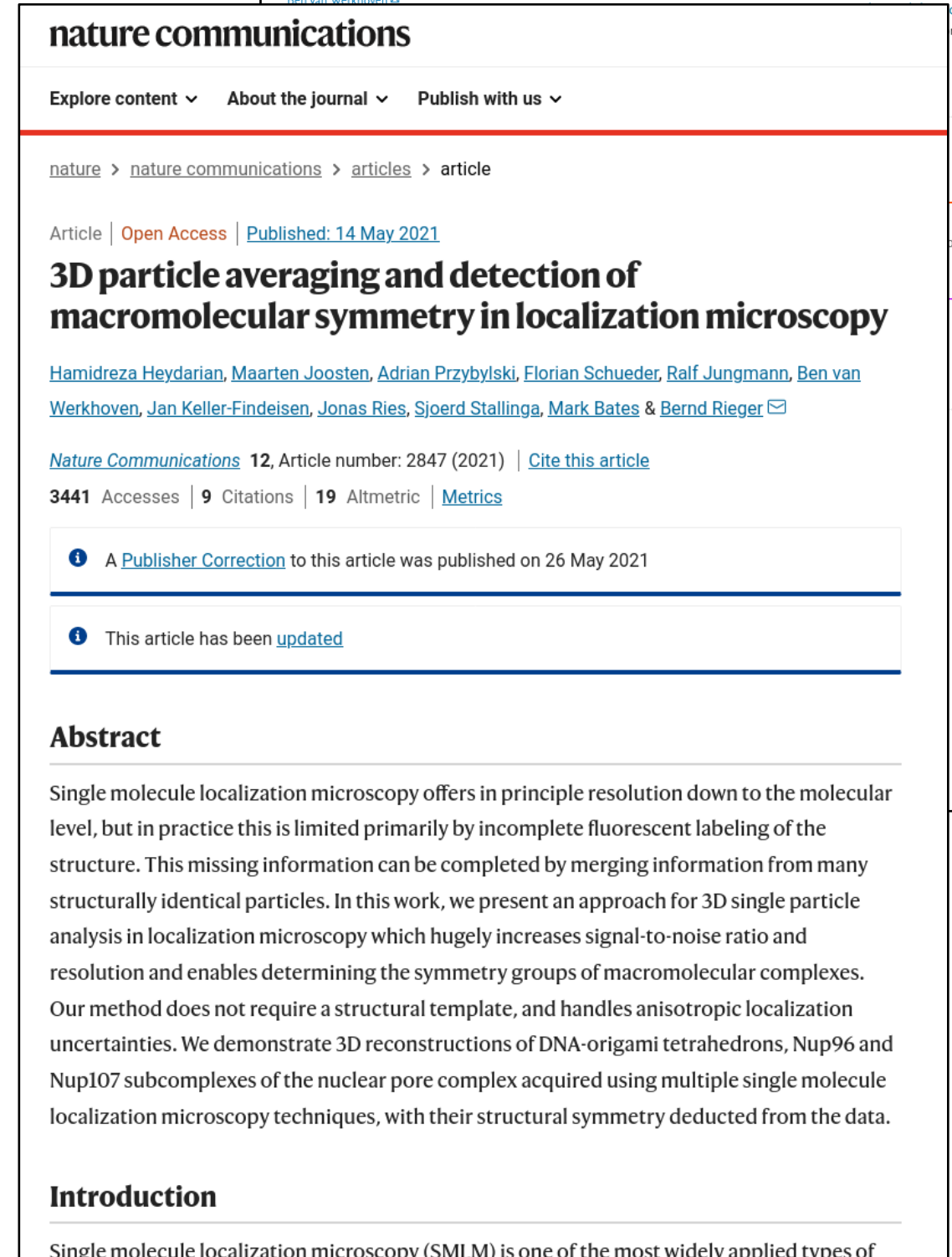
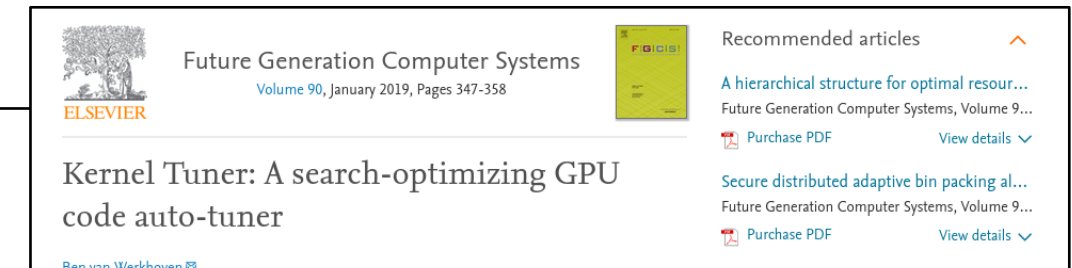
videos



