

ScienceWise

SCIENCE MAGAZINE OF THE AUSTRALIAN NATIONAL UNIVERSITY



Winter 2010

- The drumming parrot
The extraordinary behaviour of Cape York's palm cockatoos
- Getting amongst nature
Following a science career outside the lab
- Understanding the Dance of electrons
Applying quantum mechanics to chemistry
- Pluto and the potatoes
Could there be ten times as many Dwarf Planets as we currently think?
- Mastering the hazards
New course aims to train natural disaster managers
- A singular problem
Mathematics in the search for the origins of the universe
- Saving an evolutionary icon
How atmospheric nuclear weapons testing may help conservation of the lungfish

Volume 7 No.3



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4

THE DRUMMING PARROT

The extraordinary behaviour of Cape York's palm cockatoos



7

GETTING AMONGST NATURE

Following a science career outside the lab



8

PLUTO AND THE POTATOES

Could there be ten times as many Dwarf Planets as we currently think?



12

MASTERING THE HAZARDS

New course aims to train natural disaster managers



14

UNDERSTANDING THE DANCE OF ELECTRONS

Applying quantum mechanics to chemistry



16

A SINGULAR PROBLEM

Mathematics in the search for the origins of the universe



18

SAVING AN EVOLUTIONARY ICON

How atmospheric nuclear weapons testing may help conservation of the lungfish

Back cover science quiz answers

C (01)
 V (6)
 B (8)
 B (7)
 D (9)
 A (5)
 D (4)
 A (3)
 C (2)
 B (1)

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Cover Image: Stefanie Oberprieler

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The editor's corner



What Pluto can teach us about education

Over the past few years there's been a great deal of media attention devoted to the International Astronomical Union's decision to downgrade Pluto from a planet to a dwarf planet. Why this relatively obscure piece of modern science has attracted so much attention is quite interesting, and I think can tell us a lot about the perceptions and motivations of science.

Most of us were taught at school that the Solar System has nine planets. It was one of the things everyone was so familiar with. So suddenly being told that's wrong is quite a shock. It's almost like being told that hydrogen is no longer the first element on the periodic table. But it's also different. For hydrogen to have its periodic status changed, there would have to be something fundamentally wrong with science. Pluto on the other hand, hasn't changed one little bit nor has its place in our understanding of the cosmos changed all that dramatically. Everything we know about Pluto such as its location, its orbit and its mass are pretty much the same as we believed back in 1930. All that's changed is that we now know Pluto is just one of many Trans-Neptunian Objects. So it's not any different, it's just not as unique as we once thought.

The same principle applies to things like relativity and quantum mechanics. Neither prove Isaac Newton's laws of motion wrong. They just show that Newton's laws are only one part of the big picture. True under certain conditions, which happen to be those we're most familiar with; medium scales and low velocities.

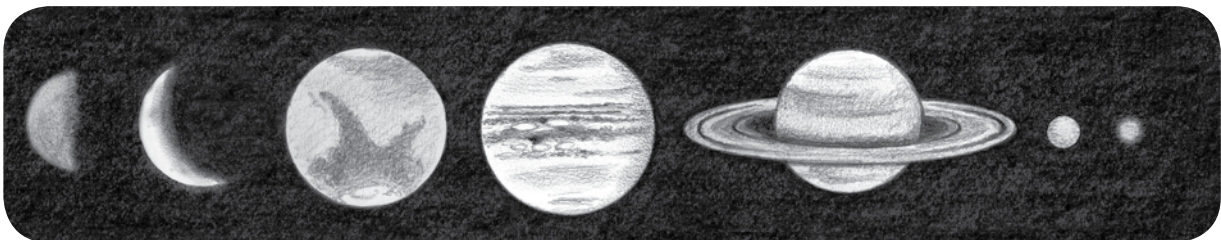
Science is just like that. It's not touted as an absolute truth, a dogmatic statement of 'this is so'. Or at least it shouldn't be! It's a summary of the present state of our ever evolving knowledge about the universe.

But I think in dismissing the furore about renaming Pluto as mindless media hype is perhaps wrong too. The fact that so many people care touches on something that we often neglect in professional science and that is the ability of the world to evoke emotional responses in us. After all, if we had no emotional connection to the world around us our only motivation to do science would be mere academic curiosity. Some of the greatest feats of science and engineering have been achieved by people who care passionately about a particular thing be it curing a disease or exploring outer space.

I think it's vital that we also look for such passion and commitment in the next generation of scientists as much as we look for academic prowess. A genius that couldn't care less is no match for a person of average intelligence who is passionately devoted to a cause. This is a point several of the young scientists interviewed in this issue also emphasise.

Different people also have different kinds of intelligence. Some of my contemporaries at university were brilliant at learning and regurgitating facts but had little ability to do independent research. Others that were mere plodders in the course-work proved to be exceptional in their later research careers. And of course there were those who were brilliant at both.

There's never going to be a one size fits all approach to education but I'm encouraged to see an increasing emphasis being placed on enthusiasm and passion. If we care about Pluto, maybe we care about other things as well!



Back in 1930 the Solar System consisted of nine recognised planets, Mercury, Venus, Earth, Mars, Jupiter, Saturn, Uranus, Neptune and of course Pluto (the microscopic dot to the right). Back then planetary science was still quite largely based on visual observations that could be made through ground based telescopes. Only with the advent of and space probes, space based instrumentation and adaptive optics have we been able to really get to grips with the true nature of our patch of the universe.

The drumming parrot

The extraordinary behaviour of Cape York's palm cockatoos

Palm Cockatoos (*Probosciger aterrimus*) are large smoky-grey parrots that can grow up to 60cm tall and weigh in at over one kg. They're native to Papua New Guinea and the Cape York Peninsula of northern Australia. We do not know the size or age-structure of the population on Cape York, and loss of habitat from mining and inappropriate fire management are possibly threatening these incredible animals.

Christina Zdenek is a Fulbright Postgraduate Fellow undertaking a graduate degree at the Fenner School of Environment and Society. She's studying Palm Cockatoos with aims to conserve the species, but the wider project aim is to ensure conservation benefits for the whole of Cape York Peninsula.

"It's really important to be able to track individuals within a population in order to do effective conservation," Christina says. "Palm cockatoos, and parrots in general, are very long-lived species and because of this, any impact on the species could be masked for decades by a persistent, but aging, population. Exacerbating this problem is the fact that palm cockatoos are very slow breeders and also have low reproductive success, so recovery would be slow, if even possible at all. So if we just monitor the number of individuals, without knowing their age or how many are breeding, we could easily be missing a big part of the story. So what I'm looking to do is develop a way to identify individual birds without harming them or interfering with their normal lives in any way."

With some species this can be a relatively simple thing to do – trapping them and putting a coloured leg-band on them or fitting a temporary tracking collar. However this doesn't work well with parrots in general and especially with palm cockatoos because they are very difficult to catch and become highly over-stressed when they are caught.

"Palm cockatoos are quite sophisticated birds. They have an enlarged forebrain, compared with other birds, which presumably gives them enhanced cognitive abilities. This may explain why they react so poorly to trapping and tagging," Christina explains. To avoid such problems, she is developing a non-invasive identification technique based on the calls of individual birds.

"Palm cockatoos are socially complex and their vocal repertoire reflects this," she says. "On Cape York, Palm Cockatoos have a vocal repertoire made up of various syllables that are mixed and matched in different combinations. This mixing and matching of syllables in their vocal repertoire may be unique among the cockatoo family. Their calls are also not raucous,



Christina Zdenek takes notes in the field. Photo by Roland Seitre

harsh calls like other cockatoos (picture the Sulphur-crested Cockatoo calls), but instead are pleasant-sounding whistles. Palm cockatoos even appear to mimic two other local bird species– something that is common in captivity but has rarely been noted for parrots in the wild. One of my favourite Palm Cockatoo calls sounds almost exactly like a human saying 'hello.'"

Just like human voices, it is likely that each individual palm cockatoo has its own specific way of making each sound. The differences may be subtle but the variation in the way a particular bird makes a call is likely to be unique enough to recognize individuals.

