From IMAges 5,
November 2008

Nano
Nano

Nano-maths

Mathematics and nanotechnology are ideal partners, according to Dr Shaun Hendy of Victoria University and IRL. Anna Meyer explains.

What happens to physics when things get really small? How can we investigate structures so tiny that each individual atom is important? And how can useful nano-devices be built? Mathematics and computer simulation are helping to answer some of these fundamental nanotechnology questions.

"Using computer simulation, we can study materials right down at the nanoscale," Dr Shaun Hendy explains. "We might be interested in a nano-device containing millions of atoms; we can use the simulation to visualise how each of these atoms behaves." Part of the advantage of this 'silicon-laboratory' approach is the ability to see exactly what is going on at incredibly small scales, which is normally very difficult, expensive and time-consuming.

The computer simulations complement laboratory work by other research teams. "I work with several experimental groups in the MacDiarmid Institute for Advanced Materials and Nanotechnology, including Simon Brown's at the University of Canterbury."

"Simon's team builds nano-electronic devices using very small particles called nanoclusters. We're doing a lot of the modelling behind the manufacturing, to help figure out new and better ways of doing it. Some of the work we've done has led to new patents for his spin-off company."

Dr Hendy's team is one of the biggest computing consumers in New Zealand, using the University of Canterbury's Blue Gene supercomputer, the most powerful in the southern hemisphere. But even this is not always enough for the types of modelling the team is doing.

"We could use all the computing resources in the world and it would not be enough," said Dr Hendy, "so we're always trying to come up with clever ways of using the computer, of re-casting the mathematical problem in a slightly different way."

The team also constructs more traditional mathematical models of events at the nanoscale. In the world of the very small, even physics itself is different, and this can be used to make new types of devices. For example, surface tension becomes very important, as objects at that scale have very high surface area to volume ratios.

"We have had a lot of fun just constructing mathematical models of quite common phenomena, such as melting, and then seeing what happens when surface tension takes over," said Dr Hendy. "It's surprising how your intuition, which is tuned for a human-sized world, can get things completely wrong when you try to guess what will happen at the nanoscale."

The group also work on what are known as homogenisation problems. "These are similar to what happens when you put batts between the wooden beams in your roof, creating a heterogeneous or mixed up layer of insulation in your ceiling. You may want to know how well this mixture of batts and beams insulates your roof on average."

"A similar situation occurs at the nanoscale, where atoms of different types are arranged in patterns. We are interested in how these patterns of atoms lead to the overall properties of a nanomaterial." NZIMA-funded postdoctoral fellow Dr Philip Zhang and PhD student Nat Lund have been active in this area.

Another focus is nanofluidic devices – tiny pipes already used for applications such as rapid DNA sequencing. As the pipes are made smaller, the pressure needed to push fluids through them increases dramatically. "People make these lovely little devices, but then the pump needed to run them is the size of a table – it's very embarrassing. Again, the problem is surface tension – the drag on the fluid increases as you make the channel smaller. We are trying to help reduce this problem."

Finally, NZIMA-funded PhD student Dmitri Schebarchov has been working on understanding the details of very small capillaries, such as carbon nanotubes. He and Dr Hendy have discovered a way to fill and unfill them with metals, which has not been achieved before. "This will be important for building different types of nanostructures," explained Dr Hendy, "and also has relevance to controlling nanotube growth, which can be difficult."

"There's a lot of fun to be had, and it is a good place for mathematical modellers as there are a lot of new mathematical problems to be found. The work is a mix of physics and mathematics – I like the challenge of solving mathematical problems for their own sake, but I also like the fact that there are applications at the end of it. It's also a field that is developing really rapidly. You certainly don't get bored - there's always something new that you can work on where you can make progress."

Shaun Hendy, left, and Dmitri Schebarchov.