projects



https://github.com/KernelTuner/kernel_tuner



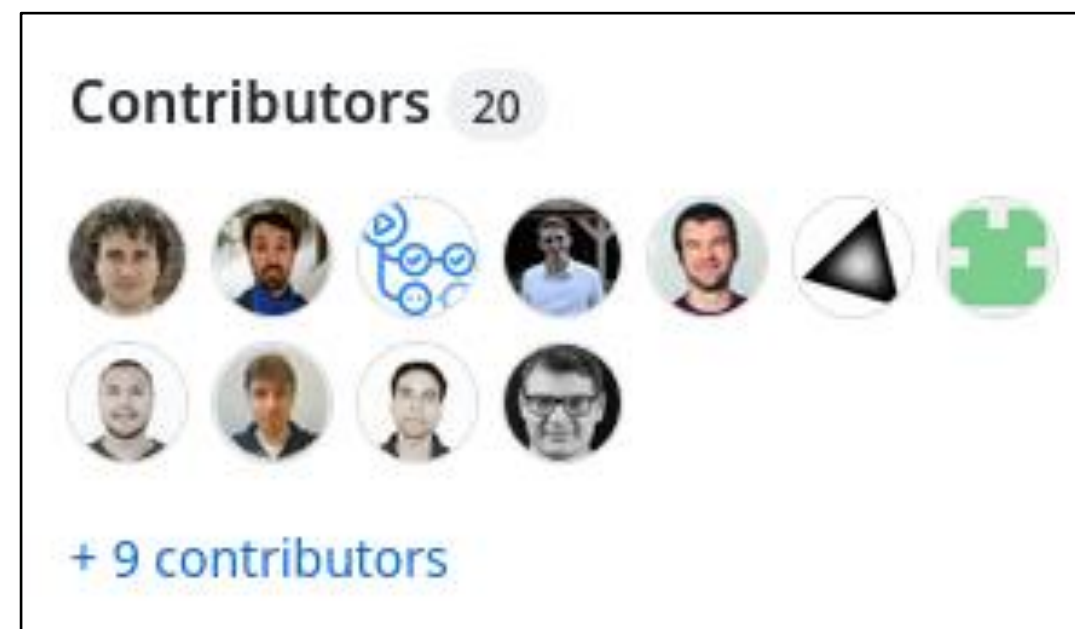
publications



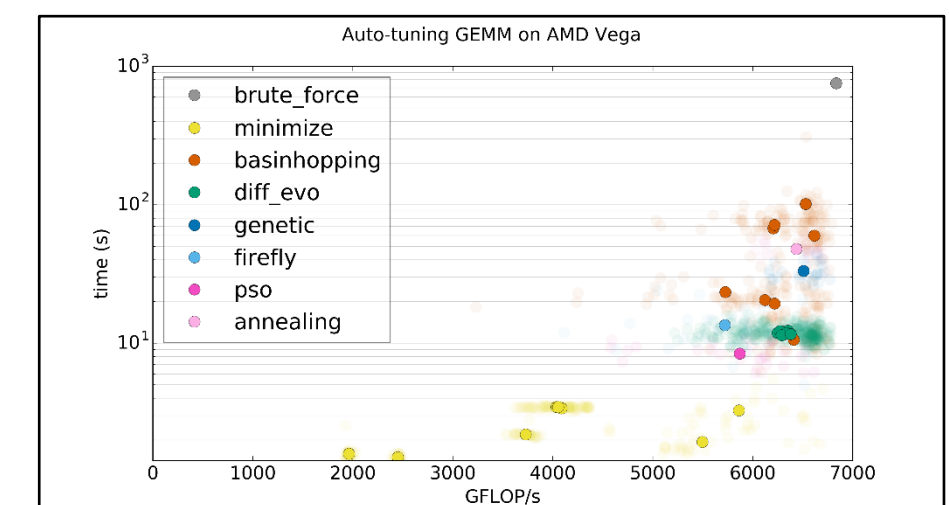
tutorials



participating organizations

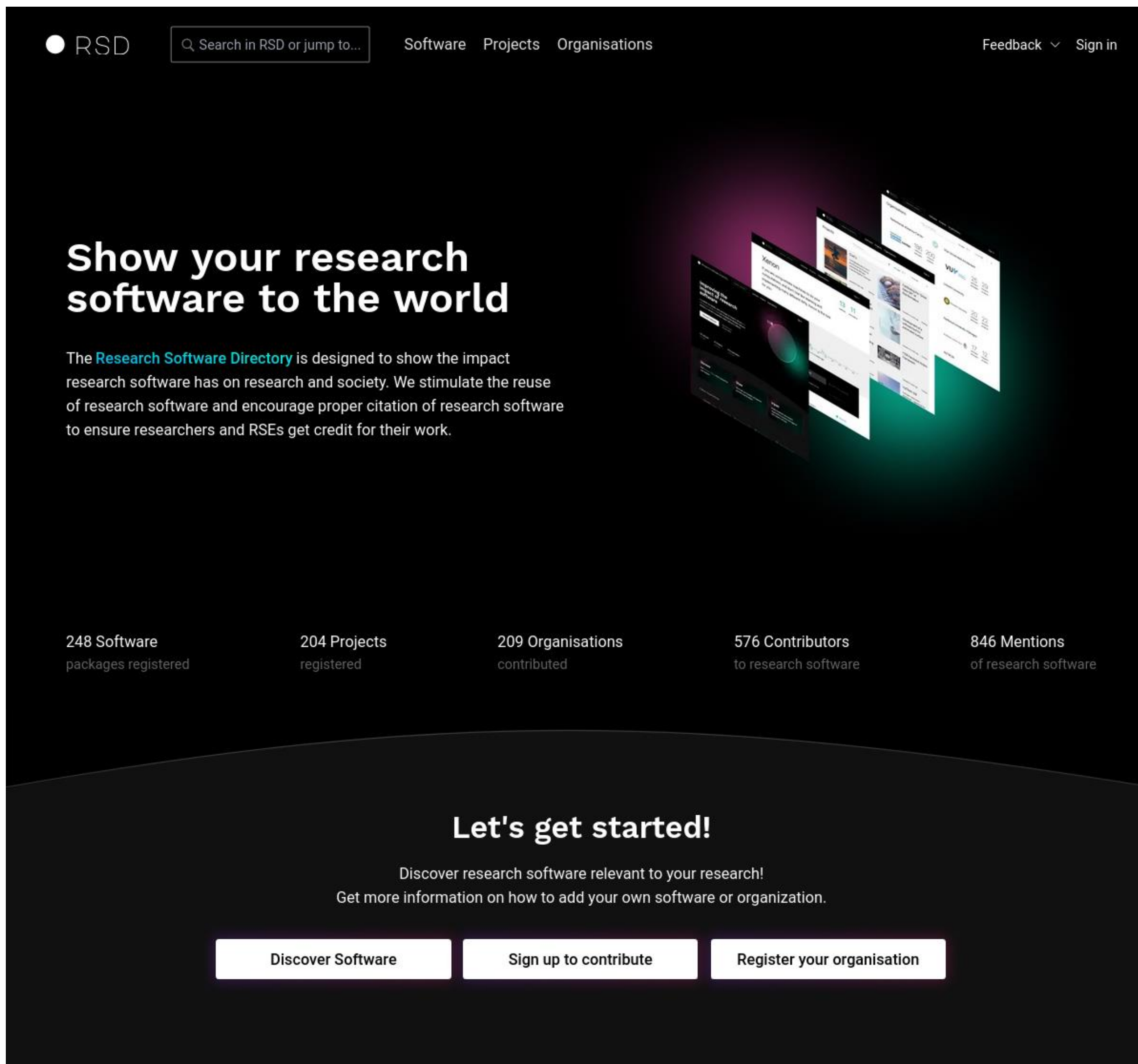


RSEs & other contributors



datasets

The Research Software Directory



The screenshot shows the homepage of the Research Software Directory (RSD). At the top, there is a navigation bar with the RSD logo, a search bar, and links for Software, Projects, Organisations, Feedback, and Sign in. The main content area features a large heading 'Show your research software to the world' and a subheading explaining the directory's purpose. Below this, there are five statistics: 248 Software packages registered, 204 Projects registered, 209 Organisations contributed, 576 Contributors to research software, and 846 Mentions of research software. A 'Let's get started!' section follows, with a call to action and three buttons: 'Discover Software', 'Sign up to contribute', and 'Register your organisation'.

