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Open Research Case Studies: Faculty of Engineering and Physical Sciences

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Open Research Case Studies – School of Chemical and Process Engineering with Alastair Baker

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Nuclear Engineering: Alastair Baker is currently on two projects; one of them is a scaling up the recycling of uranium using pilot plant scale solvent extraction equipment. The other project is for The Clothworkers' Company collaborating with the <u>Leeds Institute of Textiles</u> and <u>Colour (LITAC)</u>. That project is about recycling cellulose, which is used as cotton in t-shirts, so we would not need to spend large amounts of land and water growing cotton.

How does your research use open research practices?

I conduct a lot of engagement on the nuclear fuel cycle online on Twitter. There was recently a <u>Nature paper</u> which said there should be an additional Twitter's blue verification badge, for accounts of public interest, and function for scientists, and I would like to think that I conduct myself in a way in which that would allow me to have that access to authority in terms of holding discussions openly.*

With regard to publishing my research openly, not behind a paywall, I got lucky in the last project I worked on, and it turned out that I was expecting to pay thousands of pounds in article publishing fees (APCs), but the School of Chemistry has an agreement with the <u>Royal Society</u> of <u>Chemistry</u> that covers Open Access fees for all affiliated authors, so the APC was covered.** If I have an EPSRC-funded (Engineering and Physical Sciences Research Council) PhD student, they can apply for funding for open-access publication. If a researcher is ever in need of advice on publishing and APCs, I encourage them to contact the University's library***, as they have always answered my queries. Publishers like the Royal Society of Chemistry are also always happy to answer author queries about Open Access and the many institutional agreements they have in place to support authors in the UK.

Another way I would like to openly share my own research practices would be to contribute to Wikipedia, but there is no aspect of that in my job that requires me to do it. I conduct myself in the same way for both public engagement and outreach; I will always try and engage with events with the public, especially when it is on campus.

* The interview took place in July 2022 when the Twitter blue check was free and a way to verify official accounts like governmental bodies.

**Just to note that for research articles, our RSC APCs are in the range of £850-£1,800.

*** https://library.leeds.ac.uk/info/1800/contact_us/161/contact_the_library

"It is very frustrating that there are so many unspoken ways of how to do things the right way, such as, how many authors should be on a publication, who comes first, and what contributions deserve merit on it."

How do you deposit your work?

After publication on a journal's website, I post links to my work on my personal <u>Twitter</u> and <u>LinkedIn</u> to gain social medial attraction. I use social media to gain attraction. I also update

my accounts on other bibliographic output databases like <u>ORCiD</u>, <u>Google Scholar</u> etc. I upload my pre-submitted manuscript (also known as a preprint) to the <u>White Rose repository</u>.

In your field, have you found it difficult or easy to identify other people's open research practices?

In chemical disciplines, making data widely available is not a common practice. You find yourself reporting your best values in your publication. Unfortunately, a lot of good and repeated research that either has null results or did not work is never reported. I would want to make my data available, but this also requires clearance and approval from my managers and stakeholders.

The last project and my current project I work on could be registered as an IP, so I cannot talk too much about the successes. I try and make the supporting information available as much as possible, even when my line manager does not encourage it.

"Open research practices are there, but we still have the research culture of 'published or perish'."

Has your attitude towards open access changed in the recent years?

I don't think I have an attitude towards open access. If the funding was from taxpayers, they should be able to read the publications for free. However, someone has to maintain those research archives; it is currently market-driven rather than institution-driven. My attitude towards open access is it depends on the funding. I will always try and make my work open access.

Have you come across any negative perceptions about open access?

The negative perception of open access is usually about the question of funding: who is going to pay for maintenance and upkeep? It is naive to think that moving everything digital has no costs, <u>even emails have a carbon footprint</u>, of 4g of CO2. There has to be a certain set of balances and checks to maintain data integrity. At the moment, there seems to be no arbiter other than letting the market decide and pay for journals to do the maintaining and archiving.



Research behind paywall. Cartoons illustrated by John R. McKiernan

Do you have any concerns about preprints?

I have mixed emotions about preprints because peer review does a very good job of improving papers and questioning narratives. I can see both sides of the discussion since peer review is an editorial process that is not particularly transparent either, so you probably just want to get through the process and have your paper published.

What does data mean in your field?

I work with raw and processed data: the raw data is quite number-heavy and could be simply logging the temperature for every minute of every day. The process data is a picture that explains your point. I work in a field where we are talking about real-time measurements, and that is a lot of data, but openly publishing it can add a layer of transparency to the research.

How do you manage your data?

The fact that I am responsible for storing and managing my data shows a lack of diligence from the research institutions. The University deploys OneDrive, but does it train staff in how to best store their data? it does not train administrators, purchasing teams, or researchers.

However, that said, I work for the <u>National Nuclear Laboratory</u>, and I had to sign a confidentiality agreement, saying that at the end of the project, all the data will be removed from the University of Leeds. I am happy using OneDrive; but managing it really comes down to me mainly when I sit down and process my data.



Do you use open datasets?

Sometimes, but I want to make my data open, so you can go to my paper and get the data so that you can build your model on it. I have seen low-impact publications that publish data sets that are then used by nuclear engineering modellers. This is what I want to achieve: make my data open so others can use it. I have not done it yet, but I want to do it.

