

An interview with Peter Sloot, professor of Computational Science

Ask the average student on the university campus to explain what Computational Science is and you will probably receive a distant glassy-eyed stare followed by some incoherent mumblings involving the word 'computers'. Most people would probably not rank it highly in the league table of sexy-sounding disciplines.

So what exactly is Computational Science?

Computational Science is a rapidly growing interdisciplinary field of study that uses advanced computing and data analysis to understand and solve complex systems and processes.

And what exactly are 'complex systems and processes'?

Ask the aforementioned average student this question and their eyes may show increasing signs of ennui followed by further hushed mumbling about 'tax forms' and 'amorous relationships'.

Complex systems, however, refer to a wide range of things from the way that molecules in a cell work together to keep the cell alive, to the way terrorists interact and function within terrorist networks.

Computational Science seeks to elucidate the complex world we live in, in which myriad small components combine to affect large macroscopic processes. By collecting data and creating computer models, computational scientists can make predictions on varying problems such as how to influence the flow of traffic, how an epidemic will spread or the likelihood of individuals in society becoming addicted to drugs.

Peter Sloot, professor of Computational Science at the University of Amsterdam, is at the forefront of this groundbreaking new discipline. In addition to his academic post, Prof. Sloot also heads the world-renowned EU-funded Virolab project, which is developing computer models to help combat HIV and AIDS. In 2010, he also received the 'Leading Scientist' president award (worth 3.6 million euros) from the Russian Federation to further expand on his innovative research and was appointed professor of Advanced Computing at St Petersburg University. In addition, he is professor of Complex Systems at the Nanyang Technological University of Singapore for three months per year.

In this interview, Prof. Sloot talks about the brave new world of Computational Science and its ability to unravel the secrets of life, the universe (and making great coffee).

Can you explain what Computational Science entails?

Computational Science is not Computer Science. There's a big difference. The idea is to see if we can make sense of complex processes by modeling them in a computer. It's very much algorithmic-driven (step-by-step procedure for solving a problem in a finite number of steps), but also involves lots of mathematics and logic. And we apply that to different research areas in the natural sciences.

In a documentary you stated we live in a monodisciplinary world, but that you find it stupid when people ask you what your field is. Explain.

It's strange that people think you can understand big problems by looking at them from a monodisciplinary point of view. They require a multidisciplinary point of view. One of the most beautiful examples where all the sciences come together is climate change. It involves Physics, Chemistry, Biology, Economics and Sociology. However, we need a basic methodology to grasp complex processes. And that's the aim of Computational Science: to see if we can describe these processes in such a way that we develop a predictive power.

The need for an interdisciplinary approach to science came up in previous interviews in this 'UvA in the spotlight' series. Prof. Henkjan Honing suggested faculties should be abolished. To what extent would you agree?

That's a tremendously interesting point. Most of our courses are monodisciplinary. We're evaluated in a monodisciplinary way and we get money from monodisciplinary funds. However, the problems are all multidisciplinary. So yes, some walls have to be broken down. However, there is also a lot of beautiful monodisciplinary research and disregarding that would be stupid. I would advocate setting up something like the Institute of Advanced Study (the interdisciplinary postgraduate center for theoretical research and intellectual inquiry in Princeton), where you bring together postdoc and PhD students with a drive to conduct advanced interdisciplinary research and disregard the boundaries between faculties and disciplines.

Your academic training was very varied, having obtained an MSc in Chemistry and Physics and a PhD in Computational Science. Was this an express choice?

I started studying Chemistry, but then I discovered there are so many fundamental processes underlying the chemical processes that I didn't have a clue about, so I started studying Physics. Then I did a PhD at the Dutch Cancer Institute. I became fascinated by the amazing complexity of biological and biomedical processes. Although we know quite a lot about the human body, there are so many unresolved issues. So I started seeing if I could model tumour growth using computers and really understand what's happening, taking physiology, biochemistry and the genetic processes into account. This didn't just involve Chemistry and Physics, but also Computational Science and Mathematics. If you put all these things together,

as if stirring them in a cauldron, you gain some new insights. This triggered me to look for basic mechanisms underlying these natural processes. Computer models and algorithms help me to understand that.

You received the ‘Leading Scientist’ award from the Russian state and are currently professor of Advanced Computing in St Petersburg. Could you explain this award and your role in Russia?

