AI 4 Science Discovery Network+

AI4SD Interview with Professor Markus Kraft
29/11/2021
Online Interview

Michelle Pauli
Michelle Pauli Ltd

12/08/2022

Humans-of-AI4SD:Interview-35

AI4SD Interview with Professor Markus Kraft
Humans-of-AI4SD:Interview-35
12/08/2022
DOI: 10.5258/SOTON/AI3SD0232
Published by University of Southampton

Network: Artificial Intelligence and Augmented Intelligence for Automated Investigations for Scientific Discovery
This Network+ is EPSRC Funded under Grant No: EP/S000356/1

Principal Investigator: *Professor Jeremy Frey*
Co-Investigator: *Professor Mahesan Niranjan*
Network+ Coordinator: *Dr Samantha Kanza*

Contents

1 Interview Details

Title	AI4SD Interview with Professor Markus Kraft
Interviewer	MP: Michelle Pauli - MichellePauli Ltd
Interviewee	MK: Professor Markus Kraft - University of Cambridge
Interview Location	Online Interview
Dates	29/11/2021

2 Biography

Figure 1: Professor Markus Kraft

Markus Kraft: 'My advice to early career researchers? Do good work and talk about it'

Professor Markus Kraft is a Fellow of Churchill College Cambridge and a Professor in the Department of Chemical Engineering and Biotechnology. He is the director of CARES, the Singapore-Cambridge CREATE Research Centre. He is also a principal investigator of the Cambridge Centre for Carbon Reduction in Chemical Technology (C4T).

In this Humans of AI4SD interview, he discusses developing the World Avatar (a world model that can hold anything that is conceptualisable), the potential of AI for decarbonisation, and his advice for early career researchers.

3 Interview

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

MK: I was born in the southwest of Germany, where the country is most beautiful, in a place called Pirmasens. I studied mathematics in Kaiserslautern with a minor in theoretical physics and computer science, and I did my PhD in technical chemistry. My doctoral research used scientific computer and stochastic methods to look at turbulent reactive flow and understand the interaction between mixing and reaction.

I then had two years of postdocs at the Weierstrass Institute for Applied Analysis and Stochastics in Berlin, where I had a wonderful time in nineties Berlin. Then in 1999, I started my position as a lecturer in the Department of Chemical Engineering and Biotechnology at the University of Cambridge, where I'm also a fellow of Churchill College. Since then, I've remained with the University of Cambridge, and in 2013, I moved to Singapore to build up the university's first research centre outside of Cambridge.

For the last eight years, I've been the Director of CARES (the Cambridge Centre for Advanced Research and Education in Singapore). I also serve as a Principal Investigator for the Carbon Reduction in Chemical Technology Programme and a project on laboratory automation with the Pharma Innovation Programme Singapore (PIPS) and the Agency for Science, Technology and Research (A*STAR).

MP: What was the appeal of CARES and what has kept you there?

MK: In 2019, I became a professor, I had my higher doctorate, and I even got a British passport. I had the feeling that I had achieved everything I could in Cambridge and that it was now time to do something new and exciting. When I went to Singapore, there was nothing there, so I had to build it from scratch with some very competent help from others. It was a challenge, being in a completely different environment, but it was an exciting journey. In Singapore, there is plenty of money and resources, but it wasn't as easy to recruit talented people as it was in Cambridge. We have to compete with two world-class universities: the Nanyang Technological University and the National University of Singapore, so it was challenging to get the best people.

What's kept me here is that if I start something, I want to see it through. Our programme now has more than 160 members, and we have a fantastic laboratory with better facilities than I had in Cambridge. I also like the weather; it's fantastic!

MP: What research are you working on currently?

MK: I was originally a combustion researcher, but now combustion is a little outdated, even though it's still very important. If you want to model combustion from first principles, you see that it's actually quite complex because of the level of nonlinearity. When you build it, you discover that there are thousands of elementary reactions involved, which you cannot simply handle with a classical approach; you need to use more advanced mathematics. To grasp the problem properly, what's needed is a unified data source to which everyone contributes, and that led us to parameter estimation, experimental design, and surrogate modelling, which all exist in the realm of machine learning.