Have you written a data management plan?

I haven't written it down, but I have thought about it quite often and I just do not have the training to put anything in place, so I will build my management of data as best as I can, like numbering file names and using ISO 8601 format for expressing dates. I would like to have time to read how to do knowledge management and employ those processes. If someone would send me on training, I will participate.

"Data and knowledge management is a fascinating field that I think is where we need lawyers and judges."

What software do you use to read data?

I write code for processing data in either <u>Python</u> or <u>R</u>, or I would use Excel, depending on how much time I had on and based on the level of training. When it comes down to something more complicated, I would have to get a piece of software that could read that specific file type, whether it is free or not. I think a nice thing about the scientific community is when there is a

barrier, either you have the money to pay to get the licensed software or you spend time working with people to get a solution to see the data as you want to see it.

Have you had any licensing issues regarding using different software?

The most frustrating thing is when you get your license, and you need someone from IT to install that software, which can take months and it delays research projects. These problems are not unique to the University of Leeds: I have come across them at each university I worked.

"I do not think individual researchers should be made guilty of not doing certain practices. It needs to start from a governing institution and on a national level."

Open Research Case Studies – School of Civil Engineering with Zhengyao Li

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Materials and Structures group project description:



Zhengyao Li's research interests and expertise include connection design for timber structures, exploring the possibility of high-rise timber structures and aiming to propose a strong and adaptable connection solution for construction efficiency and structural performance. Her research focuses on static and quasi-static laboratory-based testing of steel, timber and steel-to-timber composite structures, as well as numerical simulations on the global performance of timber buildings. She is also a member of 3DMBC (https://3dmbc.com), a research group focusing on the development of optimised and reusable steel connections using

modern manufacturing methods for modular building systems (MBS) aiming to embrace resilience and sustainability in the construction sector.

What does open research mean to you?

Open research means the ease of accessing the data or journal articles or any resources that I need for doing my research without asking for permission or paying.

How does your PhD project use open research practices?

With my research team, we share our manuscripts online on a platform like ResearchGate, and we have a website for the project that people from the industry can assess to get information about what we are doing. We provide publicly accessible knowledge and share what we can.

Li Zhengyad Master of Engin United Xingdom) eering - PhD Student at University of Leeds	Research Interest Score Citations h-index	50.1 5 2 Citalises even time	
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Zhengyao Li on ResearchGate

In your field, have you found it difficult or easy to identify other people's open research practices?

Since we are using university resources, it is quite rare to find something that has limited accessibility. Maybe it is not open to the public, but we do have the means to access and use it via the university. We have some industrial partners who sometimes would like to use the

data from the latest research, but they could not access the publication, and they would ask us to help to download the paper and share the data with them.

Do you use preprints?

In my field, we still prefer to use those peer-reviewed papers, but I do use the data, including the experimental results from preprints. We may use them, but generally, we do not trust the conclusion or any theory from those that are not officially published.

Do you have any concerns about preprints?

It depends: for my project, it acts as a barrier between open-access publications and confidential information. We want to keep the project to ourselves, but we also would like the public and the industry to know about us. The preprints, for example, a small conference paper, include general information that the people get access to, so they know what we are doing.

Has your attitude toward open access changed recently?

No, I think I have always supported open-access research.

"I work in civil engineering, and people want to keep the industry up to date on what we are doing."

As a PGR student, would you like to see more training on open research?

I think more training would be important. I did not receive any specific training but often heard about open research. I realised that there are so many aspects to it. My field is engineering, and my research project is industry-related; therefore, we always want to make it inclusive.

Have you ever developed a means to 'bypass' restricted content?

Yes, quite often, by contacting the researchers. They are happy to share the materials, but they do not mention whether I can use their data in my publication. I need to inform them because when I write to someone asking for resources, the material may not be open to the public.

Do you aim to publish your PhD research?

Yes, I would like to if I can. I do not have any legal limitations on my PhD, and I want my research to be as open as possible and make it available to the industry.

What does data mean in your field?

I have quantitative data, experimental results, and some modelling drawings created in different software.

How do you manage your data?

They are stored in the OneDrive provided by the University of Leeds, and I also have a portable hard drive where I keep copies of all my data.

Have you written a data management plan?

Yes, in the first year of my PhD. We were asked to keep the data in OneDrive and keep another copy of the data. I used the <u>template form</u> from the library's website.

"It is quite hard to control the right amount of open access."

What kind of software do you use for your research?

I use basic ones like MS Word, PowerPoint, and Excel for data management. I also use modelling and drawing software applications. For the Office applications, I use the university's license, but the drawing software has a student licence, so it is freely downloadable if you are a student. For professional modelling software and applications, we use a research license.

Have you had to work with software you did not know before?

I used <u>CAD</u> since my bachelor's degree and the Office package of course. The other application, <u>AutoCAD</u>, I started to use in my PhD, so it's quite new to me.

Is there anything you want to share about your project, particularly concerning open research?

We have been developing a product of which we want the public and other researchers to be aware. But we also have to protect our design and be quite careful when we publish anything because we are trying to <u>patent it through the University of Leeds</u>. If we publish anything before the patenting is finished, we have to be sure that there aren't any details of our design released. At the moment, it is not open to the public, but we want the result of our research and why we are developing this product to be accessible. Even if we would like to publish anything open access about the design, we have to wait until we get the patent.

