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Making materials matter

THE AUSTRALIAN NATIONAL UNIVERSITY

New ways of knotting networks

You'd be amazed what a twist in space can do

(left) Toen Castle holds up a basic knot: "A knot is a loop in space that you can't straighten out into a normal circle in space without passing it through itself"

Toen Castle believes we have much to learn (and gain) by subtley modifying the connections between the nodes that make up a network, be that network a crystal lattice or a molecular material. His specific interest, which forms the basis of his PhD studies in the Department of Applied Maths (RSPSE), lies in understanding how networks of points can be entangled without changing the basic order of connection. These networks are connected in the same way but possess completely different properties.

"Understanding the connections between a set of nodes can give you an understanding of how the system works," says Mr Castle. "I've always been amazed by the way you can connect nodes and the networks they form. I'm particularly interested in the subtleties of the connections between nodes. Each node may only connect to a few neighbours but it's the nature of the neighbourhood and its context that can be just as important. That neighbourhood may connect to other neighbourhoods in such a way that the global behaviour of the entire network changes. So, it has big implications for how things work.

"For example, in our global village today things are very different to how they once were. In times gone by it might be that you know 500 people but they all live in neighbouring villages. But now you might know 500 people equally well but some are scattered all around the world and some are local. All these networks function at different levels, scales or hierarchies depending on which models you're viewing them through. However, if you look at what the connections mean for things like disease transmission or information dispersal, you can see that this global structure can make a massive difference even though on an individual basis we may not be in communication with more or less people than we previously were."

Embedded in space

"This field of research started with people looking at networks that are embedded in space," explains Mr Castle. "These approaches are relevant to a lot of physical systems such as crystals because crystal lattices are simply networks of atoms and bonds embedded in space.

"However, while quite a large amount of interest has been directed towards considering what is connected to what in these networks, not so much attention was given to the more subtle effects of the manner in which connections could be made. This is what I focused on for my PhD.

"And when I looked at how connections might vary I began to concentrate on features that these bonds within the network can have. It's possible to conceive of a tangling of complex structures, of things being connected in ways that are knotted or linked.

Knot basics

"A knot is a loop in space that you can't straighten out into a normal circle in space without passing it through itself," explains Mr Castle. "Knottedness is a fundamental property of a loop in space. Either it's just a simple loop, like a circle, or else it's got

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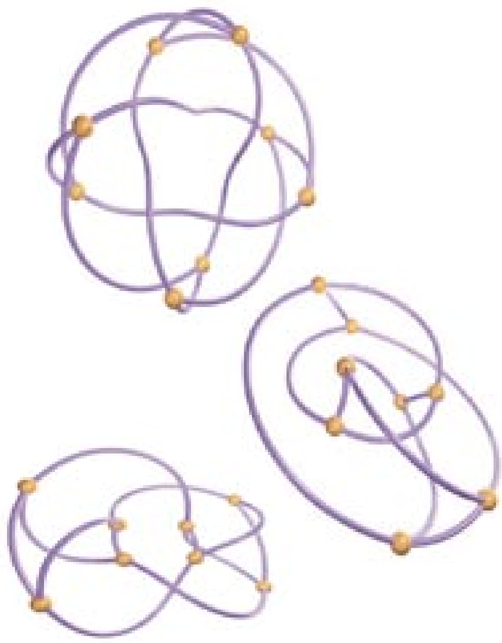

Each of the knots pictured here has the same connectivity as a cube (8 nodes connected by 12 edges) yet each arrangement is startlingly different. By understanding the language of loops and knots Toen Castle believes we can create materials with new properties.

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some form of structure in it that can never be removed unless you pass edges through each other.

"If that's prohibited, say in a chemical you've got two hydrocarbon chains that can't physically pass through each other, then you can see the relevance of the mathematical concept to the practical situation.

"Links are related but fundamentally different structures to knots. In the case of the link you have two separate components and they're joined together but unable to separate, which is a very similar thing, but involves two components instead of the one.

Knots and links add a whole new dimension to the manner in which a network performs. You can have two networks with the exactly the same connectivity but which are linked or knotted in different ways making them behave in different ways.

