Marvellous **motion:** predicting the behaviour of large systems

Accurately predicting how large systems behave – how they move and change over time – is very desirable in many areas of physics and chemistry. This has historically been very difficult, largely due to the need for accurate mathematical methods. Anna Meyer investigates.

Robert McLachlan
Photo: Graeme Brown

Large, complicated systems are everywhere around us – from the motion of planets in the solar system, to the collision of molecules as they undergo a chemical reaction, to the ever-changing patterns of weather and climate. Over the last ten years, Robert McLachlan, a professor of applied mathematics at Massey University and a Maclaurin Fellow of the NZIMA in 2005 has been developing inventive new mathematical tools to make it easier to study the behaviour of large systems.

To track how large systems behave, a branch of maths known as numerical integration is used, which involves calculating and predicting movement in the system over time as a series of tiny steps, building up to an overall picture. The problem is that although the starting positions and forces can be determined accurately using the laws of physics, small errors are unavoidably introduced at each step as the movement trajectory is calculated. These errors, due to intrinsic properties of the equations used, build up over time, and so even a tiny uncertainty early on becomes magnified very rapidly. This means that it has traditionally not been possible to accurately predict the behaviour of large systems very far into the future. This was particularly true for the motion of atoms or planets, where calculation errors are usually very large.

A solution to the problem was hit upon almost by accident a little over a decade ago. "It turns out that applied scientists had been ignoring what the numerical analysts were saying, and doing enormously long runs millions of years into the future, without worrying about the errors much," says Professor McLachlan. What is more, they were getting excellent results. Intrigued, mathematicians began to study the methods scientists had devised, and discovered they had hit upon a technique that at last gave a reliable way to study motion in large systems.

Nicknamed 'leapfrog', the method is the simplest example of what has now grown into an entire class of mathematics for studying large systems, called geometric integration. The method allows the overall behaviour of large systems be studied over long periods of time. Although errors are still introduced along the way, they do not affect the overall pattern that emerges for how the system behaves. This is because the methods preserve some aspects of the physical laws exactly, with no error, for example, the conservation of energy, momentum or symmetry, or the so-called 'symplectic' property, which couples position and velocity.

Professor McLachlan's research involves designing new geometric integration methods, and studying their behaviour. The idea is to develop techniques that are faster, more reliable and simpler, and that also have a variety of specific, desirable properties.

Many geometric integration methods are now known, and are being applied to problems such as predicting whether planets will remain in their current orbits, and how proteins fold into their final shape from their amino acid sequences. In the future it may even be possible to solve more difficult problems, such as modelling climate change – a breakthrough, no doubt, that would be well received.

PRIMA donor

The NZIMA has become a founding member of the Pacific Rim Mathematical Association (PRIMA). This association of mathematical sciences institutes, departments and societies from around the Pacific Rim was established in 2005 to promote the development of the mathematical sciences throughout the region.

PRIMA aims to encourage wider participation in scientific activities in the Pacific Rim, share expertise and resources in the promotion of the mathematical sciences and their impact on society and the global economy, and to create a network for the exchange of ideas and the dissemination of scientific knowledge.

One of the first PRIMA initiatives is the encouragement of participation in summer schools and other meetings at reduced cost by students of its member institutions. Students from New Zealand universities affiliated with the NZIMA are eligible for subsidies.

See the PRIMA website at www.primath.org.

Milk tankers and traffic flows

Jenny Rankine explores some of the topics discussed at the NZIMA Workshop on Mathematical Models for Optimising Transportation Services in April 2005.

Milk tankers are such a regular feature in the life of dairying regions that few people give them a second thought. Farmer Smith expects one every morning, but every morning her herd produces a slightly different amount of milk. By the time the tanker gets to the Wihongi farm at the end of the road, it may not have enough space for the output of their cows, and the scheduler may have to send another tanker.

Arranging the collection of an unknown amount of milk from 12,000 farms and delivering it to more than 30 factories, without many such backtracks, is a constant headache for Fonterra's schedulers. They face it twice a day, every day of the year. Fonterra's milk collection consultant, Simon Harrison, presented the problem to the workshop and was heartened by the results.

He introduced the company's internal debate between stochastic and deterministic optimisation approaches. "A deterministic solution will always be at the boundary of existing constraints," he says, "and therefore has the biggest risk of being wrong on the day. The question is whether you can design a stochastic optimisation approach to reduce the risk of being wrong on the day at minimal cost to the mathematically optimal solution. For a business like Fonterra, that is the crux of the argument." At the time of the conference, Fonterra was evaluating software using the different optimisation models.

The workshop brought together a group of local and international scheduling experts to debate the issues in a Fonterra-sponsored panel session. "It was quite fruitful," says Harrison. "What we got from the workshop was a much better understanding of the issues, a set of questions to ask our prospective suppliers, and better tools to make sure that the path we're on is going to give us the results we're looking for." He says Fonterra would be interested in taking part in a similar session on a high priority maths problem again.

An unexpected result was that Fonterra's schedulers heard "all those brainy people struggling to model 150 pickups and went away thinking they do a really good job".

The workshop also included a stream about regional transport models, with a presentation by the Auckland Regional Transport Authority. Another expert panel considered transport models as tools for evaluating regional transport policies; how to increase Auckland public transport's share of travel time at reasonable cost; and how to plan for travel growth when forecast data is uncertain.

Workshop co-organiser Professor Andy Philpott says that traffic system models look at many individual drivers going from their origin to their destination and aiming for the quickest trip. "The models seek to construct an equilibrium where each driver is travelling by the route that gets them where they are going in the shortest time accounting for the similarly optimal choices of all the other drivers." The models allow researchers to explore the likely effect on traffic flows of changes such as expanding the capacity of a main road or motorway.

At the time, the introduction of tolls for Auckland central traffic was being debated. Professor Mike Florian from the University of Montreal told television viewers that tolls work only if there are alternative untolled routes that could then get more congested. They may not have any effect on drivers when there are no alternative routes.

A third theme of the four-day workshop was transport pricing and revenue management. The event was attended by more than 80 people from Australia, Canada, Chile, China, Denmark, Germany, India, Israel, the Netherlands, Norway, Singapore, Spain, Sweden, USA and New Zealand. It was hosted by the Department of Engineering Science at the University of Auckland and funded by NZIMA and the University's Operations Research Group. See www.esc.auckland.ac.nz/Transportation.