Christina spends up to six months of each year living in a 2-walled shelter-shed "humpy," adjacent to the rainforest in the remote wilderness of the Cape York Peninsula. The remote sites are only accessible during the dry season with a 4-wheel drive vehicle (or a motor-bike, which she will use for next field season). In the wet season the rivers swell their banks and the dirt tracks are frequently washed away or under metres of water. "One of the things I had to learn before beginning this project was how to handle a large four wheel drive in rough off road conditions," she says, "That was pretty fun."

Christina tracks the cockatoos and records their calls with a sophisticated directional microphone and digital recorder. Then back at base she analyses these sounds using software that maps the frequencies, amplitudes and timing of each call. She is using nesting birds over time to build a library of bird-calls to use for a non-invasive identification method with which to study palm cockatoos.

Although the cockatoo's calls are interesting, they are not the only way these birds use sound to communicate.

Palm cockatoos have a habit of drumming. On occasion, male palm cockatoos use their powerful beaks to fashion a



A nesting-pair of palm cockatoos change over incubating duties for the day, otherwise known as nest-exchange. Female on left, male on right. Males incubate during the day, females at night. Lockhart River, Cape York Peninsula, far north Qld. Photo by Martin Willis and Christina Zdenek

Left: Satellite view of Australia's Cape Your Peninsula - native habitat of the palm cockatoo.

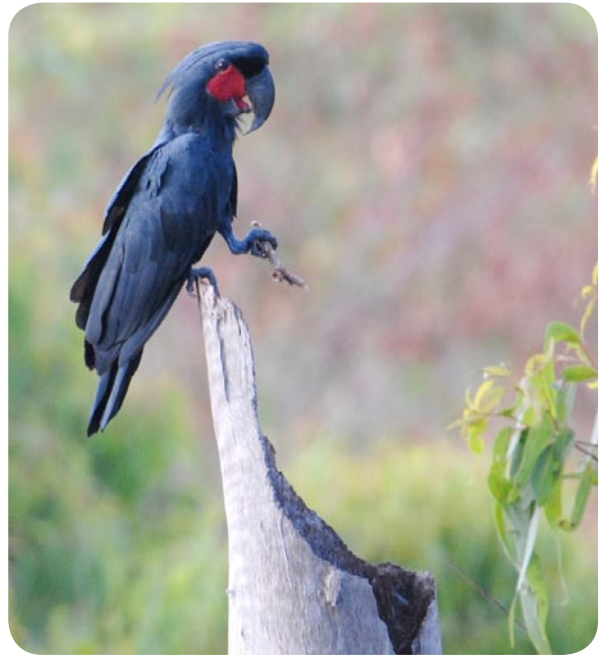
drum-tool from a live tree branch. They then fly over to a tree hollow and beat on its edge, making a distinctive sound that can be heard 100m away or more. This behaviour makes palm cockatoos particularly unique among wildlife in that they create a tool for a purpose other than eating as the end goal. "Although drumming was first described by G.A. Wood in 1984, today, 26 years later, we still can only hypothesise why they do it. Perhaps they drum to get a clue of the quality and durability of the hollow. They could be doing it to mark their territory, or maybe even to show off their cognitive abilities to a prospective mate." This wonderful mystery is something that Christina hopes to solve.

"Even though this parrot is very interesting and charismatic, we still know relatively little about them," she says, "We still don't know how long they live in the wild or when they first reproduce, which are two key factors in our understanding of their conservation status and risk to extinction. They may be threatened by bauxite mining on Cape York, but since palm cockatoos live for so long, even a major reduction in good quality nesting trees (and therefore their opportunity to replace themselves into the future) could go unnoticed until it is too late."

Aside from mining, a major threatening process is inappropriate fire regimes. Late dry season burns are typically more intense and widespread than early season pre-scribed burns because they have a higher fuel load that is also cured. This kills more trees than early season burns and even releases more carbon into the atmosphere. These late dry season burns may also lead to declines in termite populations, which are a key part of the nesting hollow-formation process. Over the course of decades, termites eat out the middle of a tree, and this forms a mud-gut that eventually gets washed out, thereby creating a possible nesting hollow. And since palm cockatoos are obligate hollow-nesters, the amount of good quality hollows determines the amount of nesting birds there can be in the population.

However, in the world of tree hollows though, not all hollows are equal. Palm cockatoos prefer to nest in slightly off-vertical hollows of live trees, as opposed to vertical hollows in dead, but still standing, trees. Presumably, a hollow in a living tree would have better and longer-lasting structural integrity than a hollow in a dead one. This would make them more immune to both fire and cyclones, which are both a part of life on Cape York.

Although now based in Australia, Christina did her undergraduate degree at the University of California Irvine, where she funded her studies with a professional basketball scholarship. "I still enjoy playing basketball but just at this point in my life my focus is on the environment and I want to devote all my energies to this. I think it's really important that



Male Palm Cockatoo drums with a fashioned drum-tool during his territorial display on a trunk-sheared hollow. Lockhart River, Cape York Peninsula, far north Qld. Photo by George Gornacz and Christina Zdenek

we understand the issues facing natural ecosystems because it's not just wildlife that depends on them, but us too. We really need to come to grips with the science so that we can be sure that the management strategies we make for preservation achieve maximum effectiveness," she explains.

"Although my specific research is focused on identification of individual palm cockatoos, what I am most passionate about with this project is the big picture of conservation across all of Cape York. Palm cockatoos are an iconic species and they can be a great flagship species to raise awareness, funding and public interest for the benefit of all the flora and fauna of the region."

As with so many environmental issues, it's only possible to make effective conservation decisions once the background science is properly understood. For example, the landscape of Cape York is a mosaic of rainforest and woodland savanna. Although Palm Cockatoos generally forage in the rainforest, they almost always nest in the adjacent woodland, where the hollows are. Knowing this enabled Christina and her colleagues to confidently recommend for the boundaries of the bauxite mines on Cape York to be at least 1 ½ kilometers before the rainforest edge, as opposed to being right at the edge of the rain forest itself. If this recommendation is taken, it would mean this ecotone would be protected, and crucial breeding habitat would be maintained for the future survival of palm cockatoos in Australia.

If you would like to receive Christina's e-newsletter, send your name and email address to ChristinaZdenek@gmail.com.

Getting amongst nature

Following a science career outside the lab

Sometimes when you think of scientists, it's easy to imagine someone sitting in a lab day in day out and never really seeing the light of day. However, such a stereotype is far from the actual lives of most young scientists, some of who travel the world in pursuit of their studies. One such person is Stefanie Oberprieler, who is in the second year of her science degree at ANU, majoring in Zoology and Ecology.

"I took a year off after finishing college because I wanted to see a bit of the world, and most importantly, have time to think about what I wanted to do with my life. During that time I worked in an animal rehabilitation centre in South Africa. This was really great for helping me decide, because I knew I wanted to work in either science or become a vet and the rehabilitation centre gave me some real hands-on experience. In the end, I decided that whilst it's really great that there are people to care for sick animals, I personally prefer being out in nature and I guess that equated to being a scientist."

Stefanie has spent a surprising amount of her career so far out amongst nature, both undertaking scientific studies and also participating in volunteer work. She recently completed a project with Volunteer Eco Students Abroad (a volunteer organization that aims to provide university students with the opportunity to do community-based volunteer work.)

"As opposed to just being a tourist you get to do hands-on stuff – in this case helping build schools and bathroom blocks in Ecuador." She says.



Zoology is not a subject for the faint hearted. A close encounter with a taranchula in South America



Stefanie Oberprieler on the Galapagos Islands

Of course like any good scientist, Stefanie rarely passes a good opportunity when it comes her way. So whilst she was in South America she decided to visit the Galapagos Islands.

"Since I was so close, I just had to visit the Galapagos Islands. You can't be a biology student without hearing about the Galapagos islands in just about every lecture so I figured I'd like to have a look for myself. It was an amazing place with animals you don't find anywhere else. It's something I just had to see."