"This is more than just academic abstraction," says Mr Castle. "For example, we've found crystals which contain linked cycles. These are cycles of atoms connected by chemical bonds; and even though neither of the cycles bonds to the other they still interpenetrate each other in space.

"There are some very subtle things occurring here and if you see two cycles that pass through each other it's very clear that physically they will behave quite differently to two separate cycles, just because they're physically linked. This same difference shows itself in comparing a chain with a bunch of unconnected metal loops.

"And you can generate these kind of networks with the same connectivity of a normal crystal."

The tangled diamond

"For another example of entanglement and connectivity we can look at the diamond crystal lattice network," says Mr Castle. "The basic diamond network has one atom connected to four others. The first is at the centre of a triangular pyramid and the others are at the corners. If you connect these up in an infinite array you get a diamond lattice.

"However, if instead you keep the three bonds which point towards the base of the pyramid, but replace the upwards-facing bond with a downwards-facing one, then you make an array out of these repeating units. You now have a diamond structure where all the layers are interwoven with the layers above and below. Clearly this structure is massively different from the standard diamond structure, and will have completely different properties, however if all you consider is whether 'this atom connects to that one' there's no difference in the two structures. There's the same connectivity between the original diamond and the tangled diamond.

"And this isn't just a hypothetical idea because the tangled diamond structure is real, it's been made. They saw the potential for it to exist so they worked out a way to create it. The tangled diamond is still an experimental material but there's a lot of interest in developing its potential."

A language of knots

"The thing is, it's very difficult to describe this area of tangled networks," observes Mr Castle. "There's no natural language that's become commonplace to describe exactly what's going on. You can wave your hands and say 'look its tangled', 'look the layers are interlocked with each other', but in terms of a quantitative science we're really searching for a unique language that describes exactly what's going on. That doesn't exist at the moment and that's what I'm trying to do with my research.

"The aim is to come up with a framework or language by which this understanding of entanglement can be taken further and applied to different networks.

"And to be a good language, it must describe the fundamental tangling features that can be present in a network. So, by finding a conceptual language that can describe the tangling you can put together words from this language and generate novel structures.

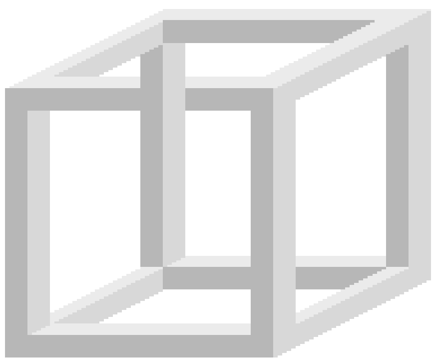
"The language we're generating is still rudimentary but we've made some real progress."

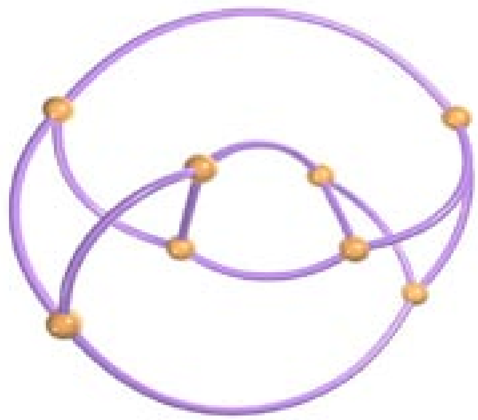
A tangled cube

To build a language of entanglement, a language of network knots, you ideally begin with a basic structure and explore what's possible in terms of entangling it without changing its connectivity. And for Toen Castle, that structure is a cube.

"Most people conceive of a cube as a solid square block with six sides," says Mr Castle. "For our purposes, ignore its volume and surface and think just of the edges as a wire frame with eight corners. The cube is a very interesting structure because it's so common and hence we have a good intuitive link with it. However, it's also complicated enough to start to display some interesting properties in terms of the potential ways to tangle it.

