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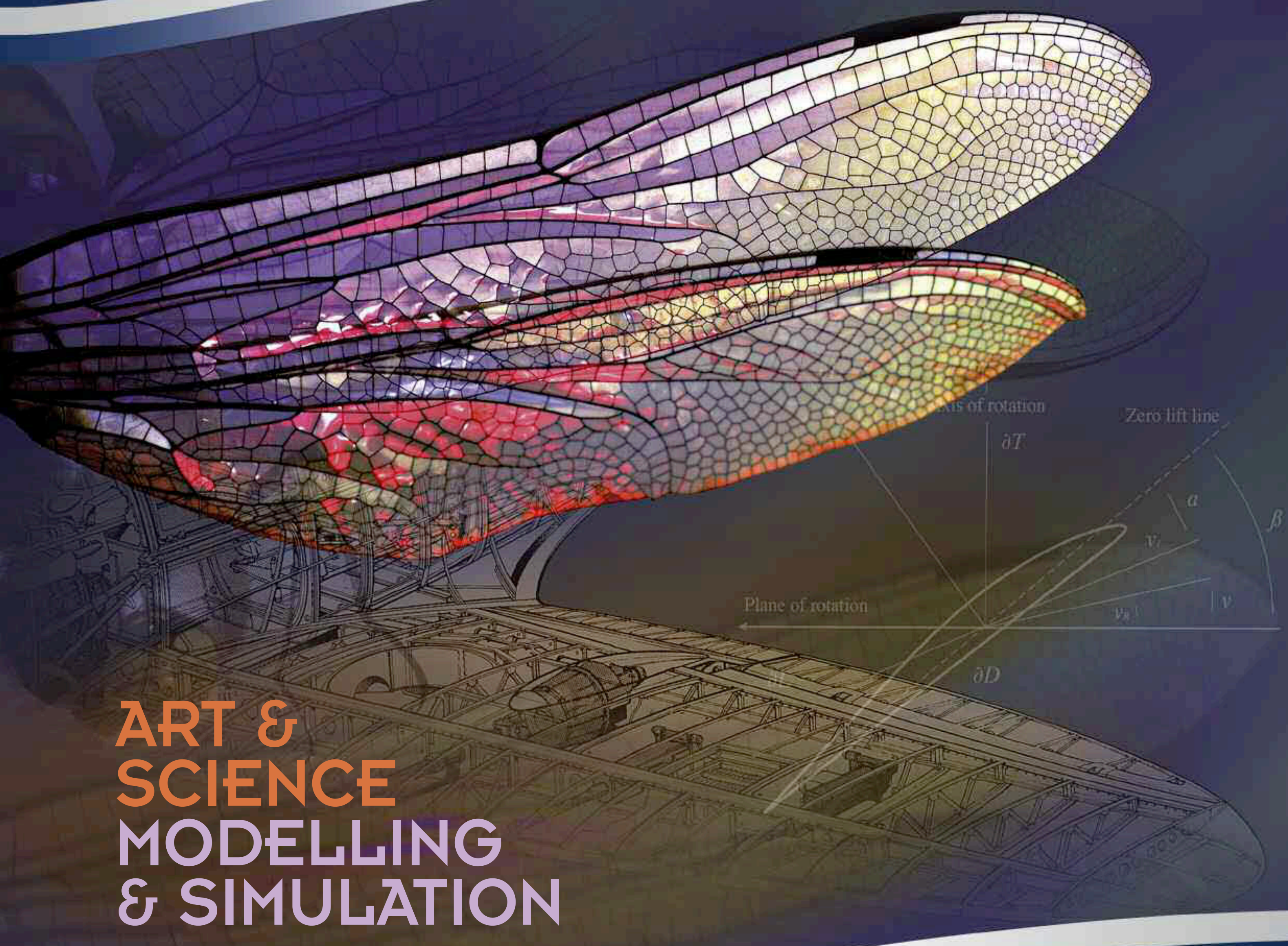

ART & SCIENCE
MODELLING & SIMULATION

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our future through science

Volume 2 Number 4 March 2008

IN THIS ISSUE...

THE ART AND SCIENCE OF MODELLING AND SIMULATION

Sowing the seeds
of leadership in innovation

CABINET APPROVED the Department of Science and Technology's (DST) 10-year plan for innovation in South Africa recently. Called 'Innovation towards a knowledge-based economy', the plan states as its primary goal South Africa's transformation towards an economy where the production and sharing of knowledge culminate not only in economic benefits, but enrich all facets of human endeavour. The plan's gauntlet to be taken up by the scientific community is five 'grand challenges', designed to stimulate multidisciplinary thinking, answer burning questions facing our nation and create new disciplines for preparing us for the future.