RSD

Search in RSD or jump to...

Software Projects Organisations

Feedback Sign in

Show your research software to the world

The [Research Software Directory](#) is designed to show the impact research software has on research and society. We stimulate the reuse of research software and encourage proper citation of research software to ensure researchers and RSEs get credit for their work.

248 Software packages registered

204 Projects registered

209 Organisations contributed

576 Contributors to research software

846 Mentions of research software

Let's get started!

Discover research software relevant to your research!
Get more information on how to add your own software or organization.

Discover Software

Sign up to contribute

Register your organisation

The Research Software Directory is an **online service** designed to **collect** and **present** this web of information in a structured way.

Enable RSEs to show the impact their software has in research and society

Help researchers to find research software they need to do their research

Encourage citation of research software in other research outputs.

Allow organisations to collect information about the research software they produce and its impact

Show your research software to the world

The **Research Software Directory** is designed to show the impact research software has on research and society. We stimulate the reuse of research software and encourage proper citation of research software to ensure researchers and RSEs get credit for their work.

248 Software packages registered 204 Projects registered 209 Organisations contributed 576 Contributors to research software 846 Mentions of research software

Let's get started!

Discover research software relevant to your research!
Get more information on how to add your own software or organization.

Discover Software Sign up to contribute Register your organisation

The screenshot shows the Research Software Directory homepage. It features a dark background with white text. At the top, there's a main heading and a paragraph explaining the directory's purpose. Below that, five statistics are displayed in a row. A central section titled 'Let's get started!' contains a sub-heading and a paragraph, followed by three white buttons: 'Discover Software', 'Sign up to contribute', and 'Register your organisation'. Three red arrows point from these buttons to labels below the screenshot: 'browse content as visitor' from 'Discover Software', 'sign up as a developer / team' from 'Sign up to contribute', and 'sign up as organisation' from 'Register your organisation'.

You are welcome to:

- browse content
- sign up as an individual / team
- sign up as an organization
- add your own software
- join the open source development

<https://research-software-directory.org>

rsd@esciencecenter.nl

**browse content
as visitor**

**sign up as
a developer / team**

**sign up as
organisation**

Research Software Directory = Open Source

RSD Search in RSD or jump to... Software Projects Organisations Feedback Sign in

Show your research software to the world

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Get more information on how to add your own software or organization.

Discover Software Sign up to contribute Register your organisation

<https://research-software-directory.org>

7/7/2022 Launched by eScience Center

Used by 8 Dutch research institutes + several international



open source and shared codebase at:

<https://github.com/research-software-directory/RSD-as-a-service>

Research Software Directory Search or jump to... Software Projects Organisations Sign in

HELMHOLTZ

Research for grand challenges.

Promote and Discover Research Software

Because software matters

Browse software

Software Spotlights

The latest outstanding software product developed in Helmholtz.

MassBank Search Contents Download Accession Go More

MassBank Record: UA002903

Atrazine; APCI-ITFT; MS2; CE: 35%; R=30000; [M+H]+

Mass Spectrum

Abundance

m/z

MassBank

MassBank is an open source mass spectral library for the identification of small chemical molecules of metabolomics, exposomics and environmental relevance.

Discover software by research topic

Energy Earth & Environment Health

Information Aeronautics, Space and Transport Matter

<https://helmholtz.software>

29/7/2022 Launch by Helmholtz

Available to all Helmholtz Institutes



User friendly data curation interface

The screenshot shows the 'Kernel Tuner' page on the Research Software Directory. The interface is clean and organized into several sections:

- Header:** 'Research Software Directory' logo, search bar, navigation tabs (Software, Projects, Organisations), and user profile 'JM'.
- Left Sidebar:** A vertical menu with icons and labels for 'Information', 'Contributors', 'Organisations', 'Mentions', 'Testimonials', 'Related topics', and 'Maintainers'.
- Software information:** Fields for RSD path (kernel-tuner), Name (Kernel Tuner), Short description (Kernel Tuner greatly simplifies the development of highly-optimized and auto-tuned CUDA, OpenCL, and C code...), Software URLs (GitHub repository), and Repository URL (https://github.com/KernelTuner/kernel_tuner).
- Description:** A rich text editor with 'MARKDOWN' and 'PREVIEW' tabs. The preview shows a list of bullet points and a paragraph describing the software's capabilities.
- Status:** A 'Published' toggle switch and a 'Publishing software page' informational box.
- Citation:** A 'VALIDATE DOI' button and a list of keywords like 'Big Data', 'GPU', 'High Performance Computing', etc.
- Licenses:** A 'LICENSES' section with an 'IMPORT LICENSES' button and a list of licenses including 'Apache-2.0'.

