Better Software, Better (Atmospheric) Research

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Promoting the values of the Software Sustainability Institute (SSI) (Fellow 2022+): www.software.ac.uk

NCAS Staff Meeting 2023, Staff-led Sessions
13th July 2023

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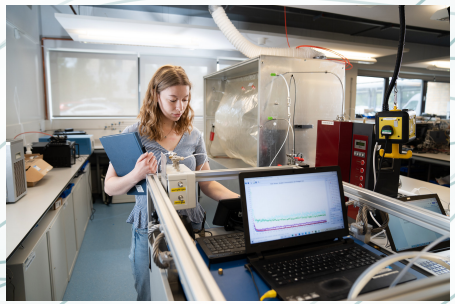
A question to start!

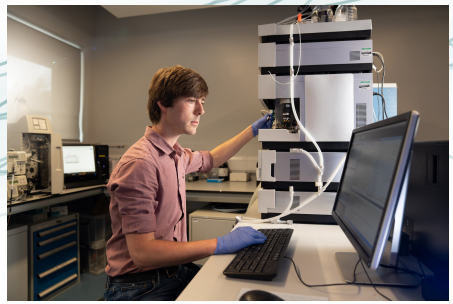
Raise your hand if you *use or develop* any *research-related** software in your work...

* Meaning not software for admin tasks or standard office-style working e.g. timesheets, browsing tools. Indirectly e.g. for observations or tools etc. towards research absolutely counts!

Software is used across most (all?) types of work at NCAS!

A cross-section of photos from the official NCAS Flickr gallery help to illustrate this and the breadth of use context...





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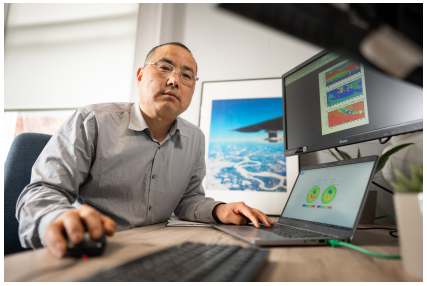

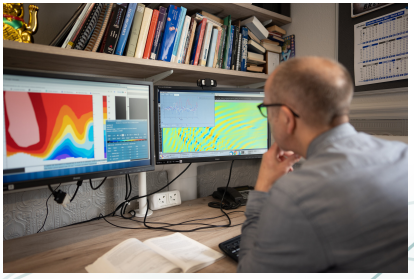

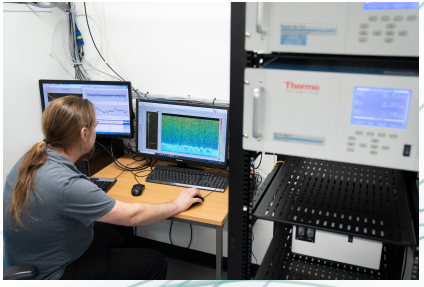



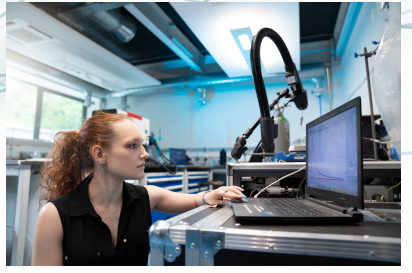

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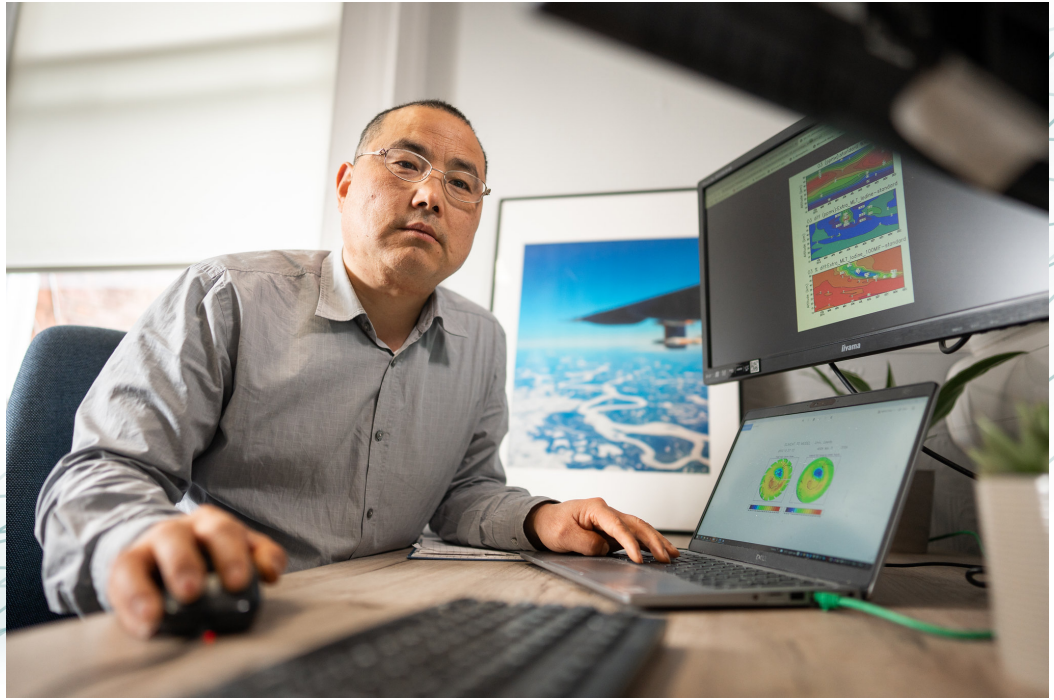
Software use within NCAS:

- By scientists i.e. for direct research, e.g. numerical modelling, data analysis and visualisation etc.;



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→ • For atmospheric observations and measurements, e.g. ground-based lab or mobile instrumentation work...

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- ...and airbourne measurements;

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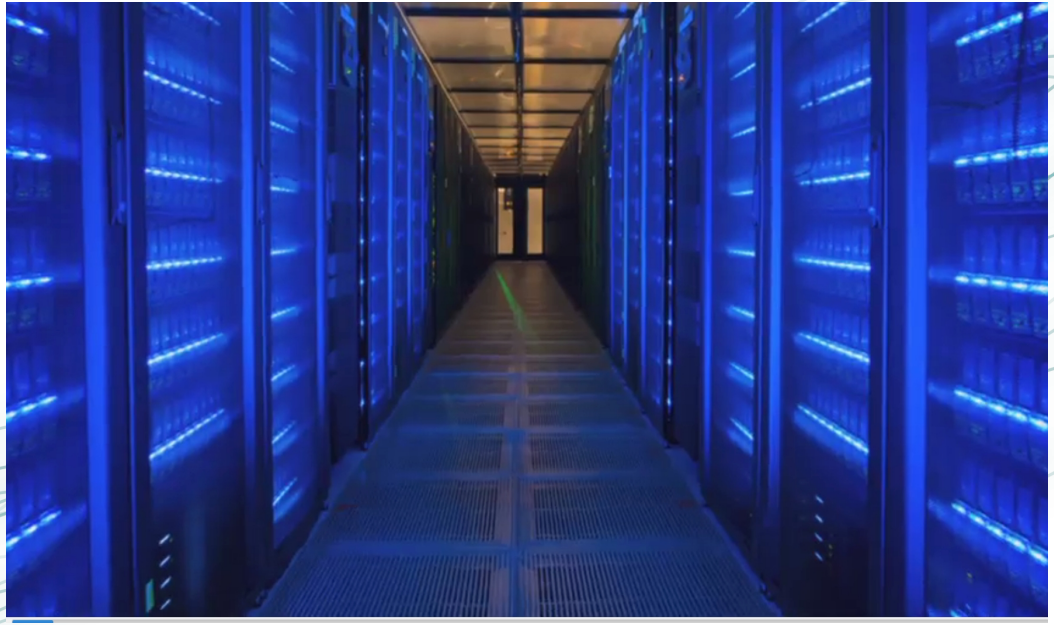
- to facilitate data considerations e.g. storage and analysis;
- to facilitate modelling, HPC and workflows;
- and indeed for services, tools and other contributions which don't come under the previous categories.



A motto and a general goal

- Sadly, in the research world, software is often treated as a second-class citizen, due to e.g. "publish and perish" culture, lack of funding for software aspects, etc.
- But many want change...

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- "**Sustainability** means that the software you use today will be available - and continue to be improved and supported - in the *future*."
- It's all very well having software that works brilliantly for you in your job right now, but how can we optimise the workflows and tools we use so that we can work as productively and collaboratively in a way that will be resistant to the constant development of science, technologies and systems?

But how does this aspiration apply to our work across NCAS, to atmospheric (and aligned domain) science, services and support?

How can we establish the highest quality software to ultimately enable the highest quality atmospheric science?

