netherlands eScience center

Open science and software best practices

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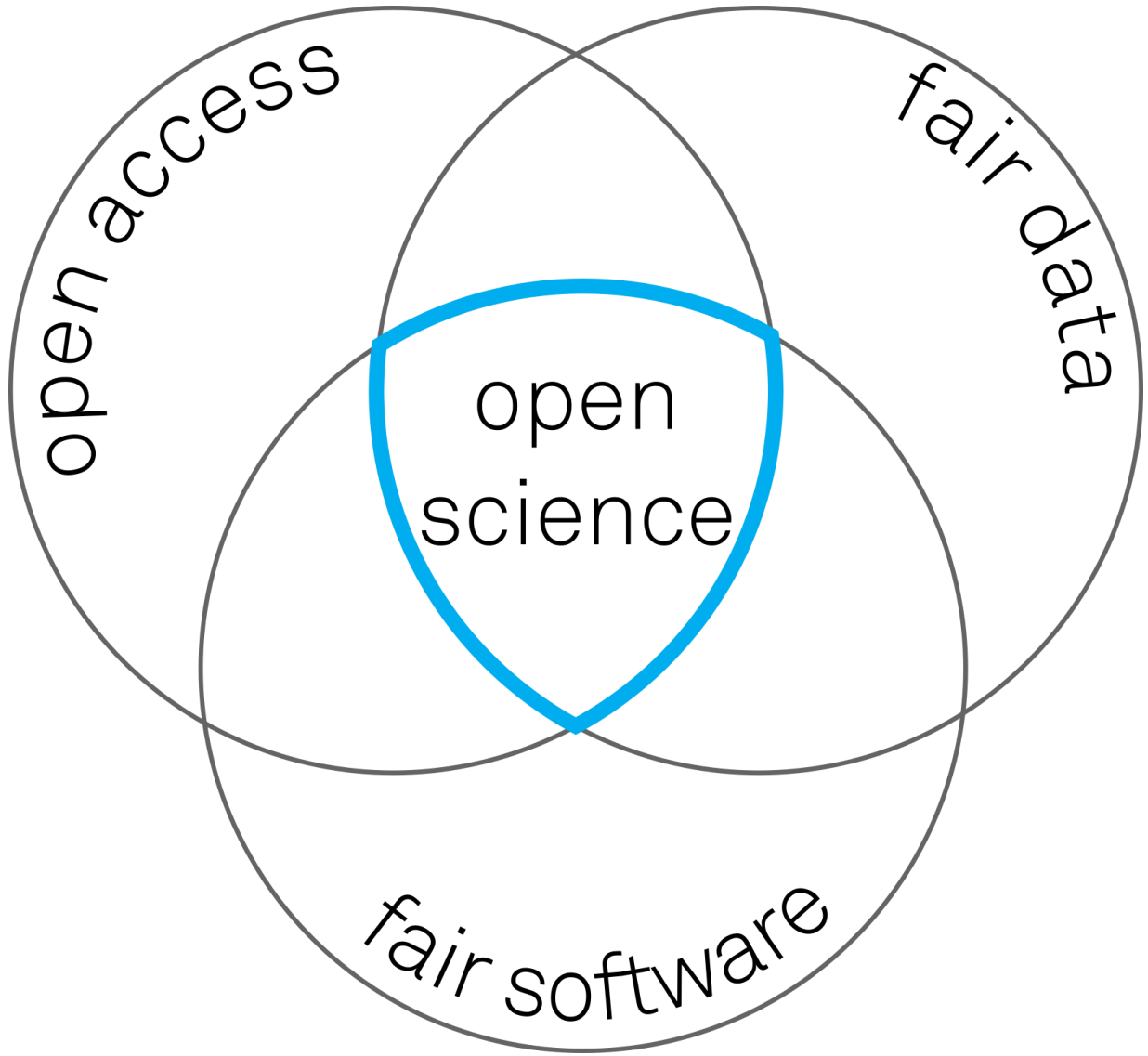
Photography: Elodie Burrillon

Netherlands eScience Center

Enabling digitally enhanced research through efficient utilization of data, software and e-infrastructure

