Software
Sustainability
Institute

SSI FELLOWSHIP APPLICATION 2019

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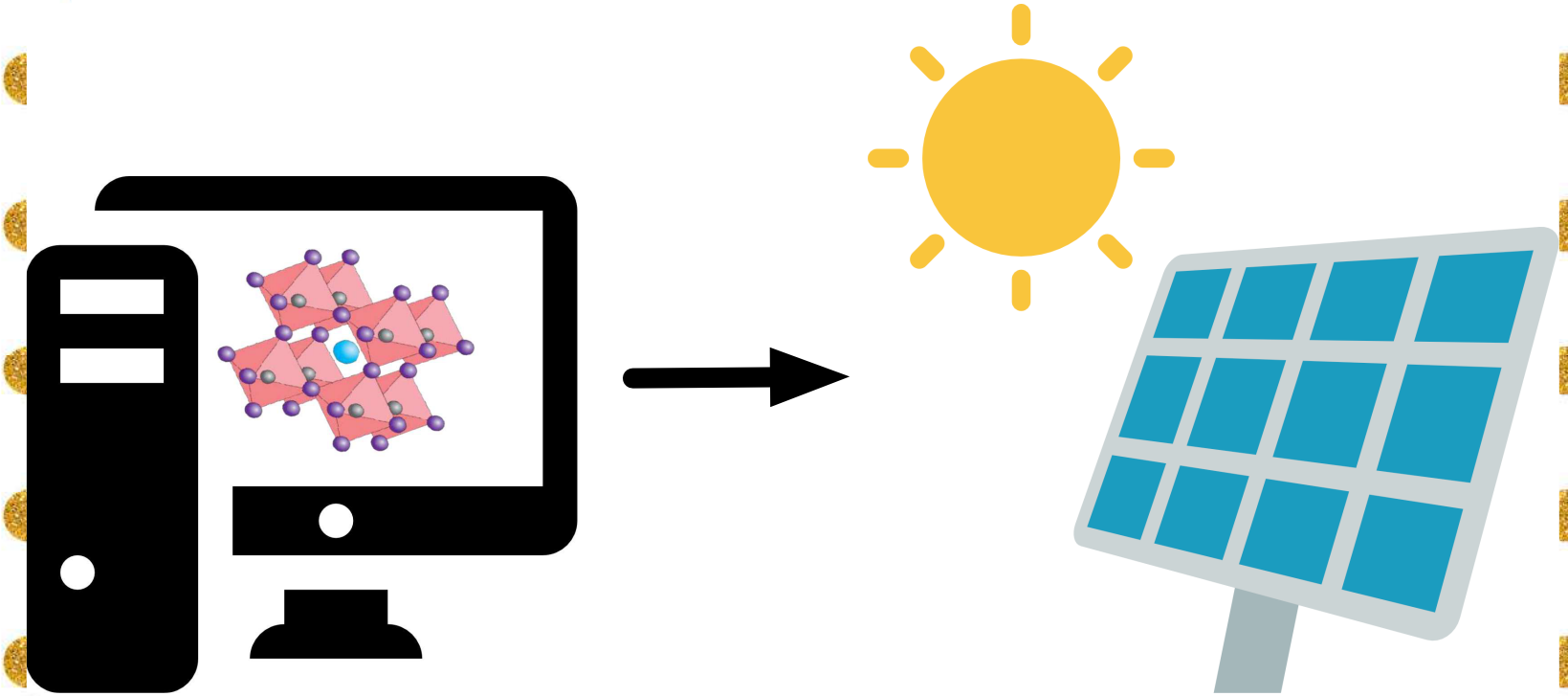
lucydot.github.io/slides

Who are you?

RESEARCHER



Objective: to optimise and design new materials for energy generation and storage

SOFTWARE..

USER

- code optimised for high performance computing,
  eg: vasp_gpu

DEVELOPER

- post-processing software, eg: effmass
- Python (NumPy, SciPy, Pandas, pytest), bash, Julia
- I try to work openly: lucydot.github.io/open

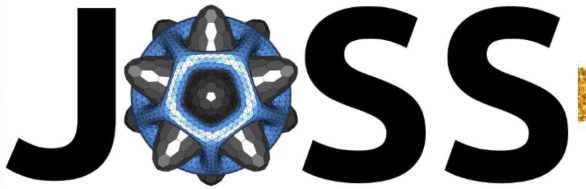
TEACHER

Ort. art and community café

What do
you do?