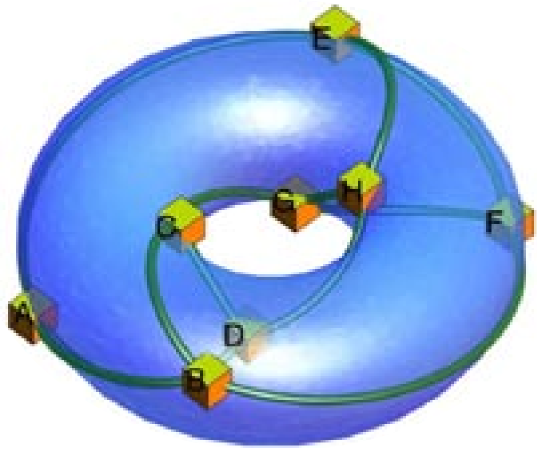
"It's also a common building block in crystal lattices. In complex structures, modern crystallographers may finds certain repeating cubic and tetrahedral units inside the crystal structure and then represent





The optical illusion of 'the impossible cube' (above), with a wire-frame version (upper right) and an embedding of the wire-frame onto the doughnut (right). An impossible cube is really a form of a knotted cube. You can't embed an impossible cube into a sphere as you can with a normal cube. However, you can embed it into a doughnut. "In terms of knottedness, the sphere isn't an exciting place to live." says Toen Castle.

By figuring out ways that simple arrangements can be knotted in different arrangements you open up rich new possibilities for networks and behaviour.



the structure in terms of those cubes and tetrahedra or prisms just to simplify their work. The work we do applies to all these basic polyhedra but we really have focused on the cube.

"In terms of knots, a cube is better to work on than a tetrahedron. A tetrahedron only has four points and six lines and there aren't actually two distinct cycles (loops) in the tetrahedron because of the constraints of the actual connectivity.

"Whereas with the cube you can see it has a top and bottom, left and right, front and back. If you think about it, that's three sets of cycles that are disjoint from each other. Because they are separated from each other you can twist them up and entangle them. Instead of being entirely separate they can interlink each with each other. And as well as that it's large enough with enough points and edges to display some interesting knotting behaviours."

How to build an impossible cube

To understand how you might tangle a cube it's helpful to consider the impossible cube. It has the same connectivity as your normal cube and yet it's completely different. It's tangled.

"Many people will have seen the impossible cube in books of optical illusions," says Mr Castle. "It's an optical enigma in which the lines and perspectives seem wrong. It seems impossible because there's no way you could embed this version of the cube onto a sphere. By that I mean that there is no way to conform the wire-frame cube onto the surface of a sphere. The cube embedded on a sphere - a normal cube - can't have any knots or links.

"If you consider every way of starting at a certain vertex of the cube, traveling along edges and coming back to your original vertex without doubling up, there's no way that you can make a cycle that will be anything other than a simple loop; there's no way it can have a knot in it, being embedded on the sphere just prohibits it. In terms of tangling, the sphere isn't an exciting place to live. Similarly, there's no way to find two distinct cycles that actually link together, they're always just on opposite sides of the sphere.

"However, it's quite easy to embed an impossible cube onto the surface a doughnut. Another way of saying that is that there's only one way you can embed a cube into a blob but there are many interesting ways you can embed that cube into a blob with a hole in it (that is, embed it into a doughnut or torus). And this is how you build your language of entanglement.

Building tangled skyscrapers

And what's the value in creating a tangled cube?

"If you give yourself an array of cubes, one sitting on top of the other, that array is going to have certain structural properties," explains Mr Castle. "Consider a sky scraper, for example. It might be modeled by a bunch of floors or rectangular prisms, each sitting on top of each other. The properties of the building might be its strength and flexibility. Or, if were talking about a molecule rather than a skyscraper, then the property we might be interested in might be its surface area or reactivity.

"However, if you were to build your skyscraper or your molecule out of knotted cubes you'd have a building with radically different properties. Of course, it's not all that easy to conceive of these different building blocks. So what we're searching for is to produce a variety of structures with different tangling properties, and various symmetries so that we can provide chemists or whomever with a database of components that they might consider.

"If researchers can link favourable chemical reactivity property with a certain structural feature, for example, then we can show them what structures they might be interested in making to produce that effect. By developing this language to describe the tangling structures and exploring possible entanglements we can provide chemists, molecule makers, and material scientists with a wealth of alternative structures to consider."

The value of this work is that if you know it's possible to build a network with a certain entanglement, you open up the possibility of that structure actually being created. The tangled diamond structure, for example, was conceived before it was created.