We have two external co-operators who have signed the confidential agreement, and I can only share data with them. Now, the only thing we can make public is the project description and some general introduction to the project.

Open Research Case Studies – School of Computing with Wisdom C. Agboh

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Robotics@Leeds project description:

Wisdom is excited about robotic manipulation. It involves robots moving their arms and hands to physically interact with objects in your environment. He develops algorithms to plan and control these robot motions.

What does open research mean to you?



For me, open research is about involving the public in the research questions we ask and in the solutions that we come up with for research problems. It is also about showing the results and making them open and accessible to everyone. Accessibility is a crucial part of this: most of the research is funded by the government, and the wider public needs to have access to that. So, open research is about how we generate solutions for those problems with engagement from the public and how we disseminate the results.

How does your research use open research practices?

Since my research is in robotics and we have different robotic tasks that we're looking into, we make sure that the code and the paper are also freely available by uploading preprints to <u>arXiv.org</u>. We usually post the code to GitHub, and we have links to the datasets in papers.

How do you deposit your work?

We use Symplectic, but we also use arXiv because it's the fastest way for people to read out work. Once we submit a preprint, it's disseminated across the web. The field of robotics and AI is very fast-moving, so it's crucial when you write something that it's out there as quickly as possible.

In your field, have you found it difficult or easy to identify other people's open research practices?

We talk a lot about the different ways of disseminating our work, for example, presenting at conferences, ensuring that the code is open and available to everyone, and writing blog posts about our work. Open research is encouraged by PhD supervisors and other academics in the Department.

How does open research inform your teaching?

I helped supervise a few undergraduate projects: we encourage students in classes and research projects to investigate ways to make their research codes and project documents open and available. It's better for the research community if people can get access to resources.

Learning to Efficiently Plan Robust Frictoional Multi-Object Grasps

All Decluttering Systems



Do you use preprints?

Yes, I read preprints and deposit them; and arXiv is the repository my field uses. We still need peer-reviewed journals that people can trust, but I think it's also important to have preprints.

Do you have concerns about preprints?

Yes, I do because it hasn't been peer-reviewed. If a preprint is in your area of study, you can have a good sense of the quality of the work because you are also a reviewer. But if it isn't in your area of speciality, then it's hard to judge the quality of the research.

Has your attitude toward open access changed in recent years?

I moved towards supporting more and more open access. Initially, I wasn't aware of the range of possibilities: if you're not in the University system, it's hard to read something behind a paywall. So, if you're just a member of the public and curious about what's happening in a particular field, it's challenging to find it out. Doing my PhD research helped me understand the problems in publishing and how I can contribute to solving those, for example, by making my work accessible to everyone.



As a recent PGR graduate, would you like to see more open research and career development training during the course of study?

It would be great to have more information and training on making data freely accessible, where to publish, which publishing houses the University have special deals with, and how we can take advantage of this. I think it's key to bring open research to the forefront for PRG training.

In your opinion, what is the current state of open access in your field?

In general, we've got a real community: we've created new conferences and journals, for example, the <u>Journal of Machine Learning</u>, <u>Robotics: Science and Systems Conference</u>, and they are all open access. Our research community is endorsing open access, and I'm happy about that.

Have you ever developed a means to 'bypass' restricted content?

Talking to the author is probably the best thing to do if you don't have access to a paper. It's the easiest, and authors usually would be happy to send you the publication.

Are there any negative attitudes toward open access you have come across?

One controversial point is how we deal with situations where someone has published a book and probably needs to make some money from it. So, my concern is how do we pay for openaccess publishing, and how do we maintain open access and be fair and support researchers?

What does data mean in your field?

Our data comes from experiments either from a simulator or a physical robot system, and we interpret the data and present the results. For example, we look at how successfully a robot moves an object from A to B, and the question is where we get that number (data) from and what was the robot motion we captured in a particular scenario? There are multiple levels to what data is, and we try to expose it as much as possible. We also have qualitative data working with human participants where people go to a virtual reality system and pass different tasks. We collect that data and try to make it open.

How do you manage your data?

We use the University's OneDrive system, which allows us to store large amounts of data. I also try to back up the data on multiple physical devices.



Parareal with a Learned Coarse Model for Robotic Manipulation (University of Leeds)

Have you deposited dataset with the Leeds's repository or other repositories?

Yes, we deposited datasets with Research Data Leeds Repository.

Have you used open data?

We don't use open data but generate it and make it available.

Have you written a data management plan?

We have our data policy, so we store it safely and come up with an elaborate plan to manage it.

How important have ethical considerations in your research?

It's crucial since we work with human participants and follow the GDPR guidelines: we only collect the data we need for particular reasons and for the time we need it.



What kinds of software do you use for your research?

We use different programming languages and physics simulators, robots, and controllers. Our projects require the integration of several components, so we use many different tools.

Has your research used open software that you were not familiar with before?

I did this during my PhD since many machine learning platforms are open source. In my research group, we use open-source tools for computation. We depend on them to make the project work: without them, we would have to go to some paid version, which we can do, but it's also great that we have open versions.