Even when at home, Stefanie likes to focus her studies outdoor where possible and her enthusiasm has on occasion paid dividends. A study she did on paper wasps yielded some interesting results and has lead to her first scientific paper published in Entomological Science co authored with her study advisor and Canberra's wasp specialist, Dr Philip Spradbery. "This publication really helped the inspirational processes of learning while travelling through Africa and aided my decision to chose to pursue a career in zoology rather than become a vet," She says, "I really enjoy discovering new things – and such research shows just how many aspects of the world remain unexplored and how much research can still be done."

Overall, Stefanie believes that enthusiasm for your subject is one of the keys to success in science or almost any other field of human endeavour. "If you end up studying something that doesn't really interest you it will be too much effort, if you follow what you're passionate about it's more fun than it is work. Science is such a broad field and so you have to make sure that you follow a path that really interests you and take any opportunity that comes your way."

Pluto and the potatoes

Could there be ten times as many Dwarf Planets as we currently think?

The five planets known to ancient people were Mercury, Venus, Mars, Jupiter and Saturn. Although outwardly star-like in appearance, their movement across the sky relative to the background stars made them objects of great fascination for many centuries. The invention of the telescope revealed their true form; spherical worlds with moons and surface features much like the Earth in many respects. No one had any reason to suspect that there may be more planets in our solar system and it's hard to imagine the surprise in 1781 when William Herschel announced that he had found a sixth planet, Uranus. The discovery of Uranus, though highly significant was really just a happy accident brought about by Herschel's prolific observations and thorough note taking.

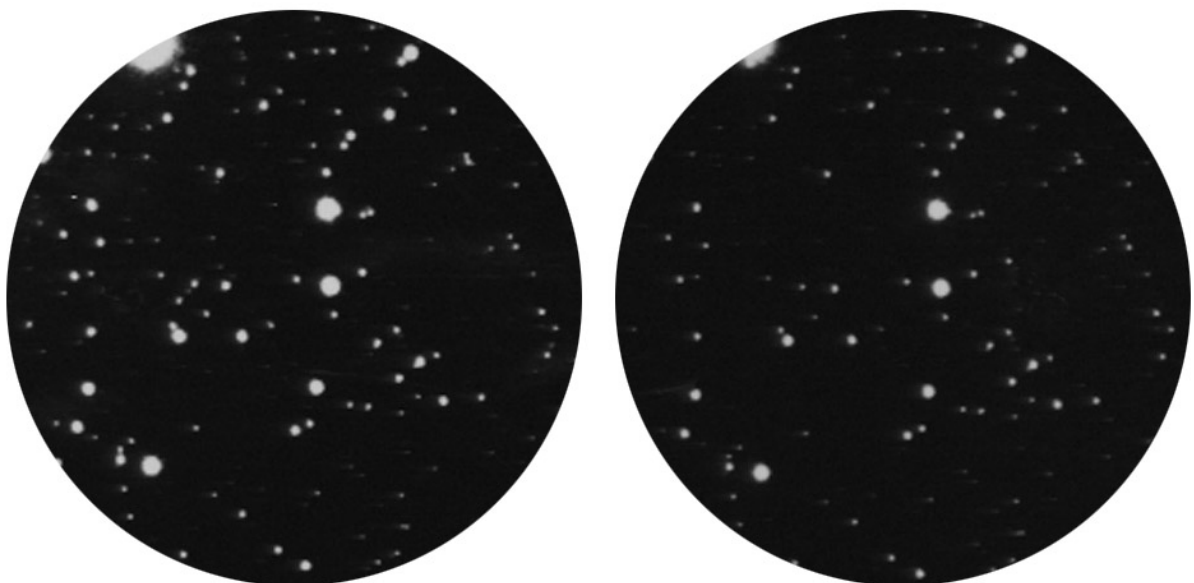
As astronomers monitored the movement of Uranus over the following century they noticed that it's orbit wasn't behaving quite as their calculations suggested it would. They supposed, correctly, that Uranus was being perturbed by the gravity of another massive body orbiting further from the sun. In an almost superhuman feat of manual calculation, the French astronomer Urbain Le Verrier correctly predicted the position of the mystery planet leading to the discovery of Neptune shortly afterwards. This was an early triumph for theoretical astronomy, it was one of the first times discovery had been

lead by theoretical prediction and underlined the value of mathematics in science.

When in later decades, the orbit of Neptune also seemed to be deviating slightly from expectations, it's no surprise that the scientific community suspected the presence of yet another planet beyond Neptune and began to search for what was termed planet X.

In 1930 Clyde William Tombaugh working at the Lowell Observatory discovered what he believed to be the illusive planet X, now known as Pluto. However as time went on all did not seem to be quite right. Pluto was too far away for its size to be measured directly but astronomers knew that it must be either very small, very dark in colour or both because it was so dim. Even the most optimistic estimates of its mass were nowhere near big enough to have any significant effect on the orbits of Uranus or Neptune. It also had a peculiar orbit, far more tilted than the other eight planets and even passing inside the orbit of Neptune at times.

In 1978 Pluto's moon Charon was discovered and subsequent observations of orbital motion of the pair enabled scientists to calculate the mass of Pluto with far more accuracy. It turned out to be miniscule at just 1/500th of the mass of the Earth. To make matters worse, other bodies of similar size began to be discovered beyond the orbit of Neptune too. Increasingly it became apparent that Pluto was merely one of the largest of a whole family of icy worlds that occupy the outer regions of the solar system beyond Neptune. Astronomers now call these bodies Trans-Neptunian Objects or TNOs.



These plates show the discovery of Pluto. Can you see the spot of light that has moved? It's difficult to do, especially when the brightness isn't exactly the same between the two plates as often happens due to differences in sky transparency. To assist in this task astronomers once used a device called a blink comparator - see right

One of the features of TNOs is that just like the asteroids that orbit between Mars and Jupiter, they have a range of sizes from small planetary bodies like Pluto down to little more than dust particles. Clearly they couldn't all be termed planets, so a decision had to be taken as to what exactly qualifies a body to be called a planet. In 2006 the International Astronomical Union decided that to qualify as a planet a body must follow three rules:

1. be in orbit around the Sun,
2. have sufficient mass to assume hydrostatic equilibrium (a nearly round shape), and
3. have "cleared the neighbourhood" around its orbit.

Pluto and the other large Trans Neptunian objects fail to qualify because although they are round, they have insufficient mass to have cleared their orbital paths of other material either by direct impact or gravitational perturbation. But in recognition of them being of sufficient size to have achieved hydrostatic equilibrium, they were designated Dwarf Planets.

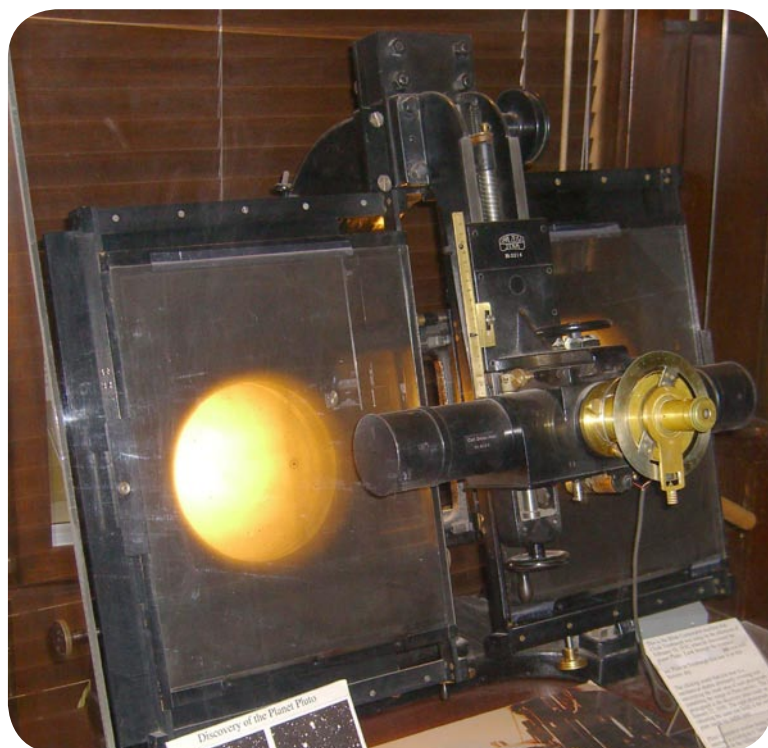
Most astronomers agree that the new classification system represents a sensible approach to classifying the many bodies that orbit the sun, especially since the mass difference between the smallest planet Mercury (3.3×10^{23} kg) and the largest known Dwarf planet Eris (1.6×10^{22} kg) is over a factor of ten.