Free to use for RSEs and researchers

- sign-in via SURFConext, ORCID (or Helmholtz AAI)

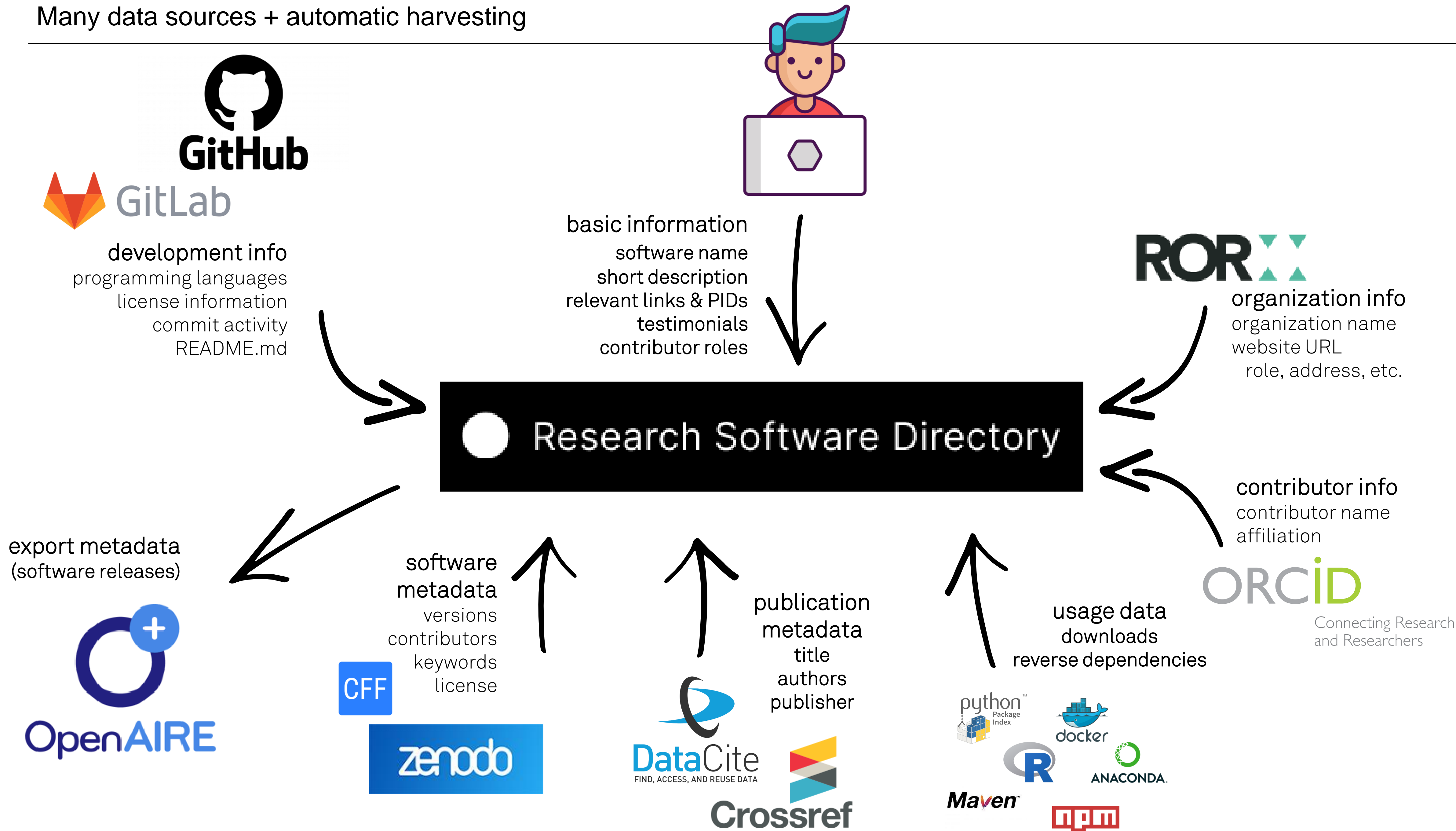
Collect all related information on software in one place

Easy to use without extensive technical knowledge

We automatically **harvest** data where possible

- Contributors via ORCID / DOI+CFF
- Organisations via ROR
- Keywords & licences from DOI
- Releases & mentions via DOI
- Descriptions via source repository in gitlab/github

Many data sources + automatic harvesting



Generated software pages (& project pages)

generated software pages

generated project pages

Research Software Directory

generated organisation pages

| Organisation | Software packages | Research projects |
|-------------------------------------|-------------------|-------------------|
| Netherlands eScience Center | 191 | 200 |
| Vrije Universiteit Amsterdam | 25 | 29 |
| University of Amsterdam | 17 | 35 |
| Utrecht University | 20 | 22 |
| Canarie | 40 | 0 |
| Digital Research Alliance of Canada | 40 | 0 |
| Delft University of Technology | 15 | 22 |
| Radboud University Nijmegen | 17 | 12 |
| Wageningen University & Research | | |
| ASTRON | | |

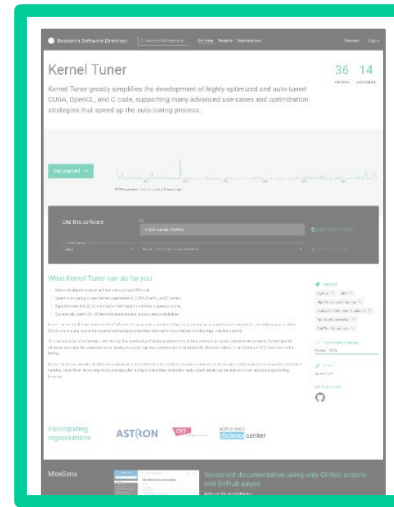
generated metrics? (TODO)

4278

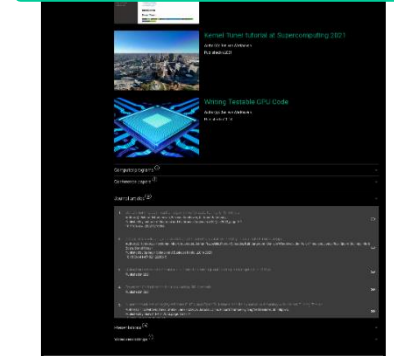
- Tweeted by 3838
- Blogged by 24
- On 895 Facebook pages
- Mentioned in 54 Google+ posts
- Picked up by 28 news outlets
- Reddited by 15
- 5 readers on Mendeley
- 0 readers on CiteULike