Knots beyond the doughnut

Having worked out a method to tangle basic structures by embedding them in doughnuts, Mr Castle is now looking to explore more complex entanglements.

"The next step in this process is to step up from the simple donut, a torus with one hole, to more complicated shapes like a donut with many holes," says Mr Castle. "This is a very big challenge because the mathematics of multiple-hole donuts is quite different to single holed donuts.

"You get a vast amount more of structural complexity when you use multiple-holed donuts. You can chop them up and peel them open up into repeating units in any number of ways giving you very interesting twisting and tangling patterns."

While conceiving a language of entanglement might sound a little abstract, Mr Castle is a firm believer in the real world application of this work.

"While this work engages with some very sophisticated concepts, there's real potential for applying this work," he says. "Indeed, I think I get the best of both worlds. I have the enjoyment of being a theoretical physicist playing with some very elegant and abstract ideas, but I know these ideas will be very useful for other scientists and engineers in coming years.

"Possible applications of this work include the creation of new crystal structures and new materials. Hydrogen storage is another big application of this work because hydrogen, being a gas, takes a lot room to store but hydrogen has an affinity to stay at the surface of some materials. So, some mineral structures, like zeolites, have lots of big rings in its structure, and are excellent for hydrogen storage. Engineers are looking to improve this storage structure and scale it up, however when they do this, the rings are prone to collapse around each other – and entangle. So, researchers are now looking to build similar structures that have the same features, but which are more stable and avoid tangling.

"And there are other ideas as well for how we might employ tangled networks and structures. Though I suspect that the best ideas on how to use this knowledge haven't even occurred to us yet."

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Understanding the many in which networks can knot may open up new ways of storing hydrogren gas.

Becoming a Master of Nuclear Science

Nuclear science is back on the national agenda and ANU is doing its best to inform the debate with a new Master of Nuclear Science degree.

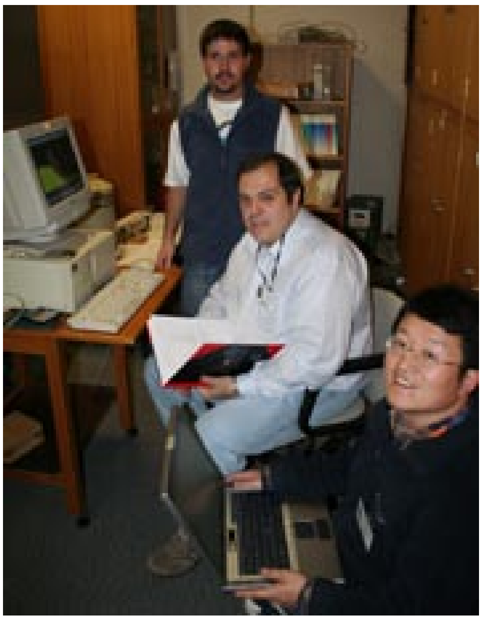
Looking down the particle accelerator, part of the university's considerable investment in nuclear technology. ANU has always led the way in terms of research in nuclear physics, now it's trying to inform the broader debate on nuclear science with a new Master of Nuclear Science degree.

That ANU is running Australia's first Masters degree in Nuclear Science probably comes as little surprise. After all, the university is one of the nation's leading research institutions in this field. A little more surprising to some, however, is that physicists don't dominate the students electing to do the course – indeed there's only one student with a physics background in the first year intake. And yet if you stop and think about nuclear science and it's role in the world, maybe that's not a bad thing at all.

In an energy-hungry world that's choking on its own emissions, talk of nuclear science is back in a big way, be it as a supply of alternative energy or a source of weapons of mass destruction. But dig a little into the rhetoric and it quickly becomes clear that there's a lot ignorance on all sides of the debate.

"It's true, nuclear science is back on the national agenda," says Professor Aidan Byrne, Head of the Department of Physics and one of the leading researchers in the Department of Nuclear Physics at RSPSE. "However, while people are very very divided about many aspects of nuclear energy, it's clear that people are not well informed about nuclear issues in general.

"Now, ANU has been for a long time the place in Australia to do nuclear physics so we saw it as a natural part of our role to make sure that we're available to educate both the public and people in government on this topic. The ANU is a credible and independent authority. It's a role that we treasure and take very seriously. We are separate from government statutory bodies and industry organisations, we are really as independent as you can be in this debate."