Biotechnology and related pharmaceuticals; climate science; energy security; space science and technology; and an understanding of the shifting of social dynamics form the heart of these challenges. As a public research institution, the CSIR has a mandate to play a leading role in the creation of wealth by seeding knowledge-based industries that will make South Africa a competitive nation by 2018, in line with the 10-year time line. While the CSIR already focuses research capacity in areas that can rise to the challenge, it will continue to establish capacity in other strategic ones such as mathematical sciences and autonomous intelligent systems. Attracting scientists in these fields from all over the world to enrich networks that are so important in this new age will also open new opportunities for learning.

But how can we generate and develop the skills needed to think across the sciences, to innovate from angles that harness our unique challenges and insights towards positive outcomes? This edition of **ScienceScope** features the art and science of modelling and simulation. Modelling forms the basis of conceptualisation, arguably the first step towards innovation. It allows people to deal with complexities, be it the dynamics of society, the development of a radical new cure or working with the fragile balances of an endangered ecosystem. As a discipline, it relies on deep knowledge of mathematics and statistics, cutting-edge computation facilities and modern approaches to software development, all elements acknowledged as key building blocks of the information age and knowledge economy. The diverse and agile use of these capabilities is demonstrated in articles in this publication.

We know that many of the challenges we face are not exclusive to Africa, but our unique context and knowledge of our continent and its people enable us to develop and deliver surprising and human-centred solutions. Modelling and simulation, and the supporting building blocks of science, will continue to enable the CSIR to blaze a trail towards a knowledge-based economy.

Dr Sibusiso Sibisi, CSIR President and CEO

The art and science of modelling and simulation

by Dr Jan Roodt, CSIR (invited guest editor of this edition of **ScienceScope**)

SOME SAY IT IS RISKY to use the words art and science in one sentence when talking to scientists and engineers. And it must be even more perilous to add the 'contentious' concepts of modelling and simulation to the brew. The immediate objection from many practising professionals in the scientific arena is that modelling and simulation are to be used only when rigour is not needed, or when people are lazy. This article and others in this edition of **ScienceScope** may bring another perspective to the discussion.

What is the aim of science? Herb Simon states in *Sciences of the Artificial* that the goal of science is to make the wonderful and the complex understandable and simple without detracting from the wonderful. Similarly, the aim of engineering is to devise artefacts (physical and non-physical) to help us solve problems. Paul Cilliers states in *Complexity and Postmodernism – Understanding complex systems* that we model (verb) in order to gain understanding. It is implied that modelling is fundamental to the scientific enterprise and that it is a tool in the hands of the investigator, thus something that could similarly be seen as the result of engineering or the tools for engineering.

We need to have a good understanding of matters in order to make appropriate decisions. When we make a good decision (through inspection of the outcomes), we expect that things will turn out well for our enterprise or effort, while also expecting that if the decision is shown to be wrong, we might not like the consequences. If we could investigate and reliably consider the outcomes of decisions before we make them, it would mitigate the risks. To be able to do that, we need some representation of the system or world to work with, to experiment with before we take the plunge in the real world. Such a representation of reality is called a model (Ackoff, 1968). More elaborate definitions exist, but I believe this one will suffice for our purpose.

Modelling is the act of constructing a model, and this is where art and science start entering the equation: We cannot develop an appropriate representation of the world without first coming to some level of understanding of the world or the phenomena we are dealing with. It relies heavily on the ability to do a scientific analysis of the phenomenon or part of the world that we are interested in. A crucial component of the scientific process is the ability to know what to include and exclude from the phenomena under scrutiny. In the case of modelling, it becomes almost an art to develop a good enough (but no better) representation of reality and to know how to check its validity so that we retain the wonderful while simultaneously gaining understanding.

A model may also be equated to an actor in a play. The actor represents a character and must mimic the behaviour and actions of that character. The actor must be consistent in how he/she reacts to stimuli from the world of the play. The actor gets directives from a script and acts within the environment prescribed by this script. It is not acceptable to have an actor in Shakespeare's *Hamlet* reciting the script from *Romeo and Juliet*. The expectation from the audience is also that some reality should hold through-out the play: When the script calls for it to be night, the actors must take cognisance of the fact that it is night. In a rather roundabout way, this is a description of the role of a simulator and a simulation. One may say the model stands in relation to the simulator as the actor stands in relation to the stage. Models are executed in a simulator and the script is known by the simulator and the models. The whole event (play) is called a simulation.