Aims of this session

- Appreciate the importance of quality software to our research and everything that contributes to it, both short-term and long-term
- Think about the software *you and your teams* make use of and whether it can be made more sustainable
- Discuss what our main barriers are to improving the software we develop and use, and any specific concerns
- Remind you of various in-house NCAS support for software matters and also provide links to some external groups and communities which champion and support better research software

Possible consequences of poor software

- Obviously, incorrect or inaccurate results
- But (perhaps) less obviously...
- Difficulty in sharing and re-using work, reducing potential for collaboration
- Maintainability nightmares
- Wasted time and effort
- Reinvention of the wheel
- Loss of staff morale: no-one wants to be working with software that's difficult or badly-designed, etc.

- *Open question: any other ideas or examples?*

Examples of good software practice

- Use of version control e.g. git to track and manage your scripts (even if you're the only one using them!) "Version/source control is the practice of tracking and managing changes to software code."
- Robust testing of code
- Thorough and *useful* documentation (again, even if you're the only one looking at your code)
- Automation of manual tasks for a better workflow

- *Open question: any other ideas or examples?*

Potential barriers to better software

- Time!
- Funds
- Staff turnover
- Lack of skills or knowledge on the issue at hand e.g. software or data skills

- *Open question: any other ideas or examples?*

‘In-house’ support in NCAS

- (NCAS-)**CMS** provides *computational modelling services* to the UK academic atmospheric and polar science community to *support numerical modelling* in climate, weather and earth-system research
- The Centre for Environmental Data Analysis (**CEDA**) provides data storage and analysis capabilities for the environmental research community
- Other in-house support...

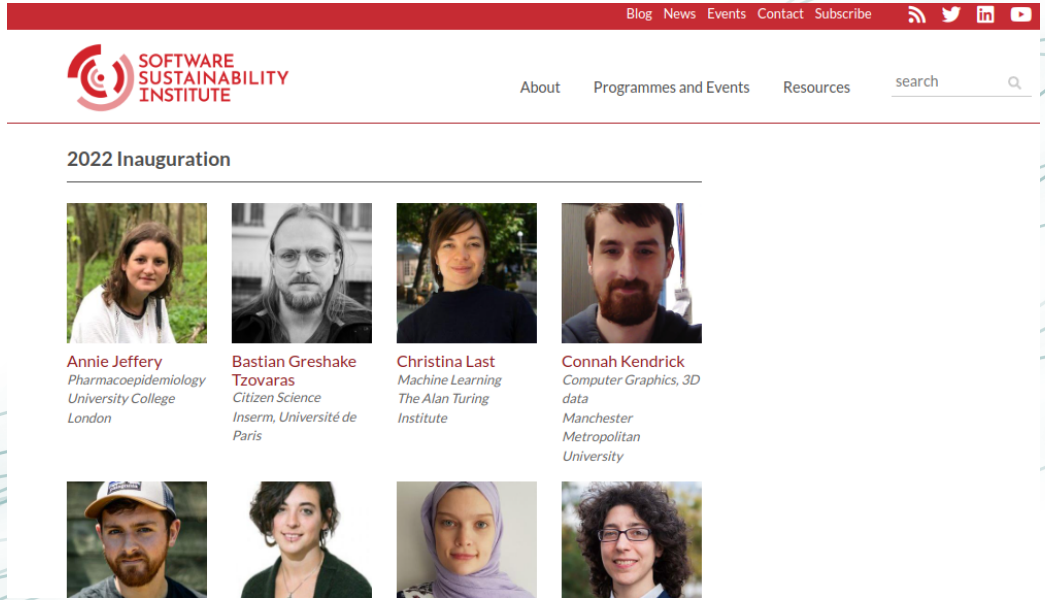
External support and communities!

- As well as NCAS support, I highly advise checking out and engaging with some external national and international communities dedicated to the aim of ‘better software, better research’
- All are cross-domain, but there are plenty of people working in atmospheric and aligned domains in these communities, including at other NERC centres
- On a personal note, these groups have been invaluable in my career professional development and path, developing competence in my work, and meeting fantastic people tackling similar issues