Software's role in open science

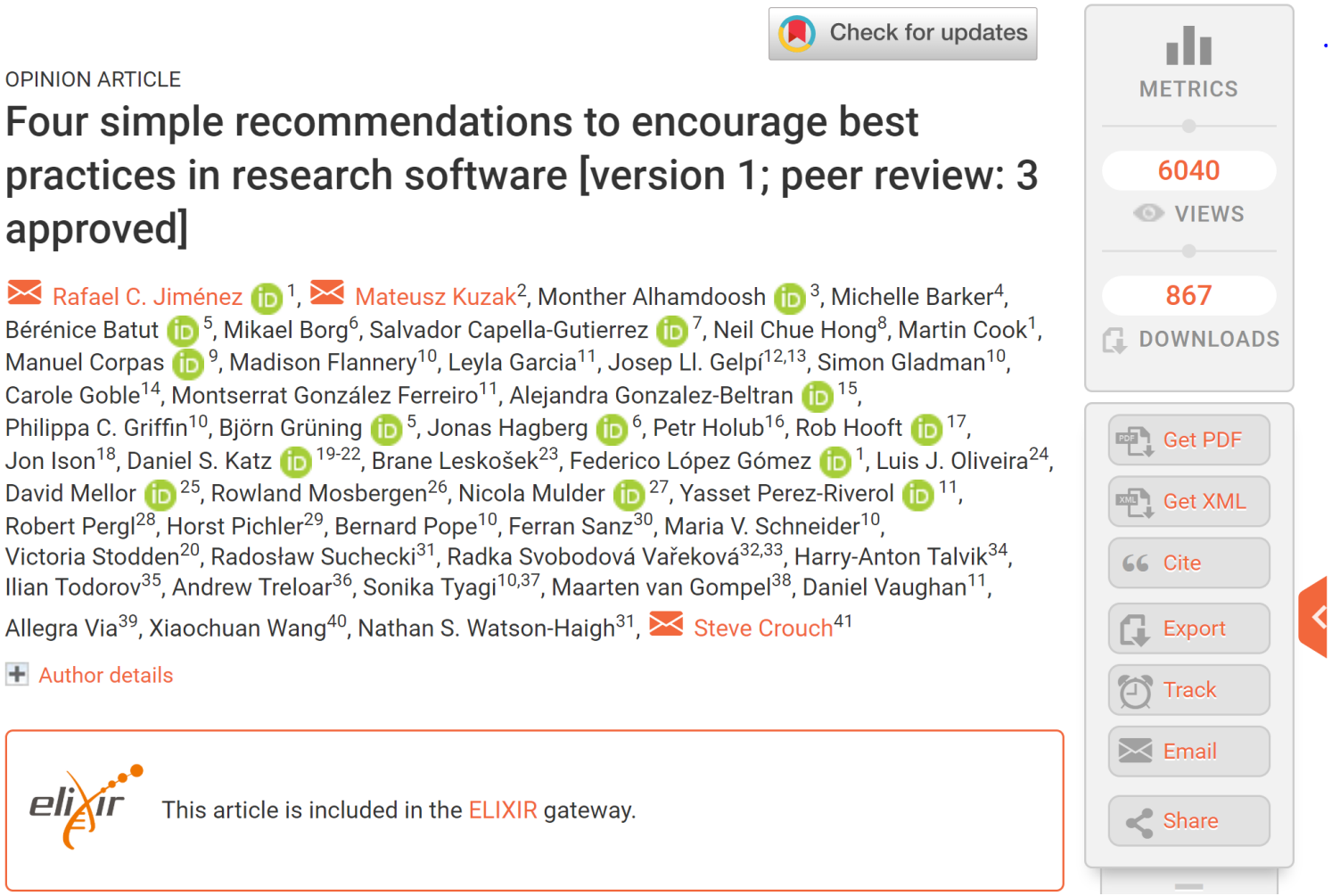


- 4 recommendations to encourage best practices in research software

- Practical guidelines

- Do you develop software?
- Do you develop on your own, or together with others?
- How do you share your software?
- What are the + and – of making code and data ‘open’?