Three aspiring students in the new Master of Nuclear Science (from the left): Chris Humphrey (from ANSTO), Rudolf Dominguez (with a background in archaeology) and Thomas Teng (with a background in geology). They reflect the diversity of people entering the new degree.

So ANU is a storehouse of nuclear expertise, but it's also a store of nuclear technology and hardware that's taken many decades to accrue.

"The Department of Nuclear Physics, under the direction of Prof George Dracoulis, is the only place in Australia that is doing experimental nuclear physics at an international level," observes Professor Byrne. "That's also something to be very proud of, that we're competitive internationally. Our facility here has been developed over several decades and that's allowed us to maintain our international credentials in the area.

"However, it's really becoming clear to us that Australia as a whole does not have much nuclear capacity. And this was really brought home to us by people coming to us asking us to help them with nuclear issues. It's very worrying to realise that there are so few people around these days who have a sound knowledge of nuclear issues.

"Now, we'd been talking for many years of creating a masters program in nuclear science but until two or three years ago there wasn't the demand for it, people simply weren't interested in supporting a nuclear science course. That changed a few years ago when people realised in terms of the bigger energy picture that nuclear power may be one of the few ways that we can generate electricity on a very large scale with a minimum, though not zero, amount of CO2 produced in the process.

"So staff in the Department of Nuclear Physics started re examining the nuclear science issue and we sat round and discussed how we might create a masters of nuclear science program that might make an important contribution to the broader debate. And we could see that it wasn't appropriate that we just had a masters of nuclear physics because ANU already trains physicists, indeed we do nuclear physics at all levels from undergraduate through to post doctoral. We're already experts in that area so our aim with this new masters was to create a qualification that's much broader. And I think we've achieved it.

"It is not just about nuclear physics, it's a multidimensional issue. On one level there's the policy, and that's another area that ANU is very strong on with our Strategic and Defence Studies Centre and the expertise there. And for that reason our masters program has a course delivered by that group about the politics of nuclear energy, the implications of the non proliferation treaty and what are the

Nuclear sleuthing

In addition to creating the Master of Nuclear Science and being proactive in the national debate on the nuclear science, the Department of Nuclear Physics also runs a variety of workshops and training course for a range of different groups. One of these courses is an annual Workshop in Nuclear Techniques for students in the Medical Physics Program at the University of Wollongong. The workshop provides an opportunity for the students to get a first hand experience in the methods of nuclear measurements and in the use of large accelerators.

"As part of the workshop, the Wollongong students actually drive the particle accelerator to figure out an unknown metal foil," says Professor Byrne. "It's quite a challenging exercise that's been developed over several years.

Greg Lane explains to a group of Wollongong University students how they might interpret the data.

"We require them to determine what an unknown foil is made from. They bombard it with the particle beam which fuses an unknown nucleus. So they've done transmutation and we've given them one ingredient, but they don't know what the other ingredient is and they have to use the nuclear techniques of detection to determine what they've made and then infer what the unknown material was. They measure the radiation from the nucleus they've produced, and this radiation is characteristic of what you've made by the energy of the radiation but also its decay properties. There are a whole lot of dimensions to this problem and it's quite a challenge to figure it out.

"This is a wonderful hands on learning experience though it takes a lot of effort on our half to set up. However, the effort is worth it because at the end of the week when they're giving their presentations you realise that they've learnt a of a lot of nuclear physics in the process.

"Our Masters students and some of our ANU PhB students also have the opportunity to go through this exercise."

The Department of Nuclear Physics has devised an exercise in which students use the massive 14UD particle accelerator (part of which is shown above) to bombard an unknown metal foil with heavy ions to deduce what the foil is made of. Aidan Byrne tutors the students on the operation of the particle accelerator.

implications of Australia selling uranium to China and India. These are complex issues.

"And another aspect that we've included is the fuel cycle and the geology of uranium, and this has implications for waste storage. Professor Richard Arculus is the person who will be contributing here and he's one of the nation's experts on uranium geology.