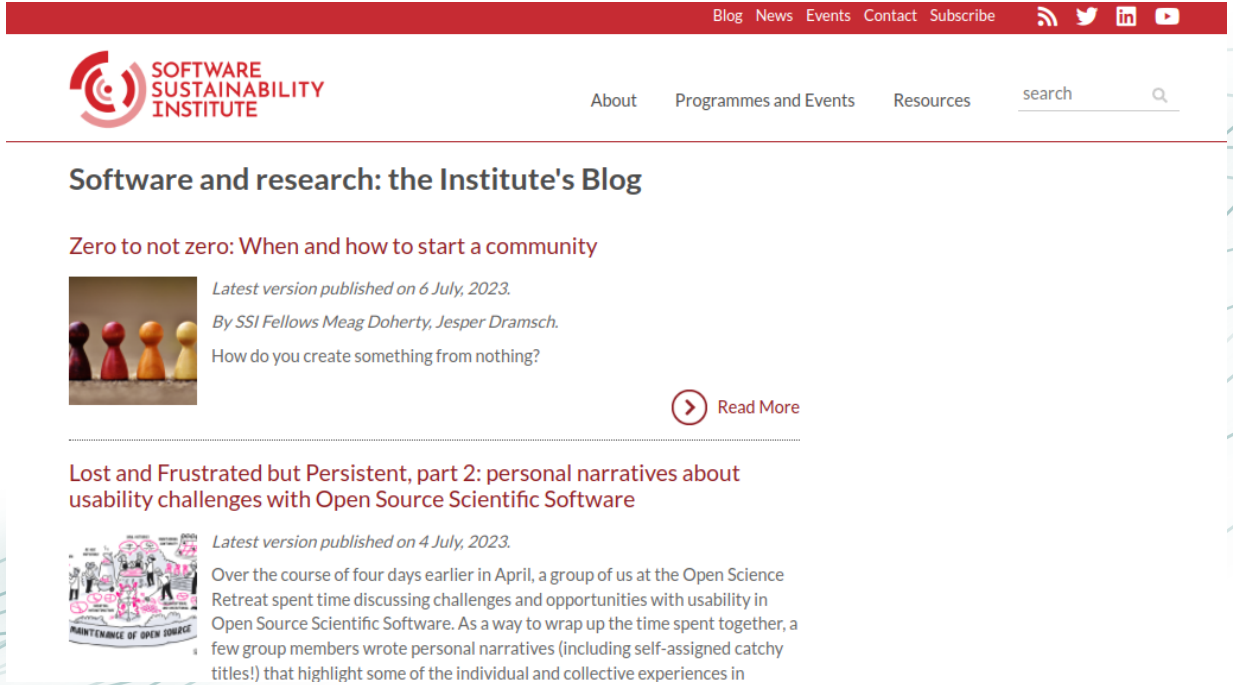
1. The SSI (www.software.ac.uk)

- A UK Institute is based at the Universities of Edinburgh, Manchester, Oxford and Southampton, with funding from all seven research councils. “Our mission is to become the world-leading hub for research software practice.”
- Provides guidance, free open resources including a blog, programmes and events...

- ...including a fellowship scheme. Myself and Luke Abraham are Fellows (2022+) and so we are keen to champion and advise on improved software practice across NCAS and aligned domains. Come and talk to us!



- Resources include a blog on good practice considerations...



2. The Research Software Engineering (RSE) community and society

- See society-rse.org
- An international community, with sub-communities e.g. national and regional groups
- Professional UK Society: SORSE. Launched 2019 but RSE community spun up in 2012. Still, all quite new!
- Events, advocacy, resources and more…
- For everyone! Not just RSEs

3. The Carpentries (carpentries.org)

- “We teach foundational coding and data science skills to researchers worldwide.”
- Provides training, ‘training training’ (training on best practice for instructing) and a myriad of open resources online covering data, software, HPC and library skills: use them to learn from, to teach from, or to extend or incorporate into your own teaching
- I highly recommend becoming a certified instructor!

For guidance on better software:

- Use in-house support via CMS, CEDA, JASMIN, etc. as a first step. We're there to support you!
- Consult external resources and engage with the communities aforementioned in your own time. I've found them incredibly useful for my work and career
- Feel free to contact SSI Fellows at NCAS, myself (sadie.bartholomew@ncas.ac.uk) or Luke Abraham (N.Luke.Abraham@ncas.ac.uk) if you have a related problem or question and we might be able to point you in the right direction for guidance and solutions

And some questions to close...

- Can you identify ways to improve the software you use or develop with?
- What is in the way of you or your team making those improvements?
- Do you know where to find support towards better software for better (atmospheric) research?

Summary and quick links

- Software (directly or indirectly) for research is crucial to most, if not all, work throughout NCAS, but in the research sector it is generally not treated as a first-class citizen.
- For productivity and sustainability, we should give software its due diligence. Better software means better research!
- We discussed some aspects of poor software, means for improving, and barriers to making improvements
- In-house support is available (CMS, CEDA, etc.) but do check out some fantastic external groups pushing for this goal and their guidance, resources, events and communities:
  - The Software Sustainability Institute (SSI): www.software.ac.uk
  - The Research Software Engineering (RSE) community and society: society-rse.org (+ regional and international groups linked within)
  - The Carpentries: carpentries.org