Have you encountered any licensing issues or obstacles when adopting software developed by the private sector?

There's a physics simulator <u>MuJoCo</u> we use for our project. During my PhD, I had to get an academic license to use it, which was very expensive, then a company bought it and made the software open source, which is great. However, I ended up paying a lot for something that is now open and accessible to all.

Have you made your code open access to others following the completion of your research?

We always ensure people have access to our codes on <u>GitHub</u> or can see what we've done because it helps with the trust in our research.

Do your codes have an open license?

Yes, they do: usually, <u>MIT</u> or Creative Commons sometimes.

"I don't have concerns about making the code open but about how: we try to ensure that the code is readable and usable for others. It requires some extra time to create good metadata."

Open Research Case Studies – Research Software Engineering with Alex Coleman

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What is your job role as a Research Software Engineer?



I am a professional service support person for researchers who are developing computational tools for their research. I help to facilitate best practices for researchers around how they develop those tools both through advice, formal training, and via consulting. Researchers can buy out my time to help directly on a research project. We are here both as people to provide support also advocates in the research community for best research practices.

How does your work use open research

practices?

We are encouraging both open research and reproducible research practices. We have computational tools that make it easy for people to build open and reproducible research in their projects. A big part of our role is making sure we signpost these resources to users because often researchers are very focused on the research and not particularly aware in the broad sense of other tools that they can use, which quite often align with reproducible research and best practice ideas like the FAIR principles.

Have you received any feedback from researchers or support staff?

In general, we get positive feedback around the training we provide, which is tailored toward reproducible practices. One feedback was about our website which is open source, and you can see the code that hosts it. We had a colleague from the library who, completely unsolicited, had found our website and had made some recommendations about web accessibility. This is the real value of openness: you can get contributions from other people to improve things. We showed researchers that if you do things in this way, you introduce the opportunity for open collaboration, which is positive for everyone.

Which Schools do you work mostly with?

We are open to everyone but there are disciplines we are interacting with more like the School of Computing, the Faculty of Biological Sciences, the Faculty of Environment, and the Faculty of Engineering and Physical Sciences. We spend less time with researchers in the Arts and Humanities, but that is not to say there isn't anyone we are interacting with from those disciplines.

What license do you apply for your codes?

I have developed codes (my personal code) that use publicly available data. I will try and assign it a license. I don't do it with all my code on GitHub because often the code isn't necessarily in a form that I would consider worthy of a license, and it's not built for public consumption. There is a good argument that it should have a license just in case, but I don't

always get around to adding one. However, I am happy to share the personal tools that I have developed.

For the work that our team does, we probably don't put as many licenses on our work as we should. I think that is probably to do with the fact that we are unsure about Intellectual property rights, given that we are employees of the University of Leeds. We are never quite sure whether it is appropriate for us to pick an open-source license, or if we should be thinking differently about that. That is a decision taken by the team on a case-by-case basis. GitHub is the main platform that I use. I also use GitLab for some codes, mainly because there are some features on GitLab that you don't get for free on GitHub. Sometimes I share codes directly with people over email or I manage it through a private GitHub repository.



Have you received feedback on your codes?

I sometimes receive feedback from the users who download or use the code. Tragically, not a lot of the personal code that I write is particularly reused. Though at work, lots of our repositories are team managed: we have procedures where people make changes, and they have to get it approved by another team member, which leads to comments if we need corrections. We share all our training material on GitHub openly as well and we encourage students to give us feedback there so that we can make improvements. In short, I have had feedback from people, but more in the context of a team where we are trying to encourage collaborative development of our tools and platforms.

Has your attitude towards open research changed since you have been in this job role?

When I first started doing development work, before as a research software engineer, I did not think about licenses. But when I became RSE I had to start thinking about these best practices to encourage people to do the same. It made me think much more about the use of licenses for the code that I write, so, I would say I have adopted an opinion since becoming a research software engineer rather than changing my opinion.

How important collaboration is in your work, especially in writing code?

Platforms like GitHub and GitLab allow people to work on the same thing and then resolve differences constructively so that we can introduce updates to the code. In 2020 and 2021, <u>worked on a project for researchers who were modelling COVID</u>, and GitHub was very important since we were working remotely and making changes and updates to the code model. We had to come up with a way of reconciling all the work that everyone was doing. GitHub allowed us to prevent people from introducing changes that would break everything in the code and manage as a team collaboratively.



Alex Coleman's GitHub profile

What kind of training do you provide?

We provide a range of training for researchers, predominantly training around getting people ready to use the HPC systems, which does not directly touch on open research or data but is part of the thread that runs through all our training around best practices.

We also have training on introduction to the R and Python programming language, and as part of that, we typically talk about issues, such as where your data live, how you treat your data, and how you manage your code.

We also do training in Git, which is that version control system that integrates with GitHub, and that is where we spend more time talking about licensing and how you would use GitHub

to share your code openly. We discuss reproducible research practices for researchers, and we touch on Git version control, documenting your code, and the options for licensing.

"Open research is very important in the computational research area, but also more widely, for research. It is something that feels like it is gaining traction. We have to keep teaching the next generation."