4 Recommendations



Check for updates

OPINION ARTICLE

Four simple recommendations to encourage best practices in research software [version 1; peer review: 3 approved]

Rafael C. Jiménez [1], Mateusz Kuzak[2], Monther Alhamdoosh [3], Michelle Barker[4], Bérénice Batut [5], Mikael Borg[6], Salvador Capella-Gutierrez [7], Neil Chue Hong[8], Martin Cook[1], Manuel Corpas [9], Madison Flannery[10], Leyla Garcia[11], Josep Ll. Gelpí[12,13], Simon Gladman[10], Carole Goble[14], Montserrat González Ferreiro[11], Alejandra Gonzalez-Beltran [15], Philippa C. Griffin[10], Björn Grüning [5], Jonas Hagberg [6], Petr Holub[16], Rob Hooft [17], Jon Ison[18], Daniel S. Katz [19-22], Brane Leskošek[23], Federico López Gómez [1], Luis J. Oliveira[24], David Mellor [25], Rowland Mosbergen[26], Nicola Mulder [27], Yasset Perez-Riverol [11], Robert Pergl[28], Horst Pichler[29], Bernard Pope[10], Ferran Sanz[30], Maria V. Schneider[10], Victoria Stodden[20], Radosław Suchecki[31], Radka Svobodová Vařeková[32,33], Harry-Anton Talvik[34], Ilian Todorov[35], Andrew Treloar[36], Sonika Tyagi[10,37], Maarten van Gompel[38], Daniel Vaughan[11], Allegra Via[39], Xiaochuan Wang[40], Nathan S. Watson-Haigh[31], Steve Crouch[41]

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https://softdev4research.github.io/recommendations/

https://softdev4research.github.io/4OSS-lesson/

1. Develop publicly accessible open source code from day one

GitHub

Bitbucket

GitLab

2. Make software easy to discover by providing software metadata via a popular community registry

What is useful metadata?

3. Adopt a license and comply with the licence of third-party dependencies

Your work is automatically protected by copyright.
No license = no reuse by others!

Source code licenses: Apache 2, MIT, BSD, GPL, …

Data licenses: CC0, CC-BY-4, ODbL, …

https://choosealicense.com/

https://blog.esciencecenter.nl/a-license-to-science-cd8030a4a145

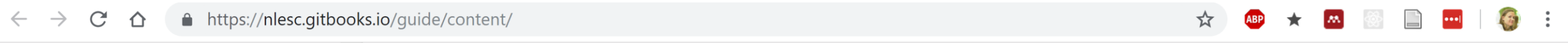
4. Have a clear and transparent contribution, governance and communication processes

How can people contribute to your project ?

How can they contact you ?

How can people ask for new features?

Can anyone push changes to your repo?



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Netherlands eScience Center Guide

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Guide

This is a guide to software development and projects at the Netherlands eScience Center. It both serves as a source of information for exactly how we work at the eScience Center, and as a basis for discussions and reaching consensus on this topic.

This Guide is a work in progress

The source of this book can be found on GitHub: https://www.github.com/nlesc/guide

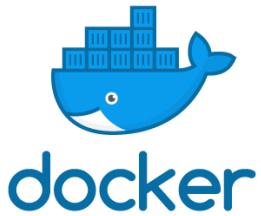
https://nlesc.gitbooks.io/guide/content/

- User documentation (README, tutorial…)
- Code documentation:
  - Python: docstring, Sphinx
  - R: roxygen

Use a consistent coding style:

- Python: pep-8
- Install *linters* for your editor (R: lintr)

- Make your code installable
  - Python: setup.py
- On GitHub: version tagging
  - Semantic versioning
- Create DOI: e.g. Zenodo
- Add Citation file
- Distribute your software:
  - Python: PyPi, Conda
  - R: CRAN
  - Generic: Docker



https://guide.esciencecenter.nl/best_practices/releases.html

- Write (unit) tests
  - Python: pytest / nose
  - R: testthat
- Continuous Integration: Travis
  - Automatically runs tests after new commit
  - Different operating systems / versions
  - Can also check code style, test coverage, generate documentation…

.travis.yml file:

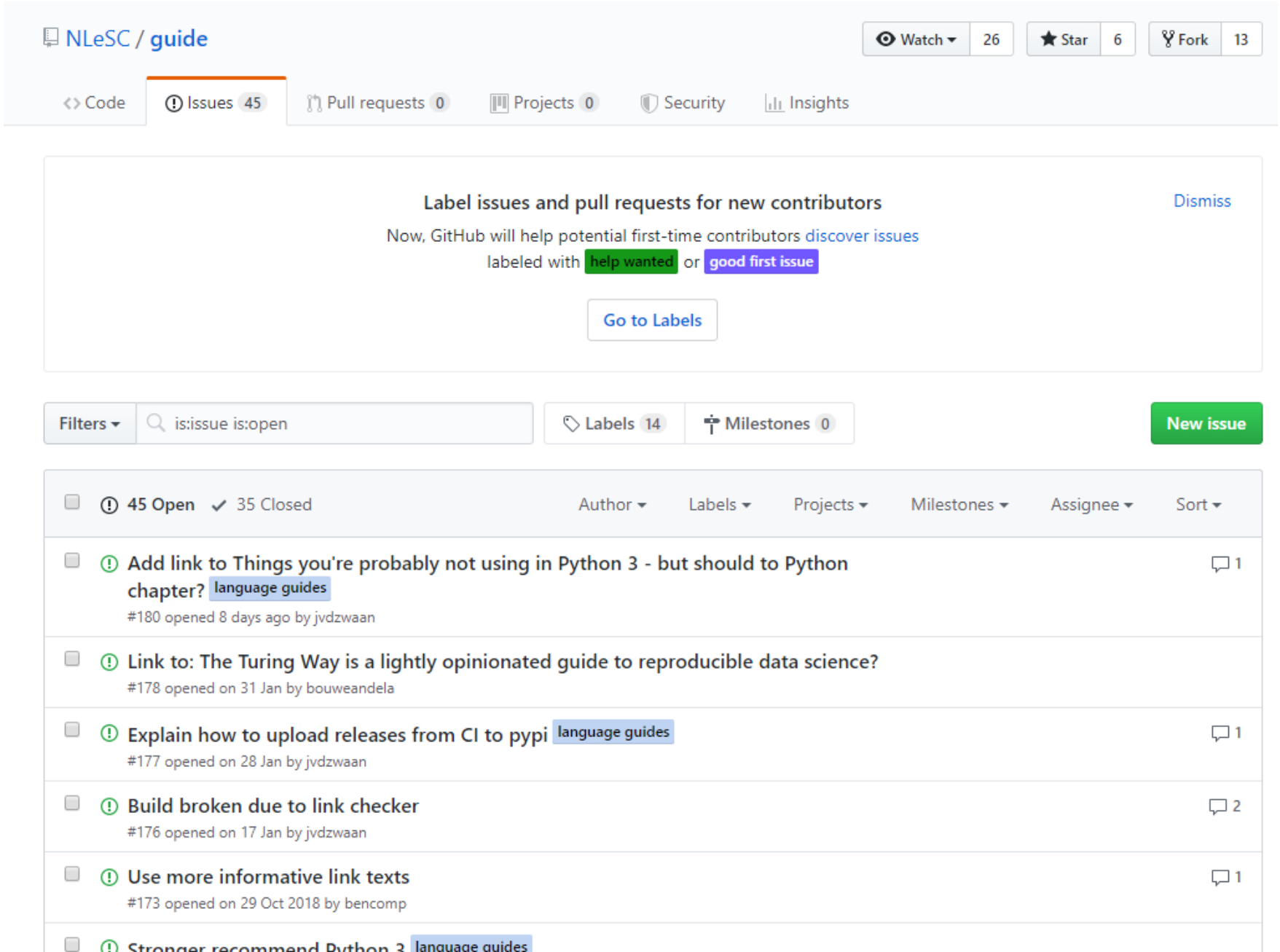
```
# Config file for automatic testing at travis-ci.org
language: python
python:
  - "3.4"
  - "3.5"
  - "3.6"

# command to install dependencies
install:
  - python setup.py install

# command to run tests
script: pytest
```

Set up empty (Python) project:

- license,
- documentation,
- Readme
- Installation
- etc…

https://github.com/NLeSC/python-template

Anything missing? Create issue



Let’s stay in touch

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