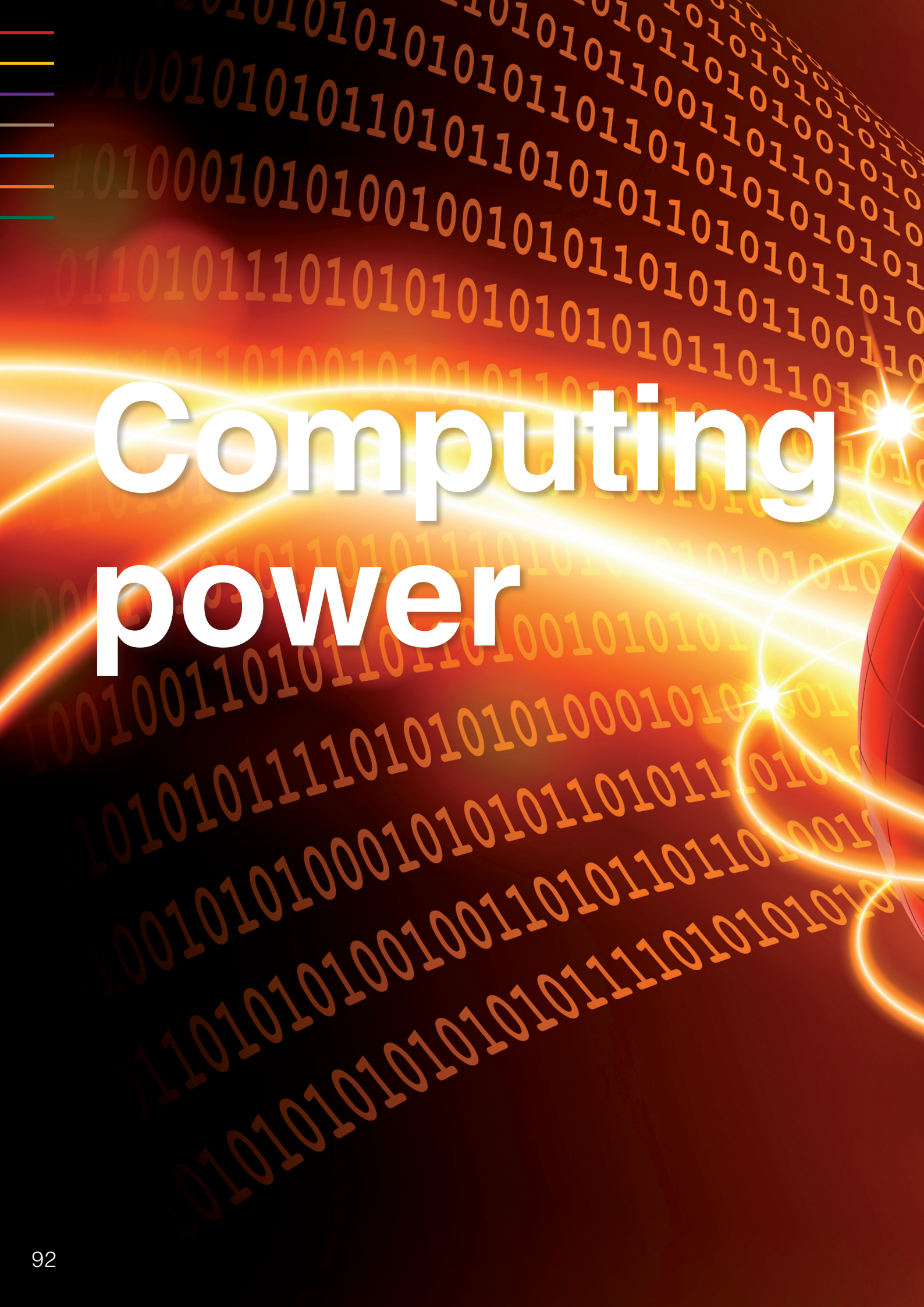


Computing power

Dazzling advances in processors and high-performance computing have allowed UCT's researchers – especially, but not exclusively, those in the natural sciences – to push the envelope in their studies. From supercomputers to cellphones, the field has opened up a slew of new prospects for scientists, some even having a hand in the development of industry-standard computing languages and software. Such are the opportunities that the university has even started its own ground-level high-performance computing infrastructure, allowing more scholars access to such capabilities.