A good play has a good script, an appropriate stage and actors who give a believable rendition of the characters that interact in the make-believe world. A good model will act like a phenomenon in nature, or a process or man-made artefact within the context of our questioning.

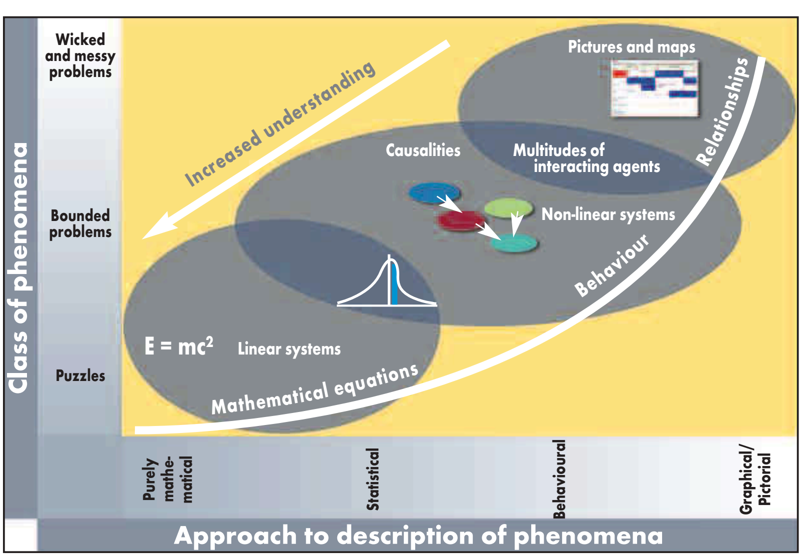
Coming back to the fact that we use modelling and simulation to understand things, to optimise a situation for decision making or predict a future state of something in nature or a process, it is evident that not all models are created equal. Some must be devised to give a specific answer when asked a specific question or when receiving a specific stimulus. The kind of phenomena referred to here is called a puzzle (Michael Pidd: *Tools for thinking – modelling in management science*). Consider the splendid model from the work of Einstein: $E = mc^2$. If we make $m = 1$ and $c = 3x10^8$, then $E = 9x10^{16}$. We know what the pieces of the puzzle are and we know that when all of these are put together correctly, it yields one, and only one, verifiable result. These models are by no means of a lesser value than any others – a complex law of the conservation of mass and energy is explained beautifully. This model is very efficient in its use of simulator hardware and software: It can be executed even in our own brains, but the answer is really useful only within the context of the work of Albert Einstein on relativity, which is a massive body of knowledge and deep understanding.

In other cases, a single stimulus might result in a range of possible outcomes, for example a statistical model using probability distributions or superpositions of distributions to generate its output. The so-called (bounded) problems (see the y-axis of the figure) may be approached via these types of models. Another technique to understand the problems is to develop models that 'behave' in a certain manner under stimulus, sometimes even generating surprising (or so-called emergent) outcomes. This method relies on the interaction of agent-like software elements, interacting in simple ways with one another to mimic highly complex behaviour. A good example is the modelling of the flocking behaviour of birds, using simple rule-based agents.

The last large group of phenomena typically considered by the modeller is wicked and messy problems. So little is understood here of the complexity that we are dealing with that it is possible to consider only relationships (pictures and diagrams) between elements that we think should be considered in an attempt to gain a better understanding. The decision on who should get what level of medication during a deadly epidemic might fall into this category. Work across several disciplines is needed to be able to generate a common basis for understanding on which to make decisions. Once we have a model that describes the wicked problem adequately however, we can start breaking the messiness down and try to model it with techniques that rely on behaviour. In turn, it might yield models and solutions that allow us, for example, to use statistical distributions. Every cycle increases the understanding of the phenomena we are dealing with, until we are able to discover the fundamental elements that rule the system.

Sometimes, and this is the artful part, we must know when more slicing and dicing of the problem will not yield more understanding, but only contribute to the confusion. This is why modelling is now recognised formally as a type of research methodology – action research. The laboratory of the action researcher includes advanced and complicated software and hardware, often developed in-house. Sometimes large government-sponsored facilities are used for the computational power needed to do research into the rational design of drugs, or to understand the turbulence patterns around an innovative wind-power generator blade.

Clearly, developing models and simulations is not for the lazy or for those looking for a quick way out. What is needed for this kind of science are individuals with competence in several fields and the discipline of scientific rigour.