Although everyone agrees on the clear difference between Planets and Dwarf Planets, it's not quite so clear where the line between Dwarf planets and large chunks of rock or ice lies. The matter hinges on rule two, being massive enough to be essentially round. But how big is that?

The rules provided no hard figure for this radius but based on observational evidence, most astronomers took it to be roughly 400km, which implies that there are five dwarf planets. Ceres with a radius of 490km is the only one in the asteroid belt and there are at least four beyond the orbit of Neptune comprising Haumea (575km), Makemake (750km) Eris (1200km) and of course Pluto with its radius of 1150km.

The question of how big is big enough is of great interest to Dr Charley Lineweaver, a planetary scientist at ANU. "I really wanted to know how big a potato-shaped object can be, before it becomes a sphere under the weight of its own gravity," He says.

The critical diameter is what Dr Lineweaver aptly terms the "potato radius" and surprisingly to date, there has been relatively little theoretical work done to establish just how big this is. What is known from observation, is that rocky bodies like asteroids and icy ones like TNOs both have quite similar potato radii.



The blink comparator used to detect Pluto is now on display at the Lowell Observatory. These instruments have been superseded by computer analysis of astronomical images. Right: Clyde Tombaugh with one of his home made telescopes

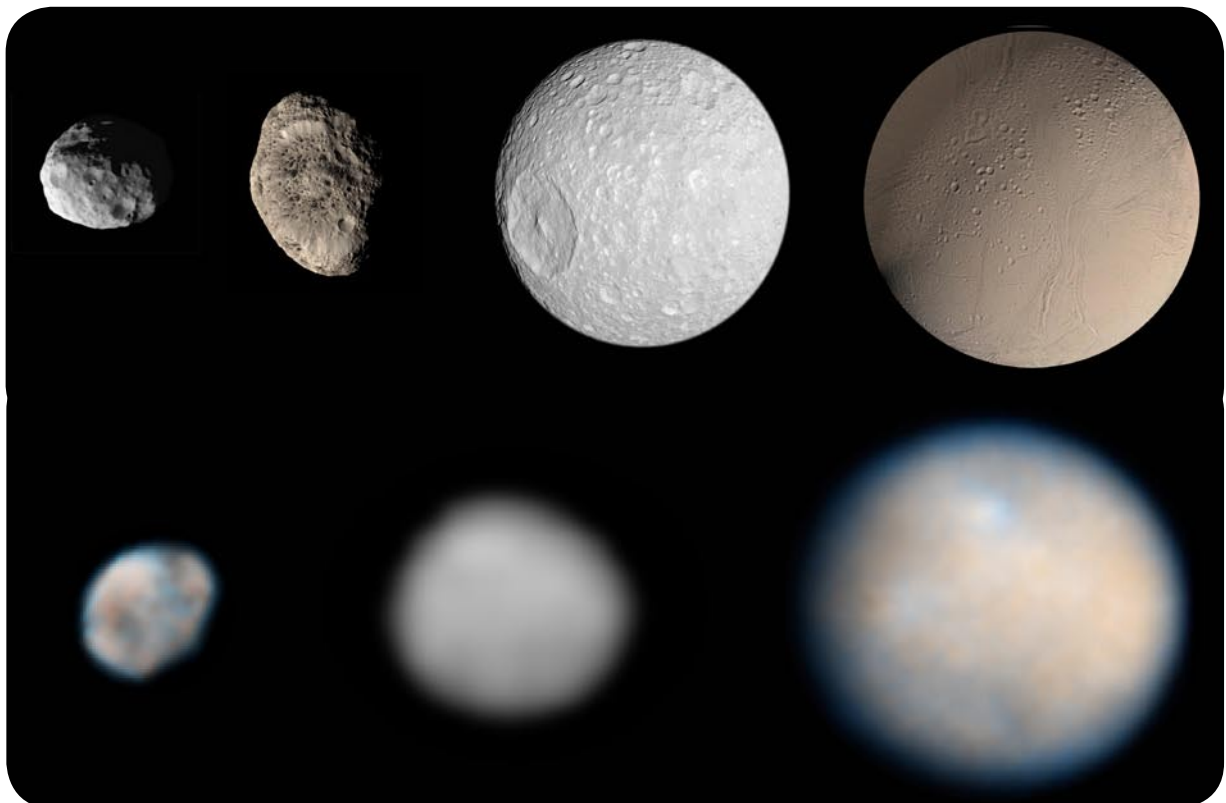
"Initially it surprised me that bodies like asteroids that are made of materials like rock and iron would have the same potato radius as trans-Neptunian objects that are predominantly made of ices." Dr Lineweaver says, "If you imagine crushing an ice cube with a pair of pliers then doing the same to an iron bolt, the bolt would be far more difficult. But the explanation is that at the distance from the sun TNOs lie, their temperature is very close to absolute zero which significantly increases the yield strength of the ice."

Because direct imaging of the shape of most TNOs is impossible with current telescope technology, Dr Lineweaver wanted to calculate the potato radius from first principles. In this way by knowing the radius of an object from its brightness and the material it's composed of from spectroscopy, it would be possible to calculate whether it would be round or not and hence whether it should be called a Dwarf Planet.

In Douglas Adams' science fiction classic "Hitch Hikers Guide to the Galaxy", to get a sensible answer out of the super computer "Deep Thought", you have to ask the right question. And in real science, much the same thing applies.



Dr Charley Lineweaver



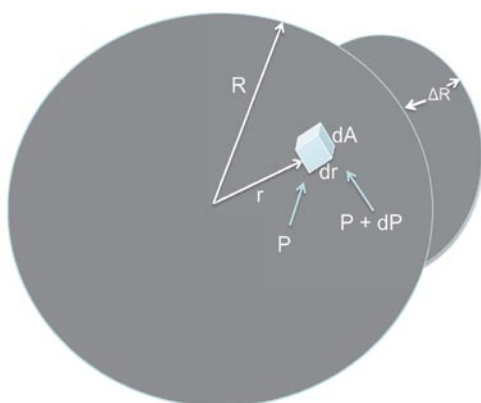
Transition from potato to sphere. Top row: Icy moons Janus, Hyperion, Mimas and Enceladus have a similar composition to Trans-Neptunian objects and transition from potatoes to spheres at about 200km radius. Bottom row, rocky asteroids Vesta, Pallas and Ceres make that transition around 300km radius.



Artists conception of the Pluto Charon system with the New Horizons probe approaching

"The first calculation I did gave a very surprising answer." Dr Lineweaver says, "A body with a structure like the Earth would need to be around 10,000km radius to achieve hydrostatic equilibrium, which is quite absurd because as we can see, many bodies smaller than that are perfectly round. It turns out that my maths was correct but what I was asking was 'what would the surface gravity of a planet need to be to deform a rock at the surface?' which is the wrong question. What I needed to calculate was 'what overburden pressure within a planet would deform rock?'"

$$\Delta P = \frac{2\pi}{3} G \rho^2 [(R_{\text{bump}}^2 - r^2) - (R^2 - r^2)]$$



For the purpose of calculating the overburden pressure, a potato can be approximated by a sphere with a bulge. If the body is large enough, the weight of the bulge will deform the interior of the body making it round

The overburden pressure is essentially the force on rocks inside a planet created by the mass of rocks above. So whilst the gravity at the Earth's surface may not be enough to deform a rock, a few kilometres below the surface the force of millions of tons of rock above being attracted to the Earth's centre is. "When I modified my calculations to incorporate overburden pressure the potato radius turned out to be about 200 to 300 km." Dr Lineweaver says, "Which is about what we see."