The many applications of computing at UCT

Arguably the pioneer of high-performance computing (HPC) at UCT, the Centre for Research in Computational and Applied Mechanics, or CERECAM, has blazed a trail since its founding in the 1980s. And its trajectory perhaps best mirrors the evolution of high-performance computing at the university.

Established in 1981 by the late Professor John Martin, it had its origins in the small Non-linear Structural Mechanics Research Unit, the group's name not even meriting the use of the word *computing*, or a variation thereof, just yet. The word didn't feature in the unit's name in 1985, either, when it became the Applied Mechanics Research Unit.

Only with its renaming as CERECAM in 1988 – when it was granted centre status by the Foundation for Research Development, now the National Research Foundation – was its tool of choice formally introduced into the moniker.

"Globally, computational mechanics and high-performance computing were just starting to take off," recalls Professor Daya Reddy, one of Professor Martin's protégés and CERECAM director. "What we were doing here at UCT was pioneering work."

Since then, says Professor Reddy, there has been a "wonderful synergy" between the growth of both computing power and the fields of theoretical computational mathematics and mathematical modelling, which underpin CERECAM's work in computational mechanics.

"Globally, computational mechanics and high-performance computing were just starting to take off. What we were doing here at UCT was pioneering work."

Researchers in the centre have sought to develop simulations of a variety of phenomena that involve the principles of mechanics. These include biomechanics, such as the study of myocardial infarctions (heart attacks); solid mechanics, for example the behaviour of metallic crystals at the micron level; the flow of particles in mining slurries; and even the interplay between electricity and mechanics in synthetic polymers such as hydrogels.

A further major area of focus is computational fluid dynamics, that is, the flow of fluids, be it gases, air around a vehicle, or biological fluids, such as blood. The centre has, for example, partnered with UCT's Department of Chemical Engineering to investigate the complex reactions between solids, liquids and gases common to the platinum mining industry.

"In many cases, the algorithms and codes that we develop can only sensibly be run on clusters or other high-performance computing platforms, which today are a necessity rather than a luxury," says Professor Reddy.

"Many of the issues we deal with are of universal concern," says Professor Reddy, "but a number are specifically South African, in the sense that they are derived from problems experienced in South African industry."

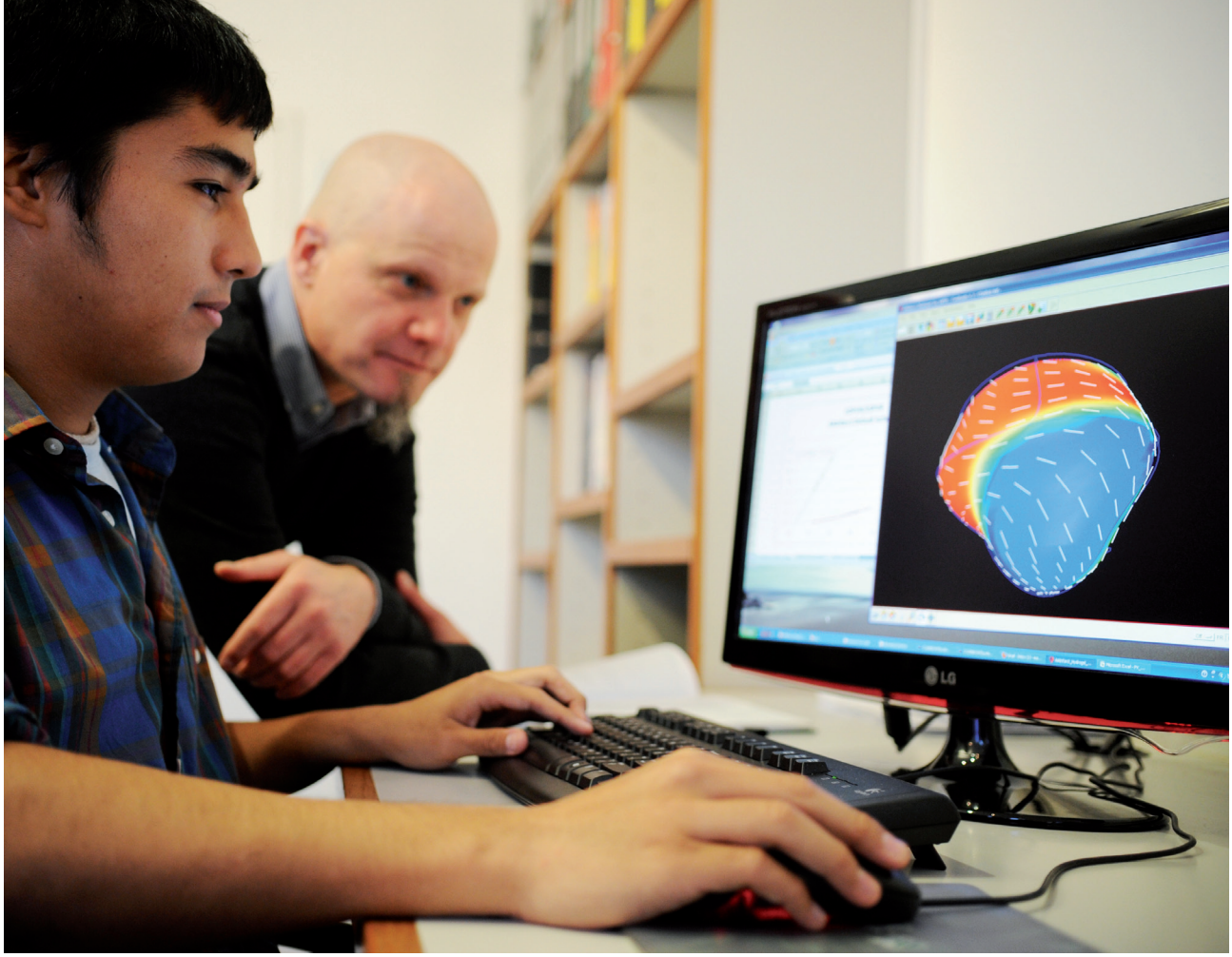
Going where no experimenter has gone before