My biggest selling point for open research and reproducible practices is that it helps you more than anyone else. These practices often make it easier for people doing a PhD when they come to write up and they look back at what they did at the start and understand what they were thinking at that time. A lot of these practices are just universally helpful, not just for others, but also for themselves.

Open Research Case Studies – SchoolofElectronicandElectricalEngineering with Dimitris Soulia

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Nanoscale tweezers for single-molecule manipulation project description:



This project is based on developing some very small tweezers on the nanometre scale based on two closely-spaced electrodes to trap single dielectric entities, such as biological molecules and, at the same time, measure the forces that we apply to such entities. So far, single molecule manipulation has been achieved with well-established techniques such as optical, magnetic, and acoustic tweezers or even atomic force microscopy. Our tweezers are developed on an electrokinetic technique, called dielectrophoresis: it is a novel type of

tweezers which offers a new way to probe forces on single molecules.

What does open research mean to you?

Open research means sharing everything with everyone, so we can tackle any problem as quickly and efficiently as possible. Under open research, we can include sharing practices from hardware to software development and even sharing scripts or a new analysis technique. It is any possible form of sharing material to tackle the research problem.

How does your research use open research practices?

Most of my first year was devoted to creating a new platform for fabricating the tweezers I described. I tried to fabricate them from all available literature, but not all the data was out there. Since I could not find all the information needed, I decided to spend some time optimising the setup even more compared to what was currently available. Now that I have completed this instrument, I am interested in publishing it in an open-access journal.

It is slightly different from the most common journals we tend to read across all the fields, which only tend to publish instruments or coding. So, this is what I have been focusing on, to publish my setup and make it available to the research community, so nobody has to go through the difficulties I did. I am also using a lot of techniques based on open-licensed software.



Directory of Open Access Journals

How do you deposit your work?

So far, I have not published anything, but I am in the process of publishing, and ORCID will be the main way to go; it is where I would put everything.

Have you found it difficult or easy to identify other people's open research practices?

I would not say that it has been difficult because in general, in the field of engineering and physical sciences, there has been a trend recently to be more open about research.

There has been a lot of development over the last ten or twenty years, but it is something that you still struggle to bring into a discussion when grants are involved or publishing your work to prestigious journals. It is hard sometimes to convince others about the benefits of open research.

Do you use preprints?

Yes, I am working in a group where we have the tradition to upload everything as a preprint on either <u>arXiv</u> or <u>bioRxiv</u> so that everybody can see it and we can get some early feedback before we submit it to a journal.

When you go to conferences, people will show you their new data. Sometimes they would have just uploaded it to arXiv or another repository.

"It takes a lot of time to reach the final point of publication through peer-reviewed journals, so preprints are a very good and easy way to see interesting and new data and discuss with others and provide feedback. "

Do you have any concerns about preprints?

I am aware that some groups have some issues with preprints, but I do not. I think it's a good practice: you expose your work to the entire community, and you are always open to any feedback, which in the end, will help you pass the peer-review process. I don't think it is a process that affects your work in a bad way.

Has your attitude towards open access changed recently?

Yes, I don't think I am as careful about it as when I started my PhD. The more I get exposed to open research, the more I tend to apply it to my work. Once you start getting involved, you meet people who spend a lot of time on open research, and they inspire me to do research more openly. My research habits have positively changed over the last three years.



Do you have any restrictions from funding bodies to publish your work?

My PhD is funded by the University of Leeds; I do not have any restrictions on where I publish my research. We have big journal companies with gold open-access platforms, and I would always pick those. It might not have an immediate impact in terms of citations, but it will be more beneficial in the future, and open access will be the standard.

Has your research benefited open-access publications?

Open access has helped me to analyse my data better. There might be a technique I wasn't aware of, and I found it immediately in an open-access journal, which had all the data and all the analysis available. I could apply these to my work, so open access has positively affected my research.

As a PGR student, would you like to see more training on open research?

I am based in the field of physics and engineering, and I think we can do much better in teaching undergraduate students about open research. For example, we can make everything open access for final-year undergraduate projects. There have been steps in that direction, but there is still room for improvement.

What does data mean in your field?

I am an experimentalist, so the main objective is to collect experimental data through microscopy. Lately, I also simulate data. Data is quantitative; it is proof of the experiments that we are doing.

What kind of software do you use you analyse your data?

For collecting data with a fluorescence microscope, I have been using open-source software established by my research community. I am basing all my analysis on <u>Python</u>, which is an open-source tool. I use open-source software from data collection, and analysis, to illustration.

How do you manage your data?

I tend to store everything on the cloud services that the University is providing me, such as OneDrive.

Do you use open-source code?

As an experimentalist, you always need to be flexible with the instruments you are using. Open-source coding gives you that flexibility: you can tune any tool to your needs. I work collaboratively on codes with other PhD students who try to tackle the same problems. We would have a platform, usually GitHub, where everybody could improve the current state of a script.

Open Research Case Studies – School of Mathematics with Mauro Mobilia

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The Eco-Evolutionary Dynamics of Fluctuating Populations project description:



This project focuses on the ubiquitous situation where the eco-evolutionary dynamics of fluctuating populations is shaped by the coupling of demographic noise and environmental variability (see cartoon). The interdependence of environmental variability and demographic noise is poorly understood but of great importance in microbial communities, which are often subject to sudden and extreme environmental changes. In particular, modelling population of varying size and composition subject to changing external factors is crucial to understand the evolution of microbial antibiotic resistance. In fact,

pharmacodynamics largely focuses on the deterministic description of large well-mixed bacterial populations, but fails to account crucial stochastic effects arising in small communities.

