AI 4 Science Discovery Network+

AI4SD Interview with Professor Charlotte Deane
08/01/2021
Online Interview

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Humans-of-AI4SD:Interview-26

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Network: Artificial Intelligence and Augmented Intelligence for Automated Investigations for Scientific Discovery

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Title	AI4SD Interview with Professor Charlotte Deane
Interviewer	MP: Michelle Pauli - MichellePauli Ltd
Interviewee	CD: Professor Charlotte Deane - University of Oxford
Interview Location	Online Interview
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2 Biography

Figure 1: Professor Charlotte Deane

Charlotte Deane: 'Open science allowed a lot of the Covid-19 epidemiological modelling to move forward fast'

Charlotte Deane is a Professor of Structural Bioinformatics at the University of Oxford where she heads up the Oxford Protein Informatics Group in the Department of Statistics. At the time of interview she was the Deputy Executive Chair of the Engineering and Physical Sciences Research Council and the Response Director for UKRI Covid-19 Research.

In this Humans of AI4SD interview she discusses her journey from chemistry to bioinformatics, easing communication between the academic community and government, working fast on the Covid-19 research response and her advice for early career researchers.

3 Interview

MP: What's been your path to where you are today?

CD: I originally did an undergraduate degree in chemistry at Oxford. When I started the degree, I had thought that I wanted to be a researcher; even though I didn't really know what one was at that point in time, but I liked the idea of thinking about things. In my fourth year, I became the captain of the Blues hockey team, but I also needed to decide on a year-long research project and I worked out that the answer to fitting the research around my sports schedule was to do a computational project.

I ended up working for Graham Richards, who researched protein informatics, which was new to me because my chemistry degree had mainly looked at small molecules. That project changed my whole way of seeing chemistry because I found that working on a computer showed me possibilities that had barely been touched by others. What I could do on the machine was amazing, and it made me realise that this is what I wanted to do.

From there, I went on to a PhD at Cambridge with Tom Blundell, a deliberate decision because he has a mixed wet and dry lab, with people doing experimental and computational work. He was also known as someone who would take risks in the area of protein informatics. From that, I got a Wellcome Trust travelling fellowship, with which I went to work with David Eisenberg at UCLA. The next step involved my coming back to the UK in the final year of the fellowship. I needed to find somewhere to work and I wrote an email to Oxford on the off chance that they might invite me to give a talk or something. They wrote back to me saying that there was a job going and that I should apply for it. It was a lectureship in bioinformatics and I only had 24 hours to put together an application. I got the job and that's where it all started.

I then found myself in that wonderful position of the horror of starting an academic job where there's way too much to do, you don't know how to teach, and everything's crazy, but you're also thinking, "I've got a chance now. I just have to make this work." It was amazing because, in one sense, it was exactly the wrong decision: going to a university where no one did what I did, but it turned out excellently for me because now I am the person who does that at Oxford.

From there I built up a research group and began working with pharmaceutical companies. I had friends who had done the same PhD as me and gone to work in pharma, and from them, I realised that there was a real need for what we were doing. Working with pharma helped a lot because it gave my group stabilisation and reassured the university that I was worth keeping.

The big jump at Oxford was when I became the Head of the Department of Statistics nearly six years ago. That was, once again, a weird jump as it isn't about my research anymore. It's about how you make it possible for people to do what they love doing. When you become a head of department, suddenly your job isn't to maximise the output from your group and have as much fun as possible, but to ensure that everybody in the department can do that. Later, I was approached about whether I'd be interested in becoming the Deputy Executive Chair of the EPSRC. I realised that was an opportunity too good to miss, which would allow me to learn more about other universities. I applied for it and was successful.

MP: What kind of work have you been involved in with the EPSRC?

CD: Primarily, my role is to support the Executive Chair of the EPSRC, and the main areas I work with are related to our research strategy: Which areas should we be looking at going forward? How do we ensure we're aware of community knowledge? What programmes should we offer? It's a balance between accepting that the UK cannot be a world leader in every single area, but there are many areas in which we are fantastic. We need to work out ways of ensuring that we keep critical mass, or that we build up mass in important areas.

Running alongside that is a lot of work in relation to the spending review, and getting and retaining funding for the research council within the UKRI and from the government. The question there is about how you persuade government that it's worth funding research into, say, material science; you must make the case for the link between fundamental research and growth in the economy. They, of course, have difficult choices to make and a limited amount of money, so we have to be clear in explaining to government why something is worth funding.

On the other side, there is the research community who might not like the way something is phrased. Often, the way we describe things to government can sound quite odd to me as an academic; it's accurate, but it isn't the language we would normally use. A lot of the job is trying to ease that communication. I think I was brought in to help the academic community understand that we need to be advocates for what we do and be part of the conversation. We need the academic community to be able to explain what is important, build consensus and not fight each other, and work together to get the best research funded. There are a lot of pieces to the puzzle, but that's how it works.

MP: Does your multidisciplinary background help with communicating across these areas?

CD: It's really helped. Before I became the head of department at Oxford I was an associate head of the MPLS division, which involves spending time talking to people from other divisions across Oxford. It was amazing to me how viewpoints varied from, say, the humanities or the social sciences or the physical sciences; your whole worldview is different, and that's just inside one university. We all roughly understand the same language, but it takes a bit of bullishness to be brave enough to talk to all these people and to understand different disciplines and viewpoints.