This rule applies also to the research in computational chemistry and biophysics, which is led by Professor Kevin Naidoo, who holds the DST/NRF SARChI Chair in Scientific Computing and whose pioneering work was recently recognised when he was named a finalist in the 2011/12 National Science and Technology Forum-BHP Billiton Awards.

Bringing to bear state-of-the-art computational techniques and HPC, Professor Naidoo and his team in UCT's Scientific Computing Research Unit (SCRU) have been able to go where experiments cannot yet go. As such, they've studied everything from the physical properties of carbohydrates and a group of molecules known as dendrimers (useful as a delivery mechanism in the design of drugs), to the behaviour of metals such as platinum in the mining refinery process.

In 2011, they unravelled the mechanisms of the deadly protein ricin, a toxin found naturally in castor beans. This finding (for which they were granted a patent) will, they hope, lead to the discovery of an antidote.

However, Professor Naidoo and his team have not only focused on applications in chemistry and biophysics. Through their research supported by the Nvidia Corporation and working closely with the likes of the USA-based



Jesse Macadangdang (left) and Dr Thomas Franz of UCT's Cardiovascular Research Unit (CVRU) start preparatory work on their new collaboration with the national Centre for High Performance Computing (CHPC) and CERECAM. The three-year research project, funded by the CHPC, is an exercise in computational biomechanics and will explore possible treatments for myocardial infarction (heart attacks).

Portland Group and the Daresbury Laboratory in the UK, they have been able to not only push the boundaries of their own work, but also have a say in the technology that is used in scientific research across the globe.

"Our strategy is to spend 50 to 60 percent of our efforts on the development of methods for use in chemistry, quantum chemistry, physics, quantum physics, biology, and so on," explains Professor Naidoo.

So, for example, their insights went into the testing and development of Portland's suite of graphical processing unit (GPU) compilers – the computing translating program that drives graphics processing units, now de rigueur for high-performance computing systems and in scientific computing. Similarly, they helped Daresbury adapt their quantum software GAMESS UK into computational chemistry code.

"The application of such technology – the type that is found in gaming consoles – to science, will exponentially expand the power of the next generation of high-performance computers," says Professor Naidoo. "This will allow scientists to simulate more realistic models of natural systems, making computing as the third mode of scientific enquiry a significant reality."