What became clear was the need for a system that could hold any type of information. I started something called the J-Park Simulator, which is now called the World Avatar. This is a system known as a world model that can hold anything that is conceptualisable, so, for example, your brain would also be a world model, which, similarly, can form concepts. With the advent of the internet, standards have been developed to represent concepts in a world model through a knowledge graph. Companies like Facebook use the knowledge graph concept, mapping concepts in the world but also making sure that the processes that alter the knowledge graph are part of it too. Our aim with the World Avatar is to create a base world that represents the world as it is.

Our first exercise was looking at the chemical park on Jurong Island, and the second was then looking at cities: the buildings that are there, the emissions from ships, all in the same system. But with emissions, you also need a representation of chemistry using combustion models to estimate the emissions that are made. So, we developed a representation of quantum chemistry. One problem we have in chemistry is around the naming of chemical compounds; there have been several different attempts to do that, but there is no single nomenclature that can cover it all. With our knowledge graph, however, data is represented as a triple—subject, predicate, object—in the graph, which we can now link to an Interaction Region Indicator, which leads you to the quantum chemistry it represents. The unique aspect of this representation is that it relates directly to the quantum chemistry of the chemical compounds.

We are now connecting this to a chemistry robot, and the idea is to help the chemist to find more sustainable reactions, with higher activity and more environmentally friendly reactants that require less energy. It's an automated setup. Then you can use machine learning optimisation or mathematical methods to find the best pathways in the reaction space.

MP: Do you see this kind of automation becoming the norm in laboratories?

MK: Not tomorrow! But even if our efforts are not successful, the technology itself will be, and it'll change everything. When I say "everything," I really mean it: if everything is connected and everything can be controlled algorithmically, then everything can be optimised. You can make the world a better place. There will be people who say "You're going to need much more energy because of all the electricity you consume with the computers," but you have to assume that you have renewable energy that feeds all of this.

MP: What has surprised you in your research?

MK: I'm still waiting for the surprises to happen! One of the most fascinating aspects of this research is, that although I have a gut feeling about which direction to go in, working out how to implement something is completely different. Together with my team, I find out how to turn ideas into a reality — it's the best part of the work. This is why it's not important if you fail to produce a working system — you will have learned some really fundamental things about the world itself. Before I started doing this research, I hadn't thought as much about how everything functions, and now I find that's the best part of the work. It's not exactly a surprise, but it's definitely important.

MP: Do you think there is enough attention on the potential of AI in combating climate change?

MK: Max Tegmark, a cosmology professor at MIT, works at the Future of Life Institute, and part of the work there involves people using classical machine learning to look into climate change. With my research and the knowledge graph, we're a little more on the fringe, but there are already a large number of people using machine learning algorithms for research into climate change.

Not too long ago, there was a European project in which they tried to build the Earth's digital twin. This meant that they could have something that automatically analyses the imagery that goes into climate change and, in turn, create climate change models. In that respect, AI is already contributing toward decarbonisation, but there are also other applications.

MP: What advice would you give to early-career researchers in your field?

MK: Be lucky, of course! What I can say is what helped me in my career. When I was a student, I joined the Verein Deutscher Ingenieure (Association of German Engineers), and in their newspaper, they have a column that's been there for the last 30 years. The columnist answers questions from people who want to be successful in their careers, and he came up with a few rules to be successful in your career. The key one was to do good and to talk about it: write good papers, get them published, go to conferences, present your work, and make sure everybody knows you. You could be scientific about it: have a think about how information travels in your network; don't be afraid to post an article on LinkedIn or on ResearchGate. Make sure people see what you do. It's not enough to just sit in your room and have your eureka moment — no one will know about it unless you publish! And nowadays, it's not simply the paper in the journal, you can use social media to some extent, and also skip repositories and go straight to preprint servers. There are many ways to communicate information.

You also want to have a degree of enthusiasm, a deep motivation to do your subject. This helps guide you through what I call the valley of tears: when you don't get the job, or you're unsuccessful with an application. At the end of the day, your enthusiasm should push you because that's what you want to do. Starting an academic career because one thinks having one is something good is not enough motivation to be successful. Without enthusiasm, you'll be lost when you start having negative experiences. If you're enthusiastic about your subject, you don't have a choice, you have to carry on.