However, if Dr Lineweaver's is right and any icy TNO of greater than 250 km radius will have reached hydrostatic equilibrium, this would greatly increase the number of Dwarf Planets.

"The whole Pluto question arose when my co-author Dr Marc Norman and I were speaking to one of our graduate students, Michele Bannister. Together we counted at least 50 TNOs with estimated radii in the 250km+ range which would multiply the number of dwarf planets by a factor of ten." He says. But Dr Lineweaver isn't fixated on names.

"I don't think the whole naming debate is tremendously important to astronomers, we're not really a sentimental bunch! What's really interesting is the nature of bodies like Pluto and what they can tell us about the formation of the early Solar System. But even if you're a Pluto fan, the news is not all bad. You can think of Pluto as the second largest of a whole family of Trans-Neptunian Objects." He says.

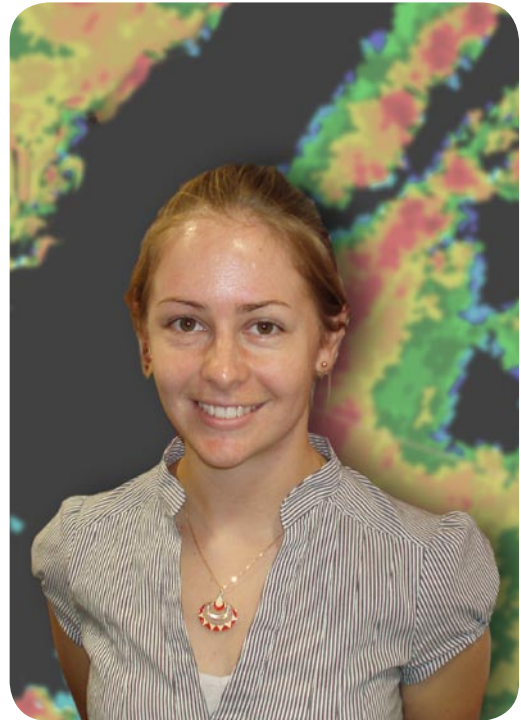
For more information see: <http://www.mso.anu.edu.au/~charley/publications.html>

Mastering the hazards

New course aims to train natural disaster managers

Volume 7 No. 3

The recent eruption of Iceland's Eyjafjoell volcano threw air transport into chaos across half of Europe and illustrates what a dramatic effect such events can have on our day to day lives. But such natural hazards are not new. Earthquakes, volcanic eruptions and tsunamis have been around longer than humans. What is new is the scale of the human impact these events have in modern times. To a large extent this is because there are a lot more humans around than there were a century ago which in turn leads to higher housing densities and taller buildings, both exasperating the effects of earthquakes and Tsunamis. There are also changes in climate and sea level brought about by human activity that may be expected to have a significant impact on the numbers of floods, droughts and severe storms in the 21st century. For all these reasons and more, the ANU College of Asia and the Pacific and the College of Physical and Mathematical Sciences have recently introduced a new Masters of Natural Hazards degree.



Christina Griffin



Sunrise against the 10 May 2003 eruption of Anatahan Volcano, Mariana Islands. Photo by A Sauter.

The course aims to provide emergency manager practitioners, scientists, policy makers and students with skills and knowledge to work effectively in the management of natural hazards. It integrates the social and scientific components of natural hazards and focuses on hazards and people in the Asia and Pacific region.

Christina Griffin is one of the first cohort of students to undertake the Masters of Natural Hazards degree. She completed her Bachelor of Environmental Science at Wollongong University and has recently worked at Geoscience Australia.

"I became interested in the course when I was studying the impact of sea level rise on Australia's coastal communities as part of my Geoscience Australia work. It led me to think about the impact of climate change in less developed countries, including how they would respond to a potential increase in the frequency of cyclone, flooding and landslide activity. Coming from a science background I was also attracted by the opportunity to study the social components to natural hazards. For example, we have studied the physical force behind tsunamis and the factors that make people vulnerable to them. The course teaches that successful disaster risk reduction requires an integrated understanding of both the physical and social sciences."

A major component of the course is an individual research project undertaken by each student. Christina intends to focus her research on the role of coastal environments such as mangroves, reefs and dunes, as natural coast defence mechanisms. "I would like to specifically look at whether these environments can mitigate the impacts of tsunami and severe storm. I would also like to research the role of community participation in the rehabilitation of these environments, and the benefits they provide communities in terms of coastal

defence and preservation of natural resources including fish."

Christina is currently in Jakarta where she plans to conduct some of her research "I find being here in Indonesia helps me better understand some of the social aspects to vulnerability that we discuss in the course."

"I hope that this formal qualification will put me in a position to be able to work in the area of disaster risk reduction. I would like to work on the management of hazards in south-east Asia, whether this is through an NGO or government organization based in Australia or the region." she says.

Although many of the people at serious risk from the effects of climate change on the frequency of natural hazards are outside Australia, Christina doesn't believe that we can simply dismiss it as not our problem.

"As a developed nation I think we have a strong responsibility to address the issues like sea level rise associated with climate change. Australia has the resources to better cope with the impacts of climate change and fewer people are directly at risk than in less developed countries. Countries in the Asia-Pacific region commonly contain large areas of low-lying coastal plains that support significant populations. This makes them very vulnerable to the impacts of sea level rise and other coastal hazards. As Australia is a large per capita emitter of greenhouse gases I think it is fair we contribute to a solution. I think meeting this challenge would mean a serious commitment from all Australians and lots of collaborative work in the region."

Aside from reducing our impact on the environment, there's not a great deal that we can do to eliminate most natural hazards but having more individuals like Christina trained to manage our response, may at least lessen the impacts on those affected.



Village hut destroyed by the May 2003 eruption of Anatahan Volcano, Mariana Islands. Photo by P Shore

