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

Accurately predicting how large systems move and change over time is very desirable in many areas of physics and chemistry. Historically this has 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.

\exp(A)\exp(B) = \exp\left(A+B+\frac{1}{2}[A,B]+\fr