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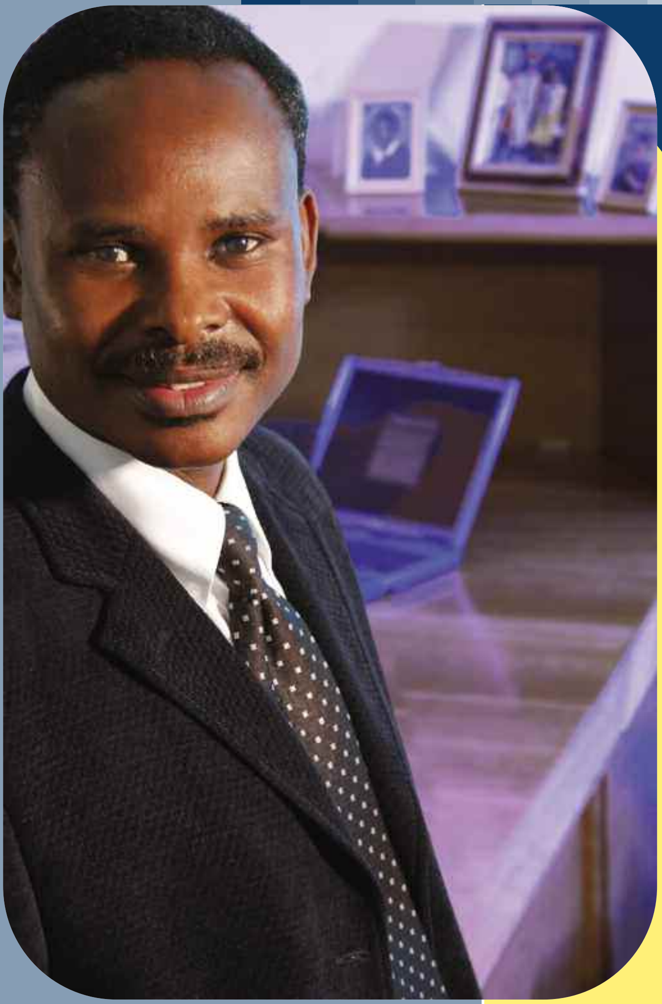
Graphical modelling

The graphical/pictorial description of wicked problems

Dr Jackie Phahlamohlaka



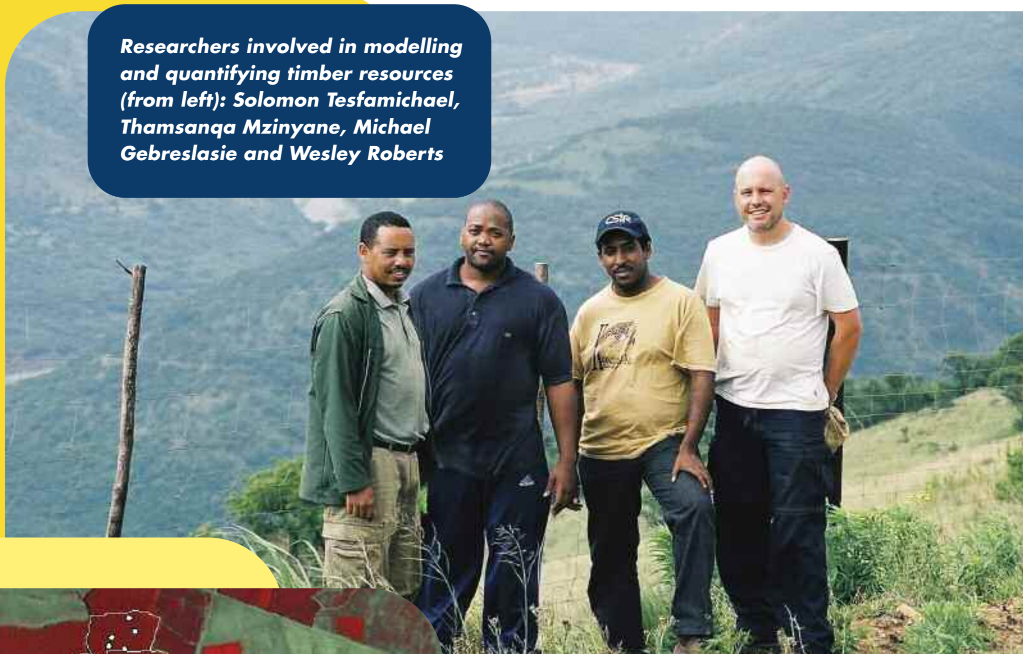
THE DISTINCTION between wicked, ill-structured or messy problems and the so-called tame problems is described in various ways in the literature; but the graphical distinction captured by Schon[1] in his extended metaphor is illuminating, contrasting the 'high ground' where problems are of great technical interest but of limited social importance, with the 'swamp' where messy and confusing problems defy technical solution. Two commonly used approaches to bringing some structure to wicked problems exist, namely mind maps and rich pictures. Mind maps are easily created by using post-it stickers (sticky notes) and then attaching meaning by rearranging and connecting these by lines. Rich pictures, on the other hand, use symbols that are grouped together in clouds, blobs and/or boxes, with arrows depicting connections. Through the use of these pictorial descriptions, the modeller is able to identify possible interactions and relationships within a mess. The goal is not completeness, but parsimony, to filter out the noise and get to the core. Successfully created mind maps and rich pictures could give to the modeller elements of structure, elements of process as well as the possible relationships between structure and process and between the processes themselves, thereby enhancing understanding of the phenomenon being studied substantially. – **Dr Jackie Phahlamohlaka**