Understanding the dance of electrons

Applying quantum mechanics to chemistry

Guy Micklethwait

Volume 7 No. 3

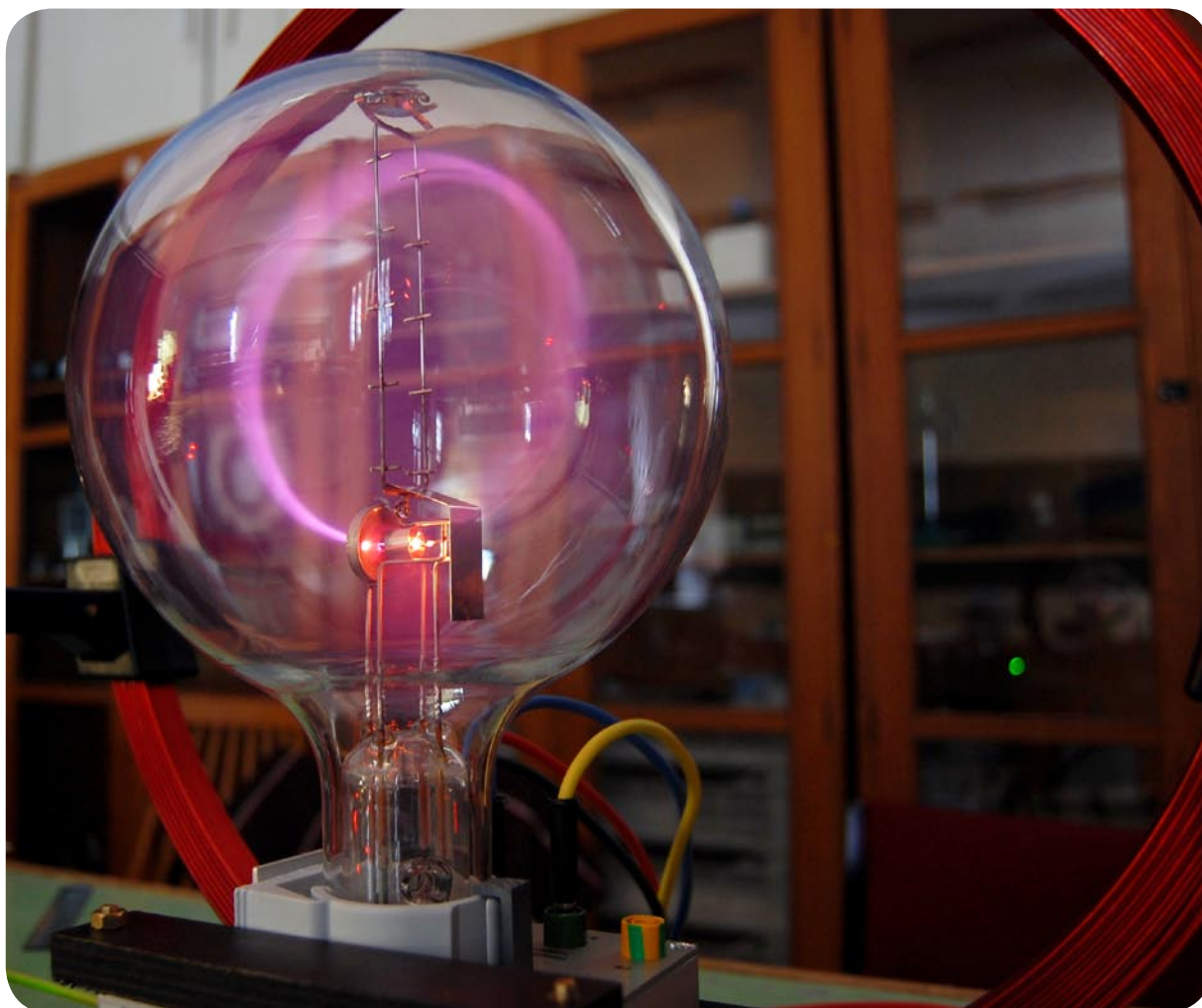
Predicting electronic structures is difficult because electrons seem to move in a very crazy and not well-understood way to avoid one another. So an ensemble of electrons all dance around like bees trying to avoid one another while staying close to the hive. Understanding this dance of electrons is called the 'Electron Correlation Problem'.

Quantum physicists currently use the Schrödinger wave equation to locate the probable position of an electron around the nucleus of an atom by considering its mass and energy. This is relatively straightforward for a hydrogen atom, as it only has one electron. However, an exact solution of the wave equation until now has never been found for a helium atom because of the mutual disturbances caused by the Coulomb interaction between the two negatively charged electrons and the positively charged nucleus.

It is similar to the 'Three Body Problem' in physics: when a planet has a couple of moons in orbit and the exact mass and velocity of each one is known, it is virtually impossible to accurately predict the location of them at other times using the laws of classical mechanics. The complex nature of the motion of the three bodies due to their mutually perturbing gravitational interactions means that scientists have never found an exact solution.

Quasixact models can be solved, such as Hooke's Atom. This uses harmonic potential to represent the electron-nucleus interaction, which is a consequence of Hooke's law. It is as if the three particles are connected by helical springs. Such computer models are very useful for predicting how chemicals will react before costly laboratory experiments have even begun. They are used in many research fields such as the development of new materials or drugs.

Dr Pierre-Francois Loos arrived at ANU from Nancy in France to begin his post-doctoral research at the Research School



Beam of electrons moving in a circle in a magnetic field (cyclotron motion). Lighting is caused by excitation of atoms of gas in a bulb. Photo: Marcin Bialek



Professor Gill and Dr Loos discuss electron behaviour outside the Research School of Chemistry

of Chemistry. His supervisor, Professor Peter Gill, gave him the challenge of studying two electrons as points on the surface of a sphere. Gill openly admits that he never expected Loos to solve the Schrödinger equation exactly. However, less than a year later their results appeared in the prestigious journal, *Physical Review Letters*.

Gill says, "What he has found is that the surface of a normal 3D sphere is not a very good model for real life; that actually the surface of the 4D sphere is the best model for real life. That is because the surface of a 4D sphere is three-dimensional... So if you really want to understand our 3D world, the best model to look at is the 4D ball's surface." This is one of the key points of this paper.

The pair have since written a paper about what happens when the sphere reduces to a point, thus crushing both electrons and this was recently published in *The Journal of Chemical Physics*.

For his next paper, Loos says that rather than increase the number of electrons on his sphere, he would like to see if he could do the same for different systems. He says, "For example, if we consider two [concentric] spheres and see what happens if we put one electron on each one."

Gill says, "We know that the real world is very complicated, but by reducing it down to this essence and understanding that perfectly, we hope we can then build up slowly from that. So that a perfect understanding of a system like this can often be the beginning of an imperfect understanding of more complicated things such as real atoms, real molecules."

In other words, if you want to understand how a hundred bees dance, you can get a pretty good start by understanding two bees.

A singular problem

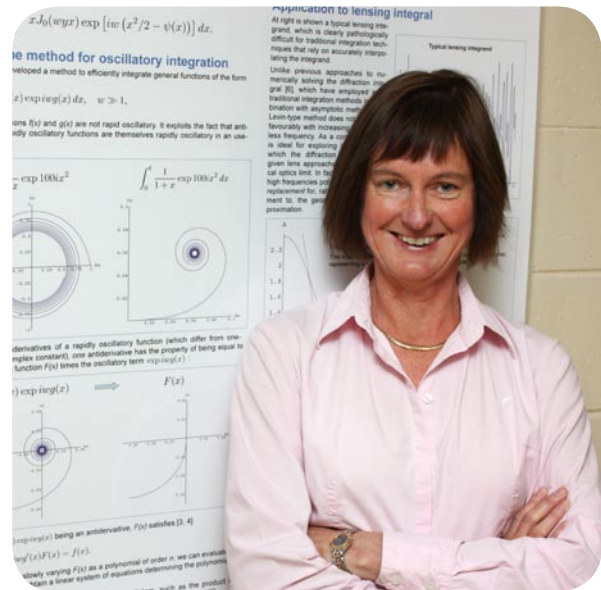
Mathematics in the search for the origins of the universe

Volume 7 No. 3

When astronomers were first able to measure the velocities of stars and galaxies relative to the Earth, they noticed a strange thing. Almost all of them were moving away from us and the further they were from us, the faster they receded. You might be tempted to think that this is because the Earth lies at some special central point in the universe, but in reality it doesn't. The universe is expanding everywhere and an observer at any point would see the exact same thing. The same is true when you look at the distribution of stars and galaxies and the distribution of the cosmic microwave background left over from the big bang. Aside from local structure, the universe looks remarkably similar in all directions. This is a property scientists call isotropy.

Why this should be so is one of the most intriguing questions in cosmology and a topic of great interest to Professor Susan Scott of The Australian National University. "There's really nothing special about where the Earth happens to be," Professor Scott explains, "so why we have this apparent isotropy is a really fascinating question. To answer it we have to better understand how the universe has evolved to the present time."