When antibiotics reduce a large population to a very small one but fail to eradicate it, surviving cells may replicate and restore infections, and these survivors are likely to develop antibiotic resistance. Owing to the small population size, the details of the outcome are subject to large fluctuations. This important example clearly illustrates the need for theoretical advances to shed light on extinction and resistance scenarios in fluctuating environments. This ambitious project aims at carrying out a cutting-edge research programme whose central goal is to develop a suite of theoretical tools that will allow us to describe biologically relevant evolutionary models, and to make testable predictions in laboratory-controlled experiments.

What does open research mean to you?

Open research means an opportunity to give broader access to our research. However, what it entails is not entirely clear: we are aware of what we are expected to do, but not how we are meant to execute it, especially in research with international collaborations.

The project has an international team (the collaboration started before the new UKRI policy on open access), and we are partly funded by UKRI and the NSF in the United States. The American collaborators are not subject to the same rules as we in the UK, which poses several questions, for example, which journals we will be able to publish in. Open research is a good idea in principle, but it has many challenges.

How does your project use open research practices?

This project started recently, so we haven't done too much yet. We want to publish in an openaccess journal. We also benefit from it since many of our resources and references are published with open access. In the coming months, we will submit papers; we have to see what the open access requirement means for our group.

For instance, one of our collaborators in the US is the Editor of an important journal, which operates on a hybrid model, and from what we heard so far, I currently don't know in which Physical Review journals we will be able to publish: most of them are hybrid, and the funding requires that the output needs to be gold open access, but the block grant cannot be used to cover the fee (article processing charge). This is, in particular, the case for Physical Review Letters, the American Physical Society's flagship publication, in which, in the recent past, we published papers relevant to this project.

"We are in this curious situation where we have funding, but we cannot use it toward publishing."

Workshop on Sociophysics - Mauro Mobilia, Serge Galam, Roberto Andrade and Sebastián Gonçalves



How do you deposit your work?

We usually publish a preprint of our work on arXiv.org and possibly elsewhere, such as bioRxiv.org or the White Rose repository. We only submit to the journal after the preprint is done. When the paper is accepted, we will update the preprints to the final accepted version, but that is without the journal's formatting.

Depending on the topics and the nature of the work, we also upload codes and data. So, in principle, we comply with everything. For us, in a sense, everything is already open access, and the requirement that it has now to be open access via a CC-BY license in a certain way makes things just a bit more of harder since now we have to figure out how we can purchase that license.

In your field, have you found it difficult or easy to identify other people's open research practices?

It is not very difficult because almost everyone is doing the same thing. It is a common practice, for example, to post preprints. I also post preprints on my webpage, and my colleagues do the same, so there are multiple places where you can access them.



Preprint: Effect of mobility in the rock-paper-scissor dynamics with high mortality

"Some people prefer to wait for the paper to be to be reviewed before putting the preprint out, in repositories like arXiv or ResearchGate. These repositories are also easy to use for senior researcher, and PGR students pick it up very quickly."

How does open research inform your teaching practices?

Sometimes in my teaching, I direct students or send them PDFs from arXiv.org, which means those are easily accessible, as opposed to some journal articles. I send them both preprints and PDFs of peer-reviewed articles so that they can compare them.

They usually think it is a very great thing to have a repository where you can access everything easily. Some wonder why we bother to publish in peer-reviewed journals if everything is already out there. That may seem a bit naive but is a sensible question.

Do you have concerns about preprints?

No, I don't have concerns. It works well in my field. What can sometimes go out of hand is if people just post anything as a preprint. For example, I was concerned when there were tons of preprints about Covid-19 at the beginning of the pandemic. But in my field, this is not the case.



Has your attitude toward open access changed in the recent years?

Yes, it has changed. But it depends on the journal. There are these mega journals where you often hear that if you pay the fee, you get published. Often the quality seemed uneven, and sometimes I wondered if a paper in those mega journals would have been published if it was not for paying the fee. On some occasions, I also had this impression when I had to review for them: I wondered whether paying to publish open access was mostly a way to collect fees to fund more expensive journals.

There are journals with great policies. I don't have an academic objection against open access, but I've practical issues with it.

Are there any negative attitudes toward open access you have come across?

The real question about open access is how we fund it, which is especially important for early career researchers who may find it difficult to publish open access if they don't have access to a major grant or hold a fellowship. There is the risk that rich journals will get richer and others disappear, which would be a pity.

There are many questions. For example, what do we do with the hybrid journals? At the moment, no one seems to know, and, depending on the area you are working on, these hybrid journals can be quite important. That's certainly the case with Physical Review Letters in my area.

In your opinion, what is the current state of open access in your field?

In areas like math and physics, we have a lot of hybrid journals, and, given the current circumstances, we are sometimes advised to avoid a particular journal. I hope to think that things will change, and they will negotiate deals. As I mentioned with this project, we have the fund to pay for open-access publication, but the grant does not allow us to do that. It is an

awkward situation where my collaborators can pay for it, and I would like to be able to say, well, I will pay the other half, but I won't pay it from my pocket.