See more details

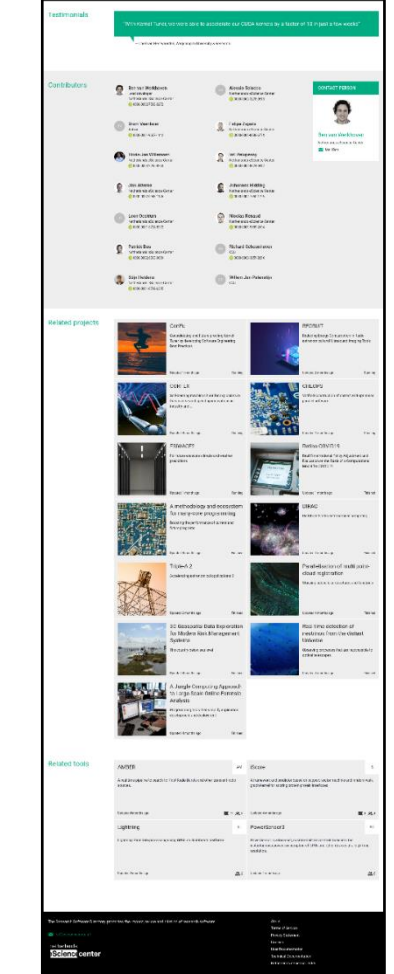
Basic information



name & description



getting started link
(to external webpage)



full page

detailed description



Research Software Directory

Kernel Tuner

36 mentions 14 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.

[Get started](#)

1239 commits | Last commit = 1 week ago

Cite this software

DOI: 10.5281/zenodo.7225842

Choose a version: 0.4.3

Choose a reference manager format:

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 10+ 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.

Keywords

- Big Data
- GPU
- High Performance Computing
- Multi-scale & Multi Model Simulations
- Optimized Data Handling
- Real Time Data Analysis

Programming language

Python 100%

License

Apache-2.0

Source code

Participating organisations

ASTRON CWI Netherlands Science center

Mentions

Versioned documentation using only GitHub actions

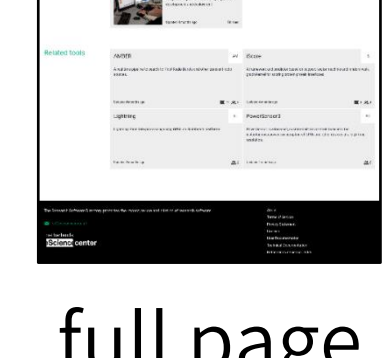
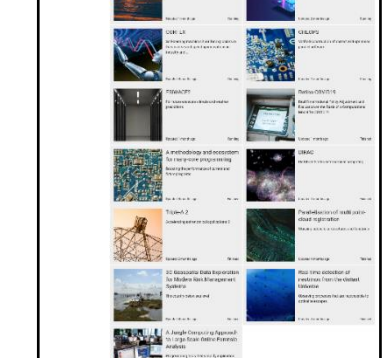
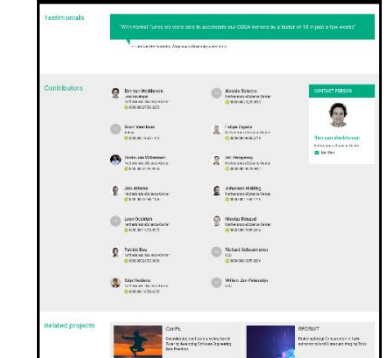
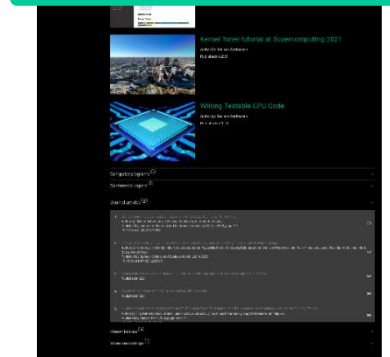
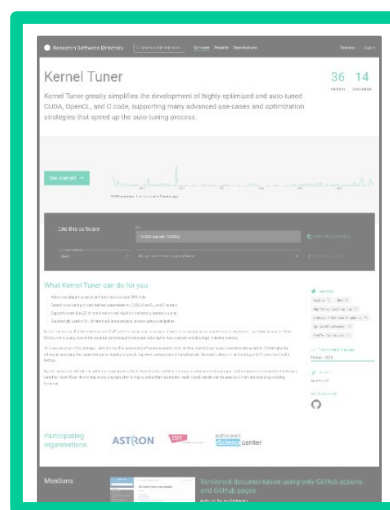
keywords

used programming languages & license

source code repository link

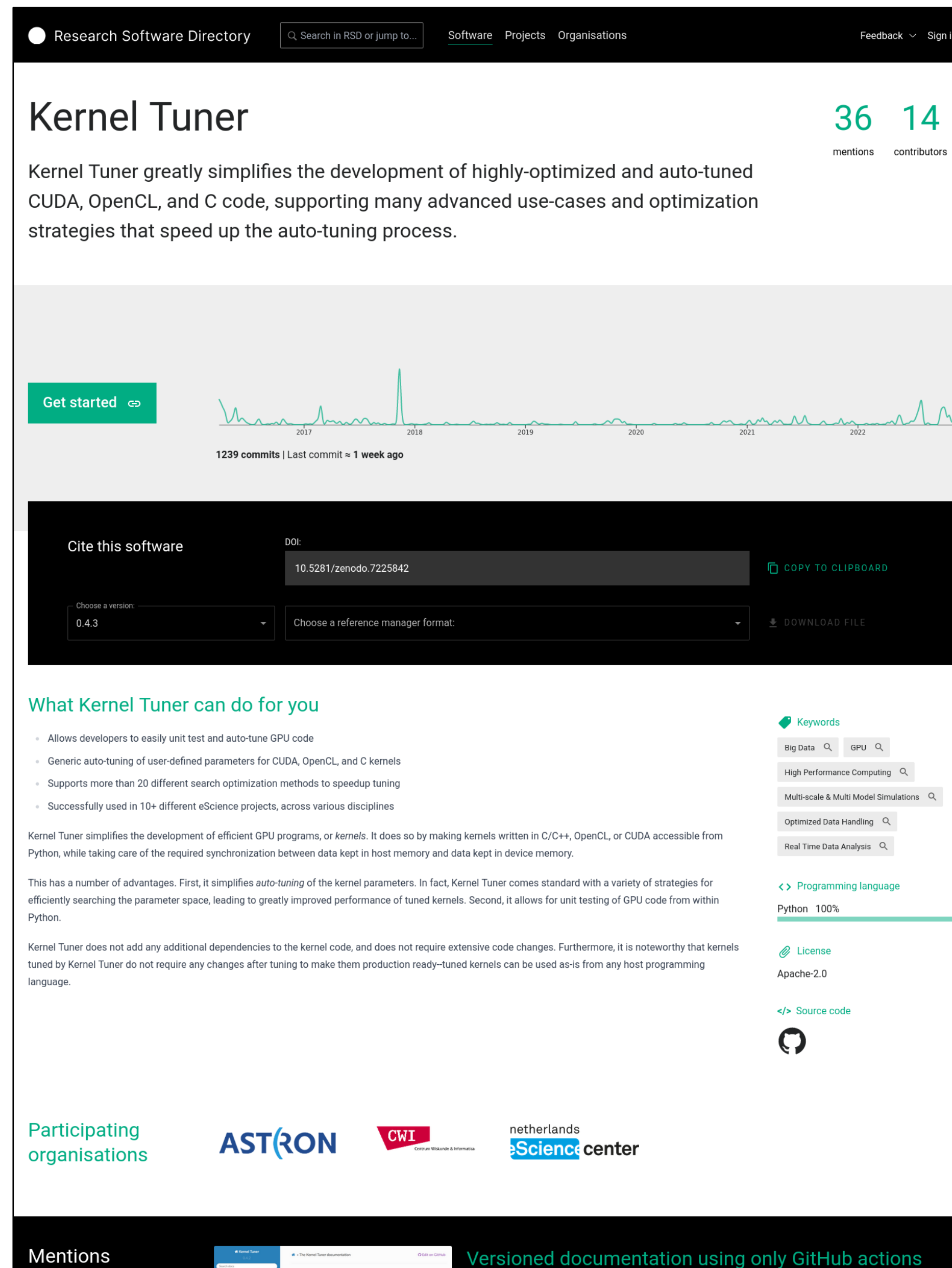
<https://research-software-directory.org/software/kernel-tuner>