It also involves having humility. For instance, I'm not an expert in social science, so there might be something that they're wanting to fund, and I have no understanding of why they would want to fund it. But if they tell me that it's good, I have to believe them, because if I told them machine learning was good, and they said "No," then I would be very angry! It's about finding the balance between understanding enough that you can speak to people from other disciplines, but not taking decisions on their behalf. You have to enable them to trust you to the same degree across the disciplines.

MP: What surprises and challenges have you encountered in your work?

CD: I went into working with research councils thinking, "You have no idea what we do," and I was wrong! It's not that they understand everything, but they work very hard to have a thorough knowledge of all the people working in different areas. I found that very impressive.

The most unexpected challenge for me was how much getting anything done still involves having to sit down and talk to people. When you're the principal investigator of a group, you can just say, "Do it," but that's not the way you get something done in an organisation, even if you're in charge. On the one hand, that's challenging because it slows things down, but on the other hand, it's right that it makes you stop and think, otherwise you can become too much of a maniac!

MP: How has the Covid-19 pandemic affected your work?

CD: Sir Mark Walport, who was the head of UKRI at that time, asked me to set up an open call for research ideas into Covid-19 projects that would have a short-term impact. These had to be projects that would make a difference within 18 months. The call had to be across all of UKRI, including Innovate. I worked with some amazing people who helped to set up the call, and we got it ready in four days, which was unheard of. I don't think it's the kind of thing we could have done were we not in a crisis; people step up in a crisis. That was the first iteration of the call, which we continuously refined. We worked with processes to ensure that grants could be assessed both rapidly and accurately. There are always risks of making mistakes when you do things fast, but in March and April of 2020, the risk of not making these decisions was probably higher than the risk of making a few bad ones.

I was also responsible for linking the UKRI research to government priorities. We spoke with GO-Science and SAGE, and listened to what they felt was important, what research needed to be done, and from there I worked out how that could percolate down to the academic community. I chaired a taskforce of senior academics and we worked to bring information together. Part of this involved rephrasing questions posed by SAGE in ways that accommodated building research projects. We also targeted specific people to get them involved or bring them together with researchers with whom they wouldn't normally work. An obvious example of this is transmission. We had to bring together experts on culturing live viruses with experts on droplets with experts in mathematical modelling. These people usually wouldn't work together, so I needed them to talk to each other and help them to understand each other's languages quickly, and build collaborations that would make a difference. There was a huge amount of willingness and openness there.

The thing that was challenging was how we needed to take things through to an impact point. Academics usually hate to share their results until they have a publishable end product, but with this, they had to share their information the minute it was available. People struggled somewhat with that because they couldn't have, say, six months to conceptualise the perfect experiment, it was go now or don't go. It didn't need to be perfect, but as long as it told us something, and there were enough checks and balances that the direction of the project could be changed later.

MP: Do you think the ways of working that developed during the pandemic will have a lasting impact in science?

CD: There are all sorts of things that might make changes. It's going to be interesting to see what happens with the virtual working environment once it's less needed. The interesting things to me are about research culture and open science. Open science allowed a lot of epidemiological modelling to move forward as fast as it did. It was brave, especially when you're in the eye of the storm and there's a lot of media attention on what you're researching, to release code and let others see the mistakes in it and rewrite it. The way that people behaved around that was so good, and the positivity that it generated in terms of how we improved the code, how much we understood, and how quickly it progressed, I'm hoping that will stay. Hopefully, more people will realise that releasing data and code is good for science, and we will move faster and improve things.

There are other impetuses too. Universities and research councils want you to have patents so you can make money out of your research, but if I do that, then I can't release my code for free. That can be a counter-incentive where, on the one hand, you have people saying, "Do open science, release everything for free!" and on the other hand, universities are saying, "How are you going to make money from this?" Those two things are often in opposition, and it's something that really needs to be dealt with. There are, of course, instances in which it makes sense not to release something for free. If you're making a small molecule, for instance, you don't just publish that on the internet because no pharmaceutical company would make it into a drug, because they can't patent it. So it's not that everything should be released for free, instead, it's that a lot more thought needs to go into where the pressures are, and what rewards you get by choosing whether or not to release something for free. I'd like to see a system where it's as good a mark on your professional record to say, "I shared this code for free" as it is to say "I got a patent."

MP: What advice would you give to early career researchers?

CD: My advice is to decide what you want to be and what you want to do and to not let other people tell you those things. For me, it was deciding that I wanted to work on computers because I found that area of research most interesting. I was told that it was a bad choice, that I should do straight chemistry or straight mathematics to get a job because there were fewer academic posts in things like bioinformatics. You can't pay much attention to that. The most important thing is to find the research that interests you and do that.

The other important thing I'd suggest is to talk to lots of people. Not to let them tell you what to do, but to get a better understanding of the big field you work in. If you go to a science talk and go, "It's not got anything to do with me," and you get bored, you're probably in the wrong career. All of it should be fascinating. The desire to understand the breadth of these things is really important. Assume that you need to learn more, because the more you have, the more tools and ideas will be at your fingertips and the more chance you'll be the person doing the next clever thing. That's all you can ask for.