What makes it even more complicated is that not the same rule applies to all, it only applies to UKRI-funded research in the UK, and colleagues from the US would have different requirements.

"We are sitting on a large pot of money, but we cannot use it to publish open access, but we are required to do something with the money to disseminate our research findings."

What does data mean in your field?

Data can be just results and figures. It can also be raw data from some simulations and analyses. We don't do experiments, so data essentially comes from simulations that are calculations.

Do you make your data open?

When we publish in a journal, they usually want a data statement saying where people can access it. We publish the data alongside supplementary information that can be some additional discussion. Usually, there is a section about computational simulation, and we discuss how we did things. Sometimes we give additional figures and results to explain how we did the research, and where people can find the codes and the metadata. It's open and available. Sometimes people come back to us and ask if they can use the data.



How do you manage your data?

For the current project, we have a data management plan, and we used the UKRI template to write it. The data management plan says that we are going to publish our work and the data. The idea is we will probably have some supplementary material and sections on computational result data uploaded to FigShare, which is a data repository. I also instructed the PGR students and postdoctoral researchers to back up the data on OneDrive.

What kinds of software do you use?

If you refer to computational tools, it is probably mostly Python, an open-source tool, and we also use MATLAB and Overleaf, which have an education license.

"I think open research is going in the right direction, but there are a few practical concerns I am pretty sure will be fixed. I don't know the answer to how long it will take. These are concerns heard across the Schools."

Open Research Case Studies – School of Mechanical Engineering with Nick Cooper

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Modelling mechanical damage mechanisms in hip replacements PhD project:



Nick's research investigates mechanical damage mechanisms in total hip replacements and receives industry funding from DePuy Synthes. He is also part of the planning committee for the Leeds hub of ReproduciliTEA which is part of the UK reproducibility network (UKRN) and supports the teaching of 3rd and 4th year modules within the School of Mechanical Engineering.

How are open research practices incorporated into your research?

At this stage, I have not gotten into publishing yet, so mostly I think about open research as in how I am handling my data and tools that are rigorous and also can help the next researcher who is going to use them. I am coming from a maximal transparency point of view, whenever it is permitted since my research is partly industry-funded, so I may not always be as open as I might like to be.

What restrictions do you have from your funders?

Everything I want to present externally or publish has to be approved by them. They would have to receive it at least a month in advance and then review it to make sure they are happy with what I am publishing.

Have you received any feedback from your supervisors regarding open research practices?

It is probably less discussed with my supervisors and perhaps partly because these open research practices are not necessarily a requirement. It can feel like you are doing the extra work. It is not a disagreement with them, but perhaps something that I do more independently from them as we will focus more on the science side of things in meetings.

"There are loads of advantages of open-source software and making it available to the community, whether it is support, development, or research."

What repositories do you use to deposit your research?

I have got an ORCID account since I was an undergraduate student: we were made aware of it then and I have had a couple of conference abstracts uploaded there. I have a profile on *Symplectic* as well but there is not much to add to it at this stage.

"My involvement in open research has been very good for my awareness of practices I will do in the future. At this stage, it has been limited what I can do."

Do you use preprints?

I would read preprints if something was relevant to me. I would like to think the preprints have the same kind of critique as a published paper. Just because something is a preprint and something is not, I wouldn't give either one more credit.

Has your attitude toward open access changed in the recent years?



I would say yes, and that is through involvement and engagement in events at Leeds, such as the <u>Open</u> <u>Lunch</u> and <u>ReproducibiliTea</u> which bring different departments and researchers together with a research interest. It is nice to talk about open research rather than just staying very isolated within my institute. It is nice to have these external viewpoints and see what happens in, for example,

the Faculty of Social Sciences, which is going to be very different from the School of Mechanical Engineering. If you are more aware across the board of what other challenges people are facing, it helps to inform your research and practices.

As a PGR student, are you happy with the training provided on open research or would you like to see more done in this topic?

I think that might only work if it is part of a requirement that the PGR students would have to do at FFPR (First formal progress review, 4 months in the PhD), transfer (an assessment to become a full PhD candidate 9 months in PhD), or APRs (annual progress reviews, 24 and 36 months in the PhD). If it is just a one-off session and there is no follow-up, then there is probably less long-term engagement with open research practices. It would have to be the case of training that gets the students thinking about open research through their PhD, as opposed to seeing it as an extra factor or a side project.

What does data mean in your field?

Part of my PhD is experimental work. I work with machines that make hip replacement components move like they're in a hip. During the test, this produces log data of movements and forces that occur. Then every couple of weeks I take a series of measurements on the changes that have occurred to the components while running tests on them, so that is raw

data that gets analysed. I also do computer modelling to predict the stresses and strains within the components. This produces a lot of data and many different outputs are possible.

How do you manage your data?

I rely on using OneDrive, which has version control and backup systems. Everything gets dated and then sorted by component number and into the three measurement techniques that I use. The other really important data to manage is my code and scripts for my analysis and computer models. I use GitHub to offer an additional layer of version control and documentation of their development. Looking after the scripts themselves is more important than any post-processed data because that can always be reproduced again. This is particularly important where model output files can get very large.