Unravelling that puzzle is the job of cosmologists. Because light travels at a finite speed, when we look at distant objects we are essentially looking into the past. This is a major reason why astronomers are always looking for larger and more powerful telescopes; distant galaxies are very faint, but the further away they are, the closer to the beginning of the

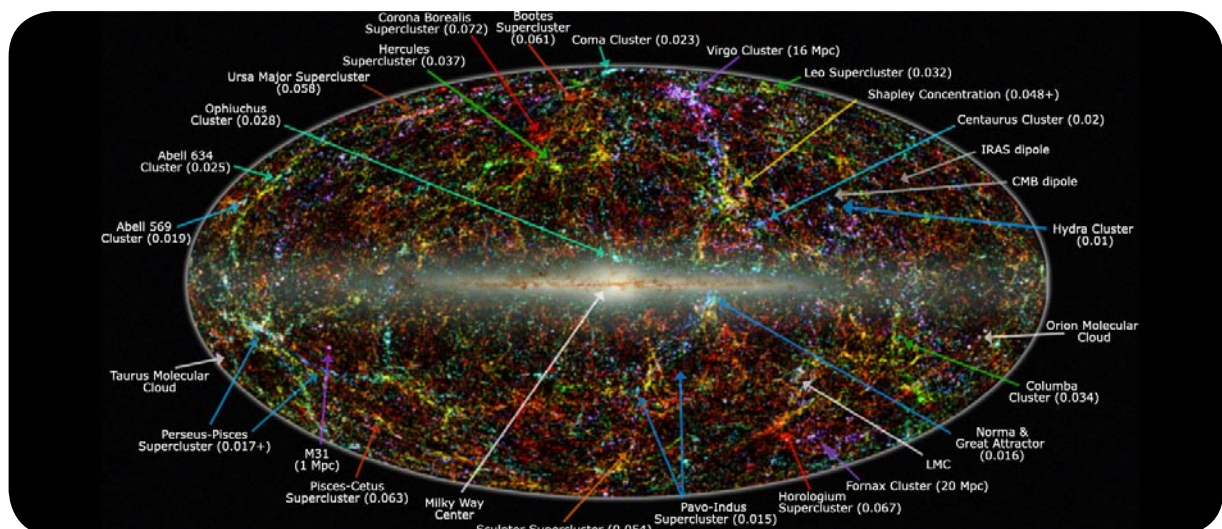


Professor Susan Scott

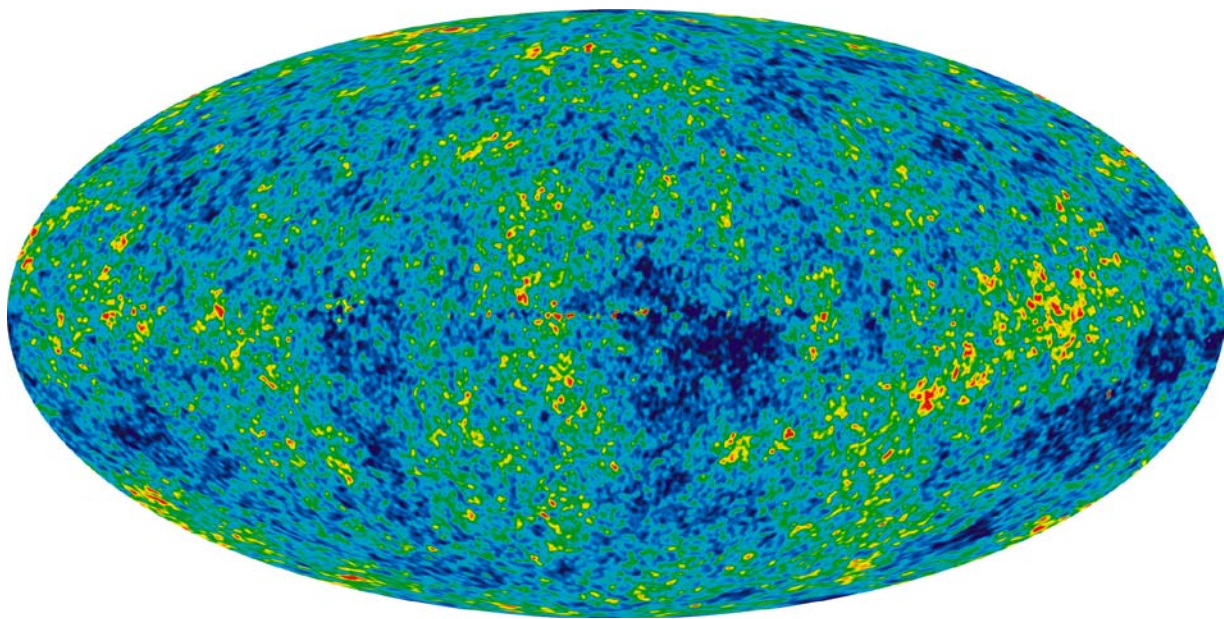
universe we see them. And of course looking at how galaxies formed over time helps us to understand the formation of the universe in general.

However observational astronomy alone, can't solve the big questions of cosmology. To do that requires highly complex mathematical models into which scientists can plug data from astronomical observation and particle physics. There are a number of competing cosmological models but they all incorporate the idea of a big bang: a point at which the universe rapidly expanded from an infinitesimally small singularity.

A simple example of a mathematical singularity is $f(x) = 1/x$. When $x = 0$ the function becomes one divided by zero which



The distribution of galaxies shows remarkable isotropy. Image: IPAC/Caltech, Thomas Jarrett



The Cosmic Microwave Background temperature fluctuations measured by the WMAP mission. The fluctuations correspond to about 0.0002 degrees. Image: NASA / WMAP Science Team

is an undefined quantity. Although the mathematics of cosmology is far more complex, the essential problem is the same.

"Solving the mathematics of the big bang as well as the final state of the universe is complicated by the initial and possibly final singularities." Professor Scott explains, "You can't do much when things go singular."

To get around this, Professor Scott and her collaborators have been working on nice regular cosmologies that don't have singularities. Although these don't directly represent the physical universe we live in, they can be designed to have what's known as conformal relationships with the physical universe. What this means is that you can solve the maths in one universe and extract results that are meaningful in another.

"An early contender for modelling the universe was Chaotic Cosmology." Professor Scott says, "This is a theory in which the universe began with a big bang and entered an exceedingly hot and highly chaotic phase before organising itself in the way we now see. The problem is that whilst this is a nice picture, it's not really compatible with either observation or thermodynamics which requires that entropy increases with time."

The more recent Quiescent cosmological model still incorporates the notion of a big bang but the key idea is that the gravitational field also has an entropy associated with it. So in effect you have an early universe in which the gravitational field is very smooth and has very low entropy whilst the first matter to condense had a very high entropy.

As time progresses the situation slowly reverses, with the gravitational field increasing in entropy as the matter cools. Of course the combined overall entropy has to increase in accordance with thermodynamics.

"Our work enables us to solve some difficult problems in the Quiescent cosmological model." Professor Scott says, "A while back we had been able to incorporate the initial singularity of the big bang. Now we've recently expanded that work to model the final singularity that might be seen in a big crunch scenario, where the matter of the universe contracts back under gravity to a single point again. However this work isn't about predicting whether the universe will continue to expand or collapse into a big crunch. The maths works equally well for both scenarios so we have to leave it to the observational cosmologists to provide some numbers to plug in."

The most recent observational work suggests that the expansion of the universe, far from slowing down with time as one might expect in a big crunch scenario, is in fact accelerating. Astronomers have dubbed this phenomenon dark energy in reference to the unknown force that may be causing it and it's a hot topic in modern astronomy.

"I think there are three really big unsolved questions in physics at the moment." Professor Scott says, "The nature of dark energy, the unification of fundamental forces and of course us, by which I mean are we unique in the universe or not?"

It may be some time before we're able to answer any of those questions but it's certain that when we do, mathematics will play a central role.

Saving an evolutionary icon

How atmospheric nuclear weapons testing may help conservation of the lungfish

Volume 7 No. 3

As its name suggests, the lungfish has primitive lungs enabling it to breathe in air. Lungfish hold a special place in evolutionary biology being a relative of the first air breathing amphibious land animals. Today living lungfish can be found in Africa, South America, and Australia. This distribution probably relates to their presence in the early super continent Gondwana that broke up about 150 million years ago and this gives a measure of just how ancient these creatures are. However the Australian lungfish is under pressure as Queensland's water resources become increasingly stretched to meet a variety of human needs. A number of dams have been constructed across the state in the past few decades and this has had inevitable repercussions on the lungfish's habitat. But establishing just how much of a threat is posed to this iconic species is complicated by the fact that scientists aren't sure how long they typically live in the wild or what the age distribution of the current population is.