I LEARN

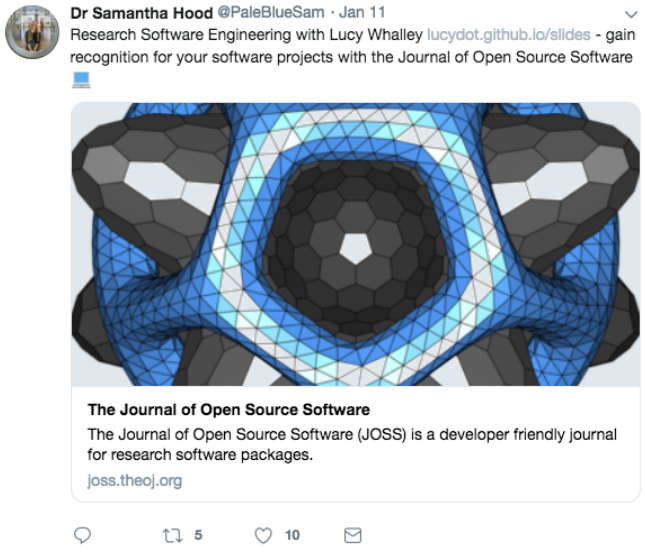
- Conferences in 2018: RSE, CarpentryCon, MozFest
- The Journal of Open Source Software: author and reviewer



I FACILITATE

- I teach programming skills: git, bash, Python
- I develop teaching materials: Pandas mini workshop
- I organise workshops: Python workshop for PhD students

I ADVOCATE



"Publishing your Software Project with the Journal of Open Source Software"

What are your fellowship plans??

I'D LIKE TO...

- Attend RSE conference and CarpentryConnect (poster/talk)
- Software Carpentry on the Orkney Islands?!

I have an idea!

THE CHALLENGE

- researchers can be reluctant to share their code
- undocumented, untested --> "single-use software"

THE SOLUTION?

Get your code publication ready

Prerequisites

Understand basic Python programming
Understand basic shell scripting
Familiarity with the version control system git
A piece of code (or perhaps an idea for a piece of code) they think may (one day) be submitted to an open source journal

Context

A growing number of researchers use and write code for their research. This code should be published to allow for reproducibility of results; however, despite a growing number of journals requiring that the code needed to reproduce results is made available, this is not currently widespread practice. There are different ways code can be made available - eg: a code snippet on a blog, emailed on request, an interactive notebook available as supplementary information. For more substantial pieces of code there is also a growing number of journals which are focused on the review and publishing of scientific software. The Journal of Open Source Software (JOSS) is one such journal, and requires that the code is tested, documented and undergoes peer review - as such, they promote best practice in development of scientific software.

The Journal of Open Source Software

The lesson is structured around the submission criteria for The Journal of Open Source Software, however this aligns well with the submission criteria for other journals such as [The Journal of Open Research Software (https://openresearchsoftware.metajnl.com/)

Course Objective

To enable researchers in the materials science community (short term) and beyond (longer term) to publish their code with an open source software journal.

Where these lessons are from

Lesson material inspired by the work of Code Refinery

Note that the testing chapter was adapted from the workshop *Python Testing and Continuous Integration* which was adapted from the Testing chapter in *Effective Computation In Physics* by Anthony Scopatz and Kathryn Huff.

Schedule

	Setup	Download files required for the lesson
00:00	1. Introduction	Why should I publish my code? What are the requirements for submission to JOSS?
00:00	2. Documentation	Why should I document my code?
02:03	3. Testing	Why should I test my code?

WHO WILL I WORK WITH?

- Audience: Materials Science initially, if successful --> other domains
- Collaborators: The Code Refinery, Jeremy Cohen (RSE Fellow 2018 / RSLondon), Adam Jackson (SSI Fellow 2018), Anna Krystalli (ROpenSci) + other SSI Fellows?

THANK-YOU!

Presentation slides + more details:

lucydot.github.io/slides