In your PhD research, have you used any software that you were not familiar with before?

Yes, quite a few. I'd done some coding before but have done a lot of Python and MATLAB now. Most software is standard university licensed; Origin Pro and SPSS were both software that I've used since starting my PhD. GraphPad Prism is the only one I've had to pay separately for which is a graphing and statistic program I first used during my undergraduate years. It does the same things as other software available but as I was familiar with it, I thought it would save me a lot of time, so I would rather pay for it.

What advantages or disadvantages do open licensing have?

I have used ImageJ in the past, which is an open-source image processing software. There are some great functions in it. You can almost get a community behind open-source software, building and developing it. A closed program might have quite high functionality since you would have a professional team dedicated to working on it but it doesn't mean it's not clunky or rigid.

If you would publish your research, what road of access would you choose?

I would have funding restrictions in terms of how open I could publish. Then there are a lot of costs associated with gold open access, so I think it would be more likely the green road; not necessarily through demand or what I want, but what is most feasible.

"If we can get students thinking about open research earlier in their journey, it is going to help a lot of them as well as their fields. Even if first just think about open research theoretically, it makes your practices so much more effective and open and transparent."

Open Research Case Studies – School of Physics and Astronomy with George Heath

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Molecular and Nanoscale Physics project description:



George's current research focuses on further developing high-speed atomic force techniques to study the structural dynamics of complex single biomolecules on the sub-nanometre scale to increase our understanding of diseases and improve medicine. One project he is working on at the moment to understand how potential drugs interact with specific proteins and how those proteins respond.

What does open research mean to you?

Open research means sharing not just publications and being open to anyone that wants to access that but sharing raw data and where that comes from and the methods so people can reproduce that work and scrutinise it.

It also entails open software and code: with that, others can see how you analysed the data and how they can analyse the data in the same way without having to do all that work again.

How does your research use open research practices?

I mainly share codes and software, so people can reproduce and build on that work. I use Atomic Force Microscope, which is produced by many manufacturers. Each has its restriction that the data can only be opened by their software. At the moment, in my field, it is a drive to make that more open because people don't share the raw data. There is a drive for the manufacturers to make that more open.

In your field, have you found it difficult or easy to identify other people's open research practices?

I would say it is difficult: in the past ten years, my field has been very closed, and nobody has shared data or software until recently. It is becoming more and more open, and more early-career researchers are starting to share software. I think that's helping.

How does your open research inform your teaching?

I don't teach open research, except that sometimes I teach protein structures and talk about the protein databank. It is an open-source databank where people can obtain 3D structures of proteins they have solved, published, and made available.

https://orcid.org/ 0000-0001-6431-2191		George R Heath		
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		DOI: 10.1016/bs.mie.2021.03.011 Part of ISBN: 9780323853743		
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George Heath on ORCID

Do you use preprints?

I haven't published my research as the main author yet, but I plan to use preprints, and I have been involved in some preprints in the past as a co-author. I think preprints are great.

Where do you read or deposit preprints?

Since my field is in biophysics, the leading repository is bioRxiv.org. Some of the papers I have been an author of are on the White Rose repository, including my PhD thesis as well though I think that's standard.

Do you have concerns about preprints?

I only have slight concerns when the media pick up on some results that have been published in a preprint and assume that it is a fact. However, this is not relevant to my research area. Within my field, I don't have any concerns about preprints.

Has your attitude toward open access changed in recent years?

Almost all my publications are open access, but I haven't published as the main author for a paper yet. So, I don't know exactly the costs, but it's a concern that the fee may be increasing and becoming very high. I don't know enough to tell you exactly, but it is a slight concern.



Are there any negative attitudes toward open access you have come across?

I think the only negative attitude is about the costs paid to journals and publishers for open access.

Have you developed means to 'bypass' restricted content?

I did not need to, as I can access most things via my university account. But I know colleagues from different universities would ask to send a paper they cannot access. I have heard that some also use Sci-Hub.

What does data mean in your field?

In my fields, most of the data is captured as microscopic images or movies, which software has to generate because it scans a tip across the surface and generates an image. We produce images through analysis as well. So, data are those images and the analysis of those.

How do you manage your data?

I store most of the data on OneDrive, where possible. Sometimes a data file is quite large, but I am not at the stage where my cloud storage is out of space. In general, I try to back everything up on OneDrive.

Do you use open data?

Yes, I often use proteins from the protein databank, analyse their structure, and compare it to my data. I have also deposited some datasets, mainly alongside a paper, and these will just be the raw values from the figures for some journal's requests.

What kinds of open software do you use?

I often use analysis software, such as <u>MATLAB</u>, which is not open; you need a university license for that. I am planning on switching to an open platform, such as <u>Python</u>, but I have been able to do it yet. Some other tools come with the manufacturers that produce the machines I use. They have software to analyse images, and you need to purchase the machine to get a license for it.

Do you use open codes?

I share a lot of codes on <u>GitHub</u> and also download other people's codes. My codes are publicly available within GitHub, where you put a license on it. In the past, I have used "GNU General Public License v3.0", "MIT License", and "BSD 3-Clause "New" or "Revised" License". It can be a bit tricky navigating which license to use.