Warwick Centre for Complexity Science

Newsletter Issue 2, Summer 2014

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Singapore Emerging as a Hub for Complexity Science

by Marcus Ong, 3rd year PhD student

The Centre for Complexity Science was delighted to help organise the inaugural Winter School for Complexity Science at Nanyang Technological University (NTU), Singapore. The school covered topics from Self Organised Criticality and far from equilibrium dynamics to networks and agent based modelling. One of the most interesting talks was given by Prof. Peter Sloot (University of Amsterdam). He introduced an EU wide project investigating the treatment of HIV which examined the benefits of developing new HIV drugs versus changing health and social behaviours. This very ambitious project saw the development of a multi-scale model of HIV from the genome to human behaviour. Using this model they discovered that in large cities social policies outweigh medical improvements in the treatment of HIV. He also introduced some fascinating work on criminal networks. By examining the illegal production of cannabis in the Netherlands, he showed that criminal networks are highly static. Consequently, if authorities target highly connected nodes (criminals), when the networks re-order they may become more efficient.

The school also provided an excellent prelude to the establishment of a Complexity Institute at the university; the first in South East Asia. Such an auspicious occasion was marked by a conference on “Hidden Connections”, with such distinguished guests and scientific luminaries as Prof. Lord Martin Rees (Astronomer Royal, University of Cambridge) and Prof. Arieh Warshel (Nobel Laureate, Chemistry 2013, University of Southern California). The first presentation was given by Prof. Doyne Farmer (University of Oxford) - “An Evolutionary View of Technological Progress”. Whilst economists have recognised that technological improvements are the primary drivers for economic growth our current understanding of how they improve are poor. Prof. Farmer develops our understanding of this process by showing that there are persistent differences in the improvement rates of technologies that have important policy implications. For example, solar photovoltaic technology has fallen by a factor of nearly five thousand over the pasty fifty years whilst nuclear power has increased in price. We were also treated to a talk by Prof. Lord Martin Rees. He took us from the Big Bang and the early stages of the Universe to how life may have evolved and the future of our planet. He discussed whether or not we are alone in the Universe and the impact we are having on our planet. Another notable talk was given by Ricard Sole (Universitat Pompeu Fabra). He delighted the audience with some fascinating developments in synthetic biology and robotic evolution; this even included a paper on re-growing a man’s finger!

The Warwick delegation thoroughly enjoyed their time in Singapore and would like to thank NTU for their wonderful hospitality. We hope this will lead to closer ties and collaborations in the future.

PhD student Mike Irvine presents a poster on “Fractals and persistence in ecology” at Hidden Connections

Big Bang – Theory and Practice

By Martine Barons, former Complexity student, and Elizabeth Buckingham-Jeffery, 1st year PhD student

Martine and Ben talk to students at the Science Fair

Several people from the Complexity Centre contributed to Warwick Science Faculty's stand at the Big Bang Fair held at the NEC in Birmingham 13th – 16th March 2014. The Big Bang Fair is a free to attend annual science fair for children aged between 7 and 19 to inspire them to study science, technology, engineering and maths subjects. Alistair Tucker, Ben Collyer and Martine Barons (now moved to Stats) helped to staff the Maths part of the stand and Liz Buckingham-Jeffery volunteered as a stand helper for mathematical themed stands as a STEM ambassador. A large variety of different companies and universities attended to present fun applications of science to students, including a make your own lip balm stand and programmable robots.

The maths stand offered a choice of 10 puzzles, including 'pick 15' which invited two participants to go head-to-head to select 3 numbers (one at a time, in turn, without replacement) to sum to 15 from integers 1 to 9. After several rounds, we asked which number was the best strategy to pick first. The 'reveal' on this activity was to show that the problem can be expressed in a different format, as a magic square with 5 at the centre. It is then obvious that the optimal strategy is to pick 5 first. This activity demonstrated, in a way accessible to the 11-15 target age range, that reframing a problem in terms of a problem with a known solution can make it more tractable.

Martine said, "We counted how many visitors we had by giving everyone a sticker. I was alone on the stand on Friday morning and saw about 100 young people. It was delightful to see the realisation dawn on their faces as we demonstrated that maths is more than doing sums! It was tiring to maintain smiling enthusiasm in a noisy environment without a break, but it was also great fun. I recommend being involved next year."