Community, development activity



full page

participating organizations



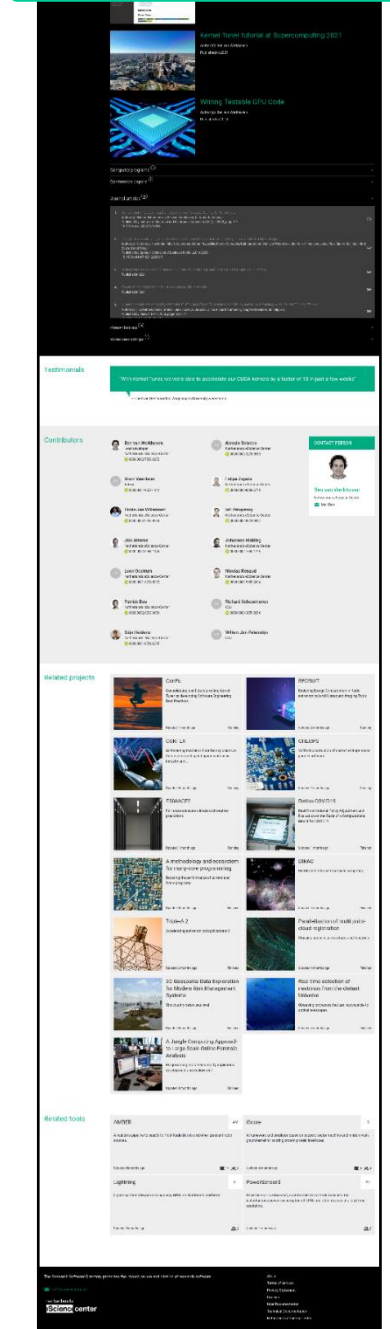
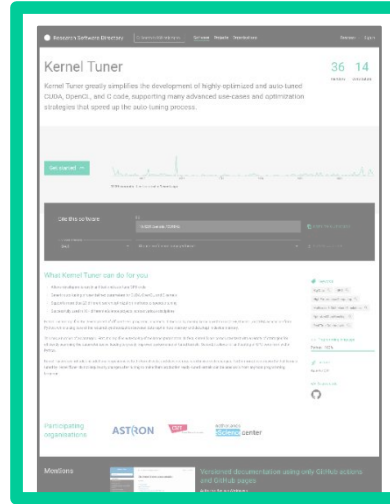
The screenshot shows the Research Software Directory page for Kernel Tuner. At the top, it displays the project name 'Kernel Tuner' and statistics: 36 mentions and 14 contributors. Below this is a 'Get started' button and a line graph showing development activity from 2017 to 2022, with 1239 commits and the last commit made 1 week ago. The 'Cite this software' section provides a DOI (10.5281/zenodo.7225842) and options to copy to clipboard or download a file. The 'What Kernel Tuner can do for you' section lists several benefits, such as allowing developers to easily unit test and auto-tune GPU code. The 'Participating organisations' section lists ASTRON, CWI, and the Netherlands Science Center. At the bottom, there are links for 'Mentions' and 'Versioned documentation using only GitHub actions'.