The award was pretty strange in the sense that I received a phone call from Moscow asking me to send my biography. Then, some months later, I was called again and informed that I had received this grant. I didn’t apply for it. What it amounts to is a lot of money to set up research into so-called ‘Advanced Computing’. The idea is to use computers to predict various types of events, from economic collapses to the outbreak of epidemics. It’s about how we combine data into computer models, which then have a predictive power that can be used to give advice to medical doctors or municipalities etc. The computer can run scenarios to predict what is going to happen, for example, in the event of an epidemic. It could help us to judge where we can intervene to stop certain events happening.

You’re best known in the Netherlands for ViroLab, funded by the EU, in which you are devising a computational model to combat HIV and AIDS. Could you explain this project?

This is an ongoing project. The question is whether or not we understand the transmission of HIV in populations and specifically the transmission of the drug-resistant part, the viruses which you cannot treat anymore. There was a fundamental underlying question posed by the EU in 2006, which was whether one billion euros could be better spent on better drugs or changing behaviour. When developing better drugs, you consider the molecular processes, the virology and biochemistry. If you think about behaviour, you consider sociology, psychology and politics. A monodisciplinary approach wouldn’t be sufficient to study these issues. This required Computational Science. For the last 10 years, we have built models with which we can study pretty much everything from the molecular process all the way to the social process.

I believe you calculated that prevention was more effective. Have the EU heeded this advice?

There’s more money going into monitoring people and giving them advice, not just giving them drugs, and following them over time. There was a beautiful study here in Amsterdam, the ‘Amsterdam Cohort Studies on HIV/AIDS’. They followed homosexual men for approximately 20 years. This was used to understand the interplay between behaviour and drugs. The weird thing is there’s an interplay between the quality of drugs and behaviour. If the drugs are good, for example, you feel better, so you tend to forget you are ill and your behaviour becomes more risky.

What are the main complexities you’re confronted with in fighting HIV or finding a computational model to combat it?

First of all, any epidemic is a complex system, where the epidemic patterns that emerge feed back into the individual interactions. This is a prototypical

complex adaptive system. The challenges we faced were on what level we would model this things. Should we model it on a molecular level, cellular level, intercellular level, organ level and on a population level, in this case the sexual network level. There's no computer that can model that process from the transcription and the entry process of the virus all the way up to the interaction between individuals, because the computational complexity is just too great. So you need to look at all the different levels and try to make models of these levels. You then see if you can understand how these models work together to explain the whole process. That's the biggest challenge and that is why it took us 10 years to do this.

How far are you now in 2012 to devising a computational model that will be affective in combating HIV?

We're pretty far. We have the entry process and the transcription, the reproduction process, the interaction with the drugs, the whole virology and part of the immunology and we have the whole sexual network level. So we can actually say how a slightly better drug will affect the transmission of resistant HIV in the total population, which is quite impressive. I wouldn't be surprised if we were able to tackle the whole HIV dynamics in the coming 10 years or so.

In one piece on your research, you mentioned there were 22 medicines to combat HIV. To what extent do you have to change that to adapt to the mutations?

That's the problem. The drugs you give in combatting HIV are patient-dependent and time-dependent. Every patient has his own set of mutations available which change over time. To design one drug for one patient is pretty hard. If you can predict what part of the virus will start to dominate then you can give better treatment. In recent research, [the findings of which were published in the scientific journal *PLOS One*](#), we combined the phylo-genetic network (the genetic network of the virus) with the sexual interaction network and from this we have learnt about completely new patterns of transmission. And it seems that certain transmissions are more dominant than other ones, transmissions of certain mutations. So you have preference pathways of certain mutations.

However, the important part of this research is that it's not only for HIV. We can use it to study other kinds of epidemics. In Singapore, where I also hold a chair, we're doing some research into Dengue, to understand how it spreads in clusters in the city. It seems we have found something fundamental in the way that epidemics spread. That's where computational science plays an important role to find the fundamental processes underlying all these things. The step from understanding epidemics to understanding criminal networks or drug-using networks is not so large. The conceptual mathematical models are very much alike.

You talk of computational models being used from combatting HIV to terrorist networks. Can Computational Science really be used for any subject, such as preventing the next economic crisis to making the perfect cappuccino?