Home-grown HPC

But although not everyone needs the high-end computing power or the ready access demanded by CERECAM and the SCRU, there is a rising demand for high-performance computing on a smaller scale around the university. However, up until a few years ago, those departments, units and research groups that did have a need for it had to borrow computing power from outside of UCT or set up their own HPC nodes.

When Izak (Sakkie) Janse van Rensburg took over as Executive Director of Information and Communication Technology Services (ICTS) at UCT, that changed. Within a short time of taking office, he had convinced the university to fund an HPC node within ICTS, a scaled-down complement to, for instance, the services offered by the nearby Centre for High Performance Computing or even the South African National Grid, which pools computing resources from institutions and centres across the country.

"We have many researchers who are either just developing their work or are moving into new areas, and need access to a smaller system at UCT like the ICTS HPC node," says Janse van Rensburg.

Research groupings associated with this theme

Centre for Research in Computational and Applied Mechanics

The Centre for Research in Computational and Applied Mechanics (CERECAM) provides a coherent focus and point of interaction at UCT for research in mechanics, by promoting and supporting fundamental research, applied research, and industrial interaction in computational mechanics and its associated disciplines. The centre's activities are multi-disciplinary, and its membership is drawn from three engineering departments, applied mathematics, physics, and cardiovascular surgery. The research interests of the centre involve the broad field of non-linear problems in solid, structural, and fluid mechanics, with a particular emphasis on the application and development of the finite element method. There is a strong emphasis on postgraduate training, at the master's and doctoral levels. The DST/NRF SARChI Chair in Computational Mechanics, held by Professor Daya Reddy, is located within CERECAM.

Director: Professor B.D. Reddy
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Scientific Computing Research Unit

The Scientific Computing Research Unit (SCRU) was established in 2009 and has as its core mission the development and application of computer code for scientific problems, specifically in chemistry, biophysics, physics, and engineering. The unit has made major technical advances in biophysical computational modelling, with the development of a generalised free energy code called FEARCF. In 2009, the unit was awarded a long-term development grant from the Nvidia Corporation to advance the SCRU programme to port quantum code to graphical processing unit-based computer clusters. The research group has strong links with international groups, particularly through its Scientific Computing International Lecture Series programme.

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Information and Communications Technology Centre for Development

The Information and Communications Technology Centre for Development (ICT4D) was established in 2008 to capitalise on UCT's unique position in the ICT domain, namely, producing world-class ICT research, but being based in a developing economy. Incorporating researchers from across the university, the centre looks to create ICT solutions that can be applied in a developing-world context. Being the only such centre in a developing country, it has been able to attract researchers and students from across the globe. The Hasso Plattner Institute Research School in ICT4D, which provides bursaries for African students working in this field, was launched in 2009 and will be based within the wider structure of the centre.

Director: Professor G. Marsden
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Centre for Information Technology and National Development in Africa

The Centre for Information Technology and National Development in Africa (CITANDA) is located within the Department of Information Systems. It brings together researchers, projects, funders, and programmes focused on the use of information and communication technology (ICT) in the service of national development. CITANDA researchers study, using a diversity of research approaches, the management, development, adoption, and impact of ICT in areas related to business, economic, and social development in Africa. The centre specifically explores and investigates information systems (IS) phenomena that arise at the nexus of interaction between information technology and Africa's business, cultural, social, and economic context, in order to advance knowledge concerning IS in organisations and society in Africa. Through CITANDA, the Department of Information Systems attracts a large cohort of PhD and master's degree students from across Africa and beyond.

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Members of the CERECAM research group.

DST/NRF SARChI Chairs associated with this theme

Computational Mechanics

Professor Daya Reddy, who holds the SARChI Chair in Computational Mechanics, is a member of the Department of Mathematics and Applied Mathematics, and Director of the Centre for Research in Computational and Applied Mechanics (CERECAM). He is a graduate of UCT and Cambridge University, and served as dean of the Faculty of Science between 1999 and 2005. The focus of the research chair is on mathematical modelling of material behaviour, for example, solids at the microstructural level and non-Newtonian fluids; and the development of algorithms for numerical simulations. The research is highly multi-disciplinary with applications in the biomedical sciences and engineering.