← contributor and mention count

← development activity

<https://research-software-directory.org/software/kernel-tuner>

Citation information

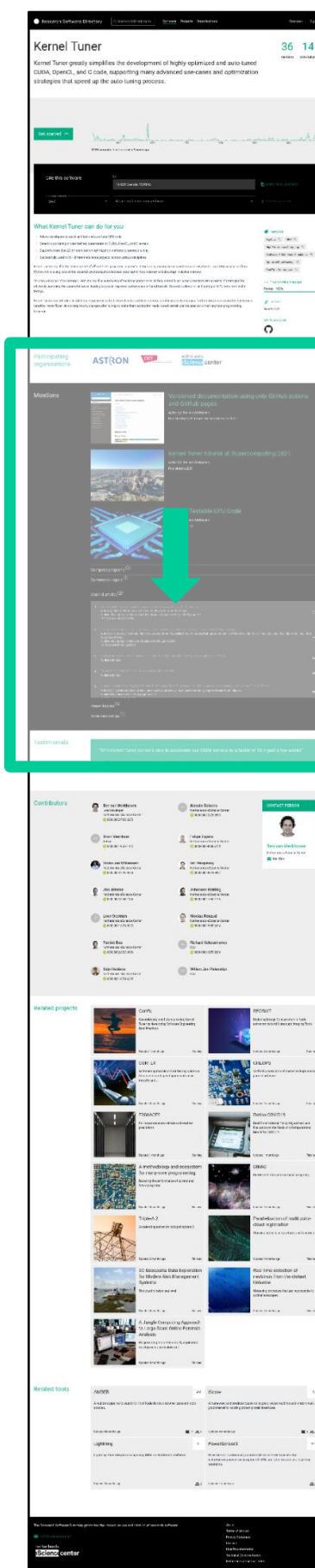


full page

A screenshot of the Research Software Directory page for Kernel Tuner. The page includes a header with the site name and navigation links, a main title 'Kernel Tuner' with statistics (36 mentions, 14 contributors), a description of the software, a 'Get started' button, a commit history graph, a 'Cite this software' section with a DOI field (10.5281/zenodo.7225842), a version selector (0.4.3), and a reference manager format selector. Below this is a 'What Kernel Tuner can do for you' section with a list of features and a 'Keywords' section with search filters. At the bottom, there is a 'Mentions' section with a list of links and a 'Versioned documentation using only GitHub actions' link.

← citation information

Mentions: related research output



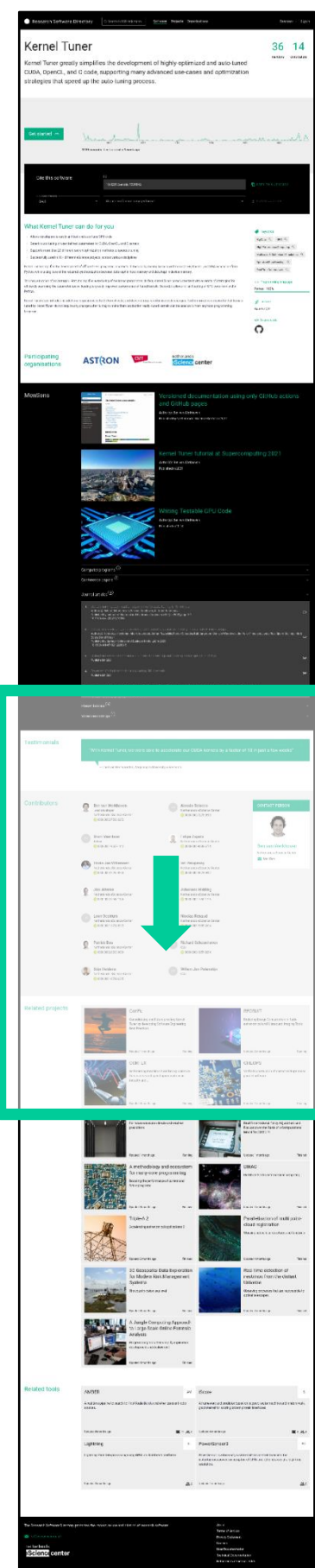
full page

highlights →

mentions grouped per type
publications, presentations,
blogs, videos, etc. →

← expanded list of
journal publications
(with links)

Contributors, testimonials, related projects



full page

user testimonials →

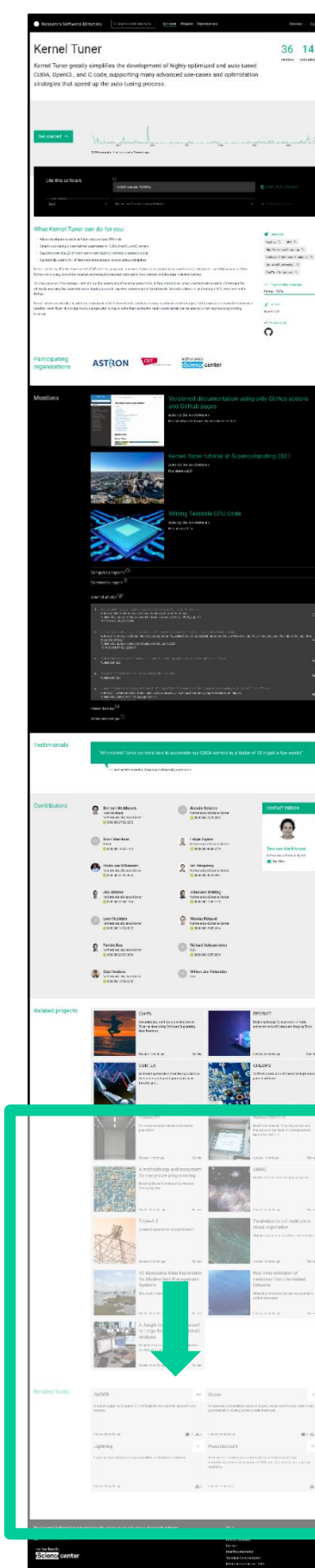
list of contributors with name, ORCID, image, **role** →

A detailed view of the website's content. The top section is 'Testimonials', featuring a green speech bubble with a quote: "With Kernel Tuner, we were able to accelerate our CUDA kernels by a factor of 10 in just a few weeks" by Chiel van Heerwaarden. Below is the 'Contributors' section, a grid of 12 contributor profiles. Each profile includes a circular ORCID icon, a profile picture, name, role, and ORCID number. A 'CONTACT PERSON' callout box highlights Ben van Werkhoven. The bottom section is 'Related projects', showing four project cards: ConFu, RECRUIT, CORTEX, and CHEOPS, each with a thumbnail image, title, description, and status.