I need to answer this in 2 steps. If we utilize deterministic processes where we can break it down into sub-components and calculate what is happening, then the answer is probably 'yes'. But what's really interesting are these problems in the field of complex systems. These can be man-made systems, such as traffic, which is a complex system, where you can get these typical complex system behaviour like 'phase transitions' (theory of traffic flow that focuses mainly on the explanation of the physics of traffic breakdown and generally has two phases: free flow and congested traffic). If you change something in the way you moderate the traffic, you can get all kinds of obscure waves as a response to that. I believe that if we can gain a better understanding of what complex systems actually amount to and develop the computational models to mimic them, we will get very close to predicting life, the universe and everything and the best coffee for that matter. Actually many years ago I did receive some money from the Italian 'Illy-coffee' brand to model the interplay between coffee granularity, suspension-flow and aroma

To what extent are other disciplines, such as Economics and Sociology, incorporating computational science?

That's happening now and happening very fast. In Economics, people like Brian W. Arthur started this idea of using agent-based models (field using computational models for simulating the actions and interactions of autonomous agents, such as organisations or groups, with a view to assessing their effects on the system as a whole) to understand the complexity of Economics. Here at the University of Amsterdam, Cars Hommes is working on that. There's this huge European flagship proposal called 'FuturICT' which is trying to work on predicting complex systems, such as the economy, through simulation. So, economists are getting there. Up to five years ago, sociologists hardly did any computer modeling. There was a lot of statistical analysis of pretty incomplete data. Things are getting easier now, with Facebook and Twitter. There are one billion people online. If you can mine that data you can really learn something from social behaviour. You need the data to pinpoint what you are going to model and make predictions.

You've talked of how complex systems function on the border between chaos and order. Explain?

If things are completely chaotic you cannot predict anything, it is something I'd like to call the entropic death. If things are completely ordered nothing happens. So, in life the interesting things happen in between those two borders, which is the place where information is registered, transferred and processed. We already know from Physics that a lot of fascinating stuff is happening in that area, but Physics was always looking at identical unchanging particles. But if you want to model human behaviour, you have to take individual adaptive behaviour into account. We're looking at this boundary between ordered systems and chaotic systems to see if we can model how information propagates through those systems. This is where the interesting stuff seems to be happening.

To what extent is computational science necessary to unlock the secrets of the universe?

I'm sure computational science will play a pivotal role in unlocking all these secrets. We see it happening. Take the complexity of cities. We know that in the coming 20 or 30 years, seven billion people will be living in urban areas. But we have no clue what a city is. There's no science of cities, as it were. It seems computational science will bring order in that field of study. It's all about being able to predict things. I believe strong computational models have this predictive power. So, for example, we can say given all the things we know now what is likely to happen next. That's important for epidemics. That's important for everything. Computational science has the promise of being able to give that predictive power to us.

You're working on a new project with the Dutch police and the Russian state looking at drug addiction. Can you explain what this involves?

The idea is that the models we are using to study epidemics and HIV, immune system models, can also measure the immunity of individuals, in terms of whether people are immune to addiction or radical ideas, such as terrorist ideas. One of the things we are looking into is the likelihood that somebody will become addicted if a person in their first circle of acquaintances is a drug addict. We are using data from LiveJournal in Russia (a social network equivalent to Facebook) which 23 million people post blogs on. We analyse the text from the people's blogs and we look for key words that are identifiers of whether they are interested in negative things and criminal things. We then try to estimate their immunity for drug addiction by analysing these LiveJournal blogs and making a personal profile based on that.

If we do that for a whole population, we can predict what part of the population will be more sensitive to drug addiction in the near future and then we can zoom in on that demographic and even on the individuals.

What differentiates the UvA from other universities?

I've spent a lot of time at different universities so I have lots of points of comparison. One of the things I appreciate at the UvA are the short lines of communication between people, disciplines and the upper management. One phone call and you have an appointment with the president of the University. And they're sincerely interested in what you are doing. They're not just administrators collecting and managing the money.

The fact that the UvA is a comprehensive university with all disciplines represented, such as the humanities and social sciences, is also vital. As I mentioned, my field requires the marriage of all these disciplines.

Links:

<http://staff.science.uva.nl/~sloot/> Peter Sloot's homepage
<http://www.virolab.org/> - Virolab homepage