"And then the other people we have on board for the program is Sue Stocklemayer and the Centre for the Public Awareness of Science, because again the perception and awareness of nuclear matters is very important in the entire debate. If Australia were ever to go down this nuclear path it'd better get its education right, and it'd better have a sensitivity to the anxieties that people have to this science.

"And one of the measures of success for that is that we're not actually getting students for this program who are physicists, we're actually getting people from a broad variety of backgrounds. That includes an archaeologist, a geologist, someone working in the area of quarantine, and a person from ANSTO.

"That's a fascinating thing about this course but from a teaching point of view it's also quite a challenge. I don't know how it will develop in the future but I think it's very important to maintain this level of information to the broader community and specifically to decision- and policy-makers in government.

"We're learning all the time, including from the students who are doing this new masters degree. And a good example of this is that one of this year's students has a background in psychiatry , and one of the questions that he is exploring is what is the psychology of the nuclear debate, what is the psychology of fear if you like. He can bring a completely different perspective than someone trained in physical science can bring to this debate, so this is a two way process."

It may be early days for the program but if you believe in the old adage that strength lies in diversity, then the new Master degree has a lot going for it.

More info:
http://wwwrsphysse.anu.edu.au/nuclear/

and click on Master of Nuclear Science under study opportunities

Chris Humphrey at work on an exercise to determine the geometry of a particle detector.

Scoping research for the next generation of nuclear reactors

Last month ANSTO ran a nuclear power technology workshop at its Headquarters at Lucas Heights, south of Sydney, to explore future possible directions for nuclear energy research and possible collaborations with Australian universities.

ANSTO, through the Australian Institute of Nuclear Science and Engineering (AINSE), intends to support integrated, multidisciplinary projects that will address research challenges relevant to the GNEP (Global Nuclear Energy Partnership) and Gen IV research programs (see box on What is Gen IV nuclear energy).

ANSTO has identified four research areas of particular interest:

-development of advanced wasteform technologies;

-structural integrity of nuclear structural materials;

-novel nuclear materials; and

-nuclear reactor performance modelling.

Clearly there is a strong materials focus in this range of topics, and materials science is expected to play an important role in developing future nuclear technologies.

The integrity of nuclear structural materials relates to the fact that Generation IV reactors will operate at higher temperatures and pressures than conventional reactors and will likely employ fast and epithermal neutrons to further enhance their performance.

Materials employed in these reactors will therefore be subjected to a radiation environment well beyond current experience, a situation that will be further exacerbated by the need for relatively long service lifetimes in such installations. Irradiation of materials is known to produce defects that cause void-swelling, phase separation and diffusion, and there is a need to develop advanced methodologies to predict micro-structural evolution and remnant life. This research area will also look at the optimisation, assessment and qualification of advanced nuclear structural and fuel cladding materials for use in these high stress environments.

Novel nuclear materials examines materials that have not traditionally been used in a nuclear engineering context. Examples include ceramics, ceramic composites, intermetallics and a range of performance enhancing thin coatings.

What is Gen IV nuclear energy

The world's current state-of-the-art nuclear reactors for power generation are advanced light water reactors or Generation III designs. Gen I reactors were the first prototypes following the Second World War and Gen II were the first commercial power stations built up until the mid 90s. While it is envisioned that superior versions of Gen III reactors will be built up until 2030, the goal at the moment is to develop the technology for new ambitious Gen IV reactors to replace Gen III reactors beyond that. The primary goals of this next generation of nuclear reactors is that they're safer, cheaper to operate, produce a minimum of waste and will prevent the proliferation of nuclear material for weapons.

According to the US Department of Energy, today there are 441 nuclear power reactors in operation in 31 countries around the world. They generate electricity for nearly 1 billion people, and account for approximately 17% of worldwide electricity generation. Another 32 reactors are presently under construction.

Participants of the October workshop. In addition to ANSTO and AINSE personnel, representatives from ANU, Curtin, Deakin, Melbourne, Newcastle, Queensland, RMIT, Sydney, NSW, UTS and Wollongong universities were present.

ANU was represented at the ANSTO workshop by Professor Rob Elliman from Electronic Materials Engineering and Dr Zbigniew Stachurski from CSEM.

Discussions on possible projects arising from the workshop are ongoing, though it is hoped that outcomes may be announced over the coming year.

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