← contact person

← list of related projects

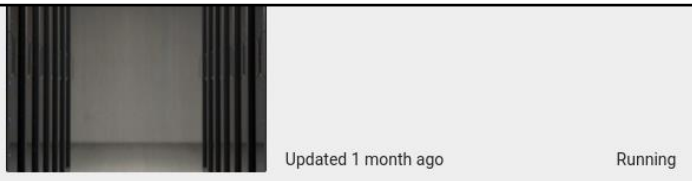
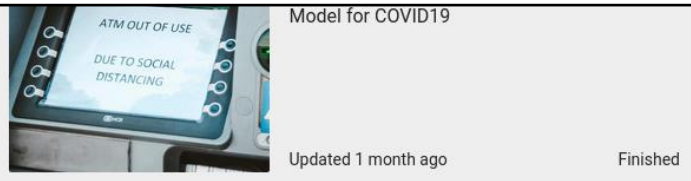
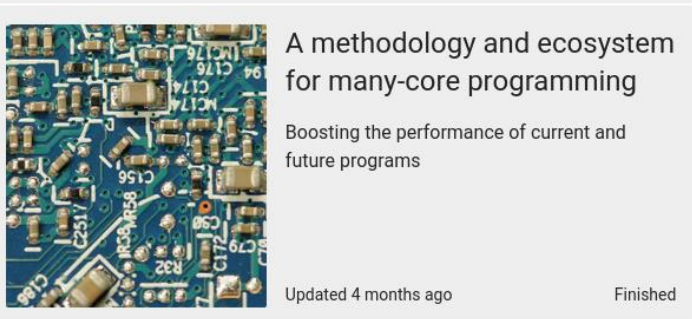
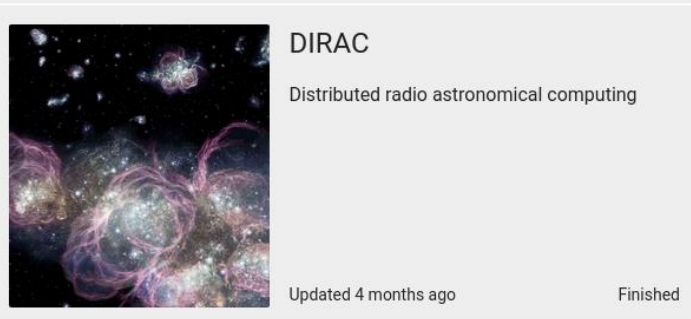
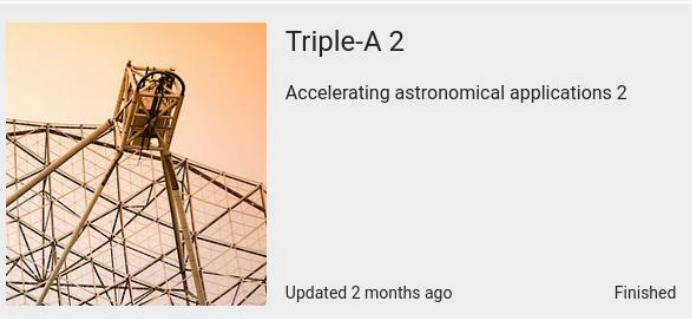

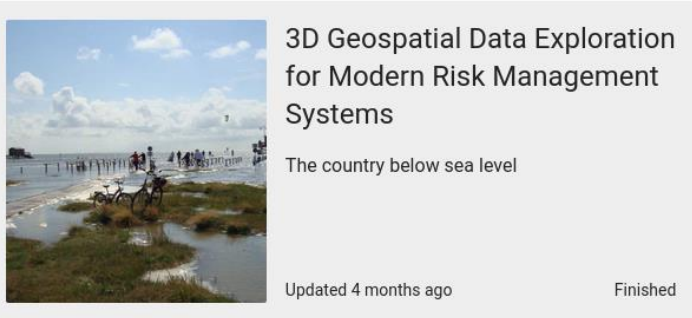


Related projects and software



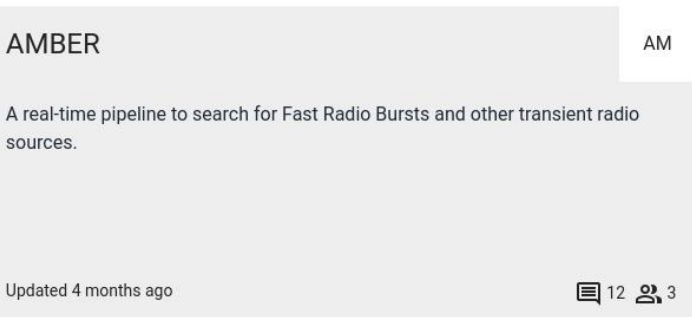
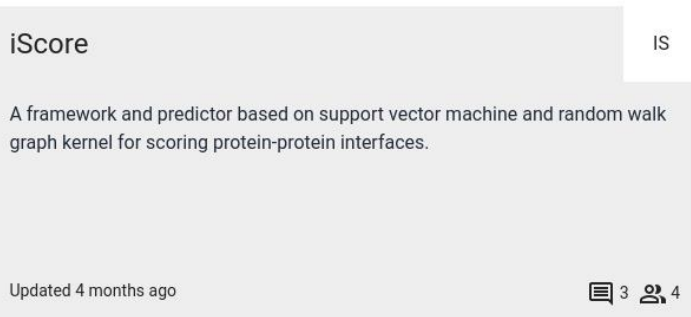

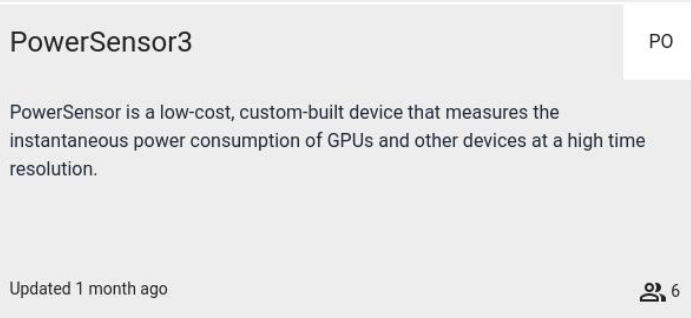
full page

list of related software



| | |
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|  | |

Related tools

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|---|---|
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The Research Software Directory promotes the impact, re-use and citation of research software. [About](#)

← list of related projects (continued)

Plans for 2023



Research Software Directory is actively being maintained and developed. Our plans for this year are:

- ✓ link to package managers, container registries, software heritage, etc., and use as data sources.
- ✓ add additional APIs to share our data with external services (REST, OAI-PMH, etc.) + connect to OpenAIRE
- ↻ improve look and feel of software pages, software highlights, etc.
- ↻ improve search, organizational overview, insight, etc.
- ⌚ harvest various indicators on software impact and quality (and figure out how to display them)
- ⌚ research community curated software collections
- ⌚ federated search between different research software directories

Questions?



<https://www.esciencecenter.nl>



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<https://research-software-directory.org>



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