ESGI 100- working on real world problems

by Diana Khoromskaia, 1st year PhD student

The European Study Group with Industry is a week-long workshop where mathematicians and industrialists brood over problems that are brought along by the companies. In April, a team of eight PhD and MSc students from the Complexity Centre participated in the 100th ESGI that was held at the University of Oxford.

On the first day the problems were presented by the industrial partners and we had the rest of the day to decide which one to work on. We were impressed by the variety of problems ranging from emotion recognition software, to optimisation of sugar beet cultivation. The most popular problem was about saturation in a coalescence filter, whose purpose is to capture small drops of liquid out of a gas. The group was entirely working on a detailed fluid dynamical model to explain saturation.

Well, not entirely... One small group of 'indomitable' Warwick students developed their very own approach in terms of Markov chains and produced a simple stochastic simulation by the end of the workshop.

It was a great experience to be part of this anniversary study group, where we got a glimpse of a broad range of mathematical problems that can have a real impact on industry and society, met academics and PhD students from all over the world, and found that going out of the comfort zone of your PhD project can be fun and inspiring. If you are interested in attending a study group yourself, please visit the webpage www.maths-in-industry.org/future/.

PhD Student Tom Rafferty presents his work to the group

Are we Cooks or Physicists?

By Davide Michieletto, 2nd year PhD student

Polymers have always played an important role in the every-day life of humans. One of the most ancient discoveries and uses of polymers took place when Egyptians mixed water and ground kamut to make a plastic yet elastic compound which, once dried under the sun, preserved the nutrients for a long time. That compound is now commonly known as "pasta". From a very naive point of view, a strand of spaghetti is just a collection of many ("poly-") single units ("-mer") of starch. Because a strand of spaghetti has two ends and no other terminal or loop, it is called a "linear polymer". There exist other kinds of polymers which can take stranger shapes. They can look like stars, brushes, tadpoles and rings for example. The shape, or "topology", of the polymers, often has deep consequences on their physical properties. For example, polymers with many branches are often used in the plastic industry to produce vulcanised rubber. Here, they increase the elasticity and reduce the plasticity of materials so they do not deform at room temperature. One of the most famous linear polymers (after spaghetti!) is DNA, although it can also occur in other forms (for example, in bacteria, DNA is often found in ring form).

The fact that we use the term polymer for everything that is a collection of units, ranging from the microscopic DNA strand to the macroscopic spaghetti strand, summarises the power of the tools employed by Polymer Physics.

It is well known that when thermal fluctuations become relevant, terminal segments of a linear polymer, like the ends of a *spaghetto*, are crucial for the motion of the chain amongst other linear chains. In fact, perhaps the most well-known theory describing this is "reputation model". Here, one imagines a very dense solution of linear polymers as snakes slithering in between other snakes. But what about polymers that have no ends? What do they do? Recently, in collaboration with Dr. Marenduzzo from the University of Edinburgh and Prof. Orlandini from the University of Padova, we have been focusing on using the tools of Statistical Mechanics to study how ring polymers cope with their lack of ends[1].

FIG. 1 Two stages of the preparation of ring shaped

We conjecture that one of the main features that distinguishes the macroscopic behaviour of ring polymers from that of linear ones is the presence of very long-lived correlations. The position of the rings in space, and that of their neighbours, matters much more than one would expect for linear polymers. This conjecture finds justification in the fact that the topology of ring polymers allows them to protrude through each-other, creating temporary, yet very strong, obstacles which hinder their free motion. We tested this conjecture by means of extensive Molecular Dynamics simulations[2].

FIG. 2 The bundles of ring shaped spaghetti after the cooking. In the background, the classical condiment for any pasta: extra virgin olive oil and parmesan.

Imagine picking a very long elastic band and threading it with another very long elastic band. The thermal motion of the first band (along its axis) is confined by the presence of the second until it diffuses away and removes the threading. This process can take a very short time if the protrusion is short and only two chains are involved. However, it could take an exponentially long time if all the chains in the system are involved and the chains are very long. The simulations we performed showed only hints of the emergence of a spanning network of inter-penetrating rings and of exponentially long relaxation times. Our findings strongly suggest that in the limit of long rings and large systems, the rings will eventually get stuck because of the many (hierarchical) topological constraints. We call this state a "topological glass".