With many fish, establishing the age of an individual is a relatively simple thing to do. Fish have structures called otoliths in their inner ears onto which layers of calcium carbonate and a gelatinous matrix are deposited each year. Seasonal variations create rings much like the growth rings on a tree and by counting these rings, it's possible to work out how old a particular fish is. However with lungfish this method doesn't work because their otoliths are too gelatinous. So instead scientists try to look for seasonal changes in the Horny scales

that cover their backs. However this is a very tricky thing to do because most of the growth is concentrated in the first, rapidly growing portion, compressing the later years into a very small area.

Ironically the solution to this conservation problem may come from the pollution created by the numerous atmospheric nuclear weapons tests conducted through the 1950s and 60s. As part of her Honours Degree, Kelly James has been working with Dr Stewart Fallon on analysing atomic bomb C^{14} residue in lungfish scales as a method of determining their age. The process involves removing some sample scales from a specimen and isolating tiny quantities of material from different points along the length of each scale. The samples can then be subjected isotopic analysis to establish the amount of C^{14} in them.

Although naturally present in the environment in microscopic quantities, the concentration of C^{14} increased significantly but temporarily, during the atmospheric nuclear weapons testing of the mid twentieth century. This means that any organism alive during that period would have incorporated some of this C^{14} into its tissues. And with tissue that continually grows such as a horny scale, that means that there is a C^{14} peak in the tissue corresponding to 1962 - the peak of bomb testing.

"On each of the scales from our sample fish we were able to detect the signature of the start of testing and the peak," Kelly explains, "We combined that with the date of capture of the fish giving us the three points we need to fit the von Bertalanffy growth curve and establish the age of the fish which in this case turned out to be about 75 years."

However although the technique sounds relatively straight forward, there is a huge amount of work associated with gathering this data. Firstly the material must be cleaned and



An Australian lungfish temporarily captured in a park ranger's boat



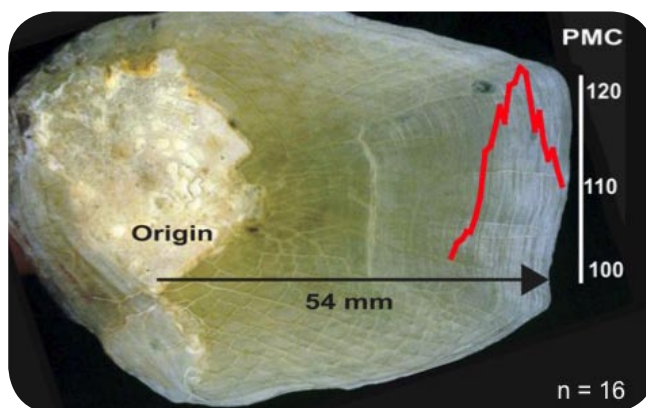
Kelly James with the complex series of cold traps that isolate carbon from biological samples

isolated to ensure that it's all from the right tissue type and isn't contaminated with other material of different age. Next the carbon needs to be extracted in the form of CO_2 gas. With organic samples like the lungfish scales this is done by a heating process. The CO_2 is then cleaned of contaminants using multiple stages of freezing and exposure to vacuum. Once the pure CO_2 sample is created it is mixed with hydrogen and heated in the presence of an iron catalyst, which generates water and graphite. This graphite isolates the carbon from the original sample in a solid mass that's easy to handle and analyse.

The next step is to determine the amount of radioactive C^{14} each of these graphite samples contain. To do this scientists use what is known as a mass spectrometer. In this case that's the dedicated SSAMS spectrometer at the Research School of Earth Sciences. The basic principle of mass spectrometry is that charged ions of any element will follow a curved trajectory when passing through a magnetic field. The acceleration depends on the charge and the field but how much deviation that acceleration produces is dependent on the mass. The upshot of this is that a heavier isotope like carbon 14 will be deflected slightly less than a lighter one like carbon 12. By placing two detectors slightly apart, scientists can then count the ratio of C^{12} to C^{14} atoms.

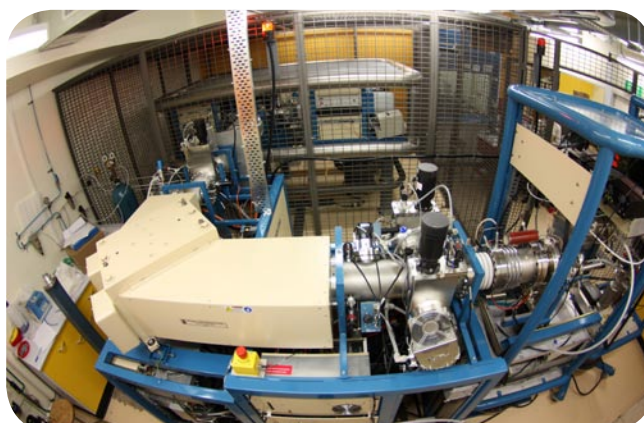
"We were delighted with our initial results" Kelly says, "One of the key things in managing the conservation of a species is establishing the basic population dynamics. How long does a particular animal live, how old are the individuals in the current population and things like that. And this technique enables us to do this reliably in lungfish for the first time. The other really great thing

about this technique is unlike counting otolith rings, we don't need to kill the fish. Simply remove a few scales and return it to the water. This is especially important when we're dealing with endangered and protected species."



Above: A lungfish scale with the concentration of C^{14} at various points superimposed on it. The C^{14} shows the classic 'bomb curve' corresponding to atmospheric weapons testing during the 1960s.

Below: The SSAMS spectrometer used to measure the C^{14} concentrations. The cage protects operators from the very high accelerating voltages.



How science wise are you? Try our quiz and see.

All the answers can be found both in the stories in this edition of ScienceWise and listed on the inside cover. The magazine is also available on line at <http://sciencewise.anu.edu.au>

- (1) Where do palm cockatoos nest?
☐ (A) In palm trees
☐ (B) In natural tree hollows
☐ (C) In nests constructed out of palm leaves
☐ (D) In dug out holes in the ground
- (2) When was Pluto discovered?
☐ (A) 1896
☐ (B) 1904
☐ (C) 1930
☐ (D) 1952
- (3) How many dwarf planets are there in the asteroid belt between Mars and Jupiter?
☐ (A) 1
☐ (B) 2
☐ (C) 3
☐ (D) 17
- (4) What is a blink comparator?
☐ (A) A medical device for testing whether each eye blinks in a similar way
☐ (B) A chemical test for potassium contamination in soil
☐ (C) A device for testing tissue density vs a standard sample
☐ (D) A device for detecting the motion of astronomical objects on film
- (5) What is overburden pressure?
☐ (A) The weight of rock compressing a given area within a planet
☐ (B) The pressure exerted by photons of light from very intense sources like lasers and the sun
☐ (C) The pressure at which a material yields
☐ (D) The pressure above which it is illegal to inflate pressure vessels
- (6) What is Hooke's Atom?
☐ (A) An isotope of platinum used in radioisotope dating
☐ (B) A old model of the atom in which the protons, electrons and neutrons are mixed in a ball
☐ (C) A theoretically predicted super-heavy stable atom with mass number of 290
☐ (D) A mathematical model of electron nucleus interaction based on a harmonic potential
- (7) What is a mathematical singularity?
☐ (A) A unique solution to an equation
☐ (B) A point at which a function becomes undefined such as $1/0$
☐ (C) A point at which a function becomes unity (1)
☐ (D) A function that remains the same for all input values
- (8) What is the potato radius?
☐ (A) The radius of a standard potato
☐ (B) The radius at which a planetary body becomes spherical rather than lumpy like a potato
☐ (C) The distance from the North Pole beyond which potatoes won't grow
☐ (D) The size beyond which a potato becomes rotten in the middle
- (9) What is a lungfish?
☐ (A) A fish with lungs
☐ (B) A parasite that invades the lungs of cattle
☐ (C) A fish that is shaped like a lung
☐ (D) A medical device that prevents water build up in the lungs
- (10) When did the supercontinent Gondwana break up?
☐ (A) 45 million years ago
☐ (B) 95 million years ago
☐ (C) 150 million years ago
☐ (D) 360 million years ago

ScienceWise

SCIENCE MAGAZINE OF THE AUSTRALIAN NATIONAL UNIVERSITY



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