

pyvale:

Lloyd Fletcher^{1,2}

Fabrice Pierron^{1,3}

¹Faculty of Engineering and Physical Sciences, University of Southampton, UK

²UKAEA, Rotherham, UK

³MatchID NV, Ghent, Belgium

Abstract

TODO

Keywords:

Metadata

The ancillary data table 1 is required for the sub-version of the codebase. Please replace the italicized text in the right column with the correct information about your current code and leave the left column untouched.

| Nr. | Code metadata description | Metadata |
|-----|---|---|
| C1 | Current code version | For example v42 |
| C2 | Permanent link to code/repository used for this code version | For example: https://github.com/mozart/mozart2 |
| C3 | Permanent link to Reproducible Capsule | For example: https://codeocean.com/capsule/0270963/tree/v1 |
| C4 | Legal Code License | All software and code must be released under one of the pre-approved licenses listed in the Guide for Authors, such as Apache License, GNU General Public License (GPL) or MIT License. Write the name of the license you've chosen here. |
| C5 | Code versioning system used | For example: svn, git, mercurial, etc. (put none if none is used) |
| C6 | Software code languages, tools, and services used | For example: C++, python, r, MPI, OpenCL, etc. |
| C7 | Compilation requirements, operating environments & dependencies | |
| C8 | If available Link to developer documentation/manual | For example: http://mozart.github.io/documentation/ |
| C9 | Support email for questions | |

Table 1: Code metadata (mandatory)

Optionally, you can provide information about the current executable software version filling in the left column of Table 2. Please leave the first column as it is.

1 Motivation and significance

TODO [1]

| Nr. | (Executable) software metadata description | Please fill in this column |
|-----|--|--|
| S1 | Current software version | For example 1.1, 2.4 etc. |
| S2 | Permanent link to executables of this version | For example: https://github.com/combogenomics/DuctApe/releases/tag/DuctApe-0.16.4 |
| S3 | Permanent link to Reproducible Capsule | |
| S4 | Legal Software License | List one of the approved licenses |
| S5 | Computing platforms/Operating Systems | For example Android, BSD, iOS, Linux, OS X, Microsoft Windows, Unix-like , IBM z/OS, distributed/web based etc. |
| S6 | Installation requirements & dependencies | |
| S7 | If available, link to user manual - if formally published include a reference to the publication in the reference list | For example: http://mozart.github.io/documentation/ |
| S8 | Support email for questions | |

Table 2: Software metadata (optional)

In this section, we want you to introduce the scientific background and the motivation for developing the software.

- *Explain why the software is important and describe the exact (scientific) problem(s) it solves.*
- *Indicate in what way the software has contributed (or will contribute in the future) to the process of scientific discovery; if available, please cite a research paper using the software.*
- *Provide a description of the experimental setting. (How does the user use the software?)*
- *Introduce related work in literature (cite or list algorithms used, other software etc.).*

2 Software description

Describe the software. Provide enough detail to help the reader understand its impact.

2.1 Software architecture

Give a short overview of the overall software architecture; provide a pictorial overview where possible; for example, an image showing the components. If necessary, provide implementation details.

2.2 Software functionalities

Present the major functionalities of the software.

2.3 Sample code snippets analysis (optional)

3 Illustrative examples

Provide at least one illustrative example to demonstrate the major functions of your software/code.

Optional: *you may include one explanatory video or screencast that will appear next to your article, in the right hand side panel. Please upload any video as a single supplementary file with your article. Only one MP4 formatted, with 150MB maximum size, video is possible per article. Recommended*

video dimensions are 640 x 480 at a maximum of 30 frames / second. Prior to submission please test and validate your .mp4 file at <http://elsevier-apps.sciverse.com/GadgetVideoPodcastPlayerWeb/verification> . This tool will display your video exactly in the same way as it will appear on ScienceDirect.

4 Impact

This is the main section of the article and reviewers will weight it appropriately. Please indicate:

- *Any new research questions that can be pursued as a result of your software.*
- *In what way, and to what extent, your software improves the pursuit of existing research questions.*
- *Any ways in which your software has changed the daily practice of its users.*
- *How widespread the use of the software is within and outside the intended user group (downloads, number of users if your software is a service, citable publications, etc.).*
- *How the software is being used in commercial settings and/or how it has led to the creation of spin-off companies.*

Please note that points 1 and 2 are best demonstrated by references to citable publications.

5 Conclusions

Acknowledgements

TODO

Data Provision

All data supporting this study are openly available from XXXX repository at: <http://dx.doi.org/XXXXXX>. The digital dataset contains the following:

1. TODO

References

- [1] Derek Gaston, Chris Newman, Glen Hansen, and Damien Lebrun-Grandié. MOOSE: A parallel computational framework for coupled systems of nonlinear equations. *Nuclear Engineering and Design*, 239(10):1768–1778, October 2009.