Unfortunately, there are strong limits on the number and length of rings that we can simulate with modern computational resources. In our case, we study rings that are roughly a thousand times shorter than the corresponding DNA molecules. On the other hand, we have (almost) unlimited provisions of flour, water and eggs. This is why we also tested our conjecture on a bowlful of ring shaped spaghetti. One way of picturing a ring shaped polymer is by taking a (cooked) strand of spaghetti and gluing the two ends together, as in Figure 1. We made handmade egg-based ring shaped spaghetti (or "linguine", to be formal) and cooked them in order to reproduce a solution of ring polymers subject to thermal fluctuations. What came out was a bundled, entangled and highly inter-penetrated network of pasta, as in Figure 2.

In this respect, our cooking experiment strongly encourages us to study longer rings and larger systems. We cannot state that our cooking experiment is the final proof that the topological glass emerges, but without doubt we can say that ring shaped pasta is much harder to eat than standard spaghetti!

[1] D. Michieletto, D. Marenduzzo, E. Orlandini, G. P. Alexander, M. S. Turner, Threading Dynamics of Ring Polymers in a Gel, ACS Macro Lett., 2014, 3, pp 255-259

[2] Davide Michieletto, Davide Marenduzzo, Enzo Orlandini, Gareth P. Alexander and Matthew S. Turner, Dynamics of Self-Threading Ring Polymers in a Gel, Soft Matter, 2014

The Centre's Annual Retreat

by James Skinner, MSc student

Students and staff from the Centre for Complexity Science recently retreated to St. Briavels, Gloucestershire, for three days of presentations, discussions and the opportunities to network and strengthen collaborative links. PhD students presented their research, sparking discussion and informing other members, particularly the MSc students, of the doctoral research being conducted. This was also taken as an opportunity to improve presentation skills; written feedback was provided by audience members enabling presenters to better understand their strengths and weaknesses.

Two external speakers were invited; Dr Allyson Reed (Warwick Corporate Relations) was able to give valuable advice on advancing as an entrepreneur, which is particularly relevant to such an interdisciplinary and real-world problem oriented Centre, and Nicholas Beale (Sciteb) gave insight into the career directions a mathematician may take outside of academia.

The Complexity retreat was greatly enjoyed by all. Improved familiarity with the work and the people in the Centre has better enabled the free flow of ideas and discussion.

Change of Administrator

by Robert MacKay, Centre Director

Jen Bowskill receiving a leaving gift as a sign of gratitude for all her help

Our administrator Jen Bowskill is moving on to the Academic Registrar's Office after nearly three years with us. We are grateful for all she has done for us and we wish her well in her new post.

We look forward to welcoming our new administrator Heather Robson, who will be joining us from the International Office. We continue to be ably assisted by Debbie Walker and are most grateful for her for holding the fort during the changeover.

New administrator Heather Robson

Recent publications from our staff and students:

- Bell, Gavin R. and **Dawson, Peter M.** and Pandey, Priyanka A. and Wilson, Neil R. and Mulheran, Paul A., Size-dependent mobility of gold nano-clusters during growth on chemically modified grapheme, APL Materials, 2, 012109 (2014)
- Andrew J. Black, **Thomas House, M.J. Keeling**, J.V. Ross, The effect of clumped population structure on the variability of spreading dynamics, Journal of Theoretical Biology, (2014)
- Manuela L. Bujorianu and **Robert S. MacKay**, Complex systems techniques for cyber-physical systems: position paper. In *Proceedings of the 4th ACM SIGBED International Workshop on Design, Modeling, and Evaluation of Cyber-Physical Systems* (CyPhy '14)
- **Davide Michieletto**, Davide Marenduzzo, Enzo Orlandini, **Gareth P. Alexander** and **Matthew S. Turner**, Dynamics of Self-Threading Ring Polymers in a Gel, Soft Matter, 2014
- **Thomas Machon** and **Gareth P. Alexander**, Knotted Defects in Nematic Liquid Crystals, Physical Review Letters, (2014)

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