Scientific Computing

Kevin J Naidoo (PhD, Michigan; postdoctoral fellow, Cornell) is Professor in Physical Chemistry and since 2007 he has been the holder of the SARChI Chair in Scientific Computing. In 2009 he established the Scientific Computing Research Unit (SCRU) at UCT. Luminaries such as Dr Neil Lane, the science advisor to the then President of the United States, Bill Clinton, have visited his laboratory. His research group develops computational methods to discover the fundamental mechanisms driving chemical reactions, and catalytic, biological, and industrial processes. In 2009, the Nvidia Corporation awarded Professor Naidoo a long-term Nvidia Professor Partnership grant to advance the group's research programme that is centered on accelerating scientific software using General Purpose Graphical Processing Units (GPGPUs). He is known for his invention of the highly successful FEARCF (Free Energies from Reaction Co-ordinate Forces) method that is used to predict dynamic properties in chemistry and biology.

"The HPC node ran its first UCT job in early 2011. Since then, it has been used across 12 departments, using 208 cores (or processors) and 45 specialised science packages."

Managed by technical specialists, Timothy Carr and Andrew Lewis, the HPC node ran its first UCT job – for Dr Ake Fagereng of the Department of Geology – in early 2011. Since then, it has been used across 12 departments, using 208 cores (or processors) and 45 specialised science packages.

The core component of any HPC system is its storage. The ICTS HPC sports an impressive 25TB scratch area – a directory to hold files and directories for short periods of time – for research data analysis and a further 25TB for archived data.

With demand steadily climbing, the service is expected to clock over 250 000 processing hours by the end of 2012.

The rise of the cellphone

High-processing computing has clearly become an essential technology for the modern university. But two UCT units are also looking at those consumers – and there are millions of them – whose needs sit at the other end of the computing spectrum.

Much of the world's computer science systems were designed in the developed world, with developed-world infrastructure in mind, explains Professor Gary Marsden of UCT's Department of Computer Science. Networking, for example, assumes a constant supply of electricity and fibre-optic cables; this is not always the case in the developing world.

Professor Marsden approaches this problem from a different perspective, calling on his background in human-computer interaction.

"Many of us were trying to apply developed-world technologies and solutions to problems in Africa, and it just wasn't working," says Professor Marsden. "So we had to go back and rethink our discipline."

To this end, Professor Marsden and colleagues set up the ICT Centre for Development at UCT. Through the centre, Professor Marsden and his team have designed applications that allow users to both draw up curricula vitae and apply for jobs using their cellphones. They are also working on two major new projects – the first will, if it works out, allow rural communities to set up their own cellphone

Master's student Ian Rogers and Professor Kevin Naidoo in the SCRU Cluster Server Room.

The newly established Samsung Mobile Innovation Laboratory at UCT seeks to develop innovative mobile phone applications in response to unique African needs.

networks without the need of an operator or network costs; the second will help such communities capture, archive and share their stories via their mobile phones.

The centre has partnered with international bodies such as the Hasso Plattner Institute in Germany and, more recently, Samsung Electronics to set up the UCT Samsung Mobile Innovation Laboratory (SMILe). The objective of the multi-million rand SMILe is to develop "innovative mobile phone applications in response to unique African needs".

African development

Apart from hosting the SMILe lab, the Department of Information Systems, through its research unit, the Centre for Information Technology and National Development in Africa (CITANDA) pursues a variety of other research interests. While still examining the role of ICT in national and continental development, CITANDA researchers do not so much concentrate on the technology per se, but on systems – taking cognisance of the interplay between ICTs and organisations, and ICTs and society.

Projects have covered, for example, information systems education and e-learning, the nature of e-commerce and e-government in Africa, the impact of ICT infrastructure expansion on human development, and on democracy, and mobile banking among the millions of cellphone users in Africa – banked and unbanked.

CITANDA has also tapped into its far-flung network of collaborators and graduates; its doctoral alumni, for example, hailing from Botswana, Kenya, and Nigeria. That geographic spread feeds into the researchers' and the centre's research goals.

"Context matters," says Professor Irwin Brown, CITANDA Director. "Nairobi and New York are very different places; if you set up a system in Nairobi or Dar es Salaam, you have to contend with a very different set of contextual issues than you would in New York."

From setting up high-performance clusters to looking at cellphone applications, that is something that UCT researchers have to keep in mind at all times.