From CSIR Defence, Peace, Safety and Security, **Dr Jackie Phahlamohlaka**'s current research interests are in ICT and socio-economic development, web-based collaboration and thinkLets within a collaboration engineering research framework.

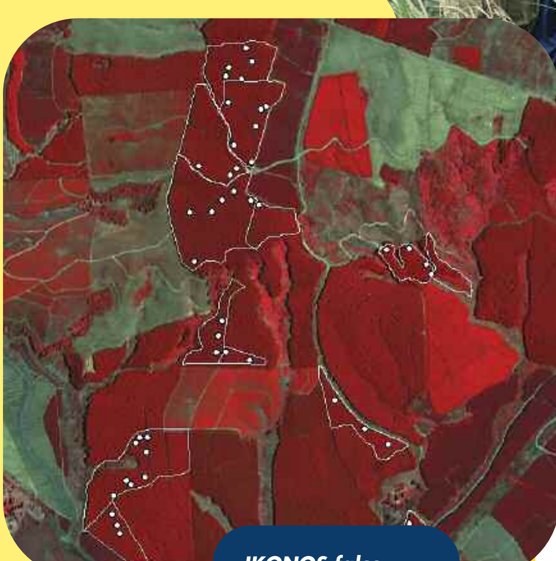
[1] Schon, DA 1987. Educating the reflective practitioner: toward a new design for teaching and learning in the professions. Jossey-Bass, San Francisco, California.

Using remote sensing and environmental data to model plantation forest attributes

by Wesley Roberts, with Michael Gebreslasie, Solomon Tesfamichael and Thamsanqa Mzinyane



Researchers involved in modelling and quantifying timber resources (from left): Solomon Tesfamichael, Thamsanqa Mzinyane, Michael Gebreslasie and Wesley Roberts



IKONOS false colour composite with timber compartments and enumeration plots

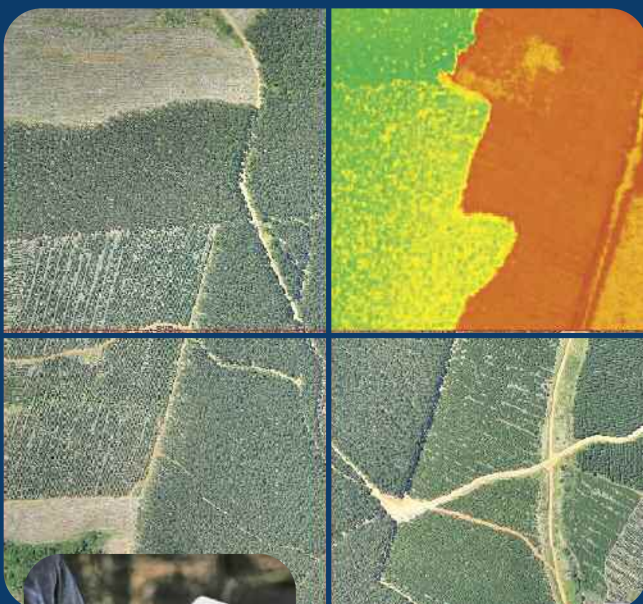
THE FORESTRY and Forest Products Research Centre (FFP), a joint initiative by the CSIR and the University of KwaZulu-Natal, and Mondi Business Paper embarked on a collaborative project in 2004 to explore the potential benefits associated with using remote sensing for plantation-related activities. Several projects were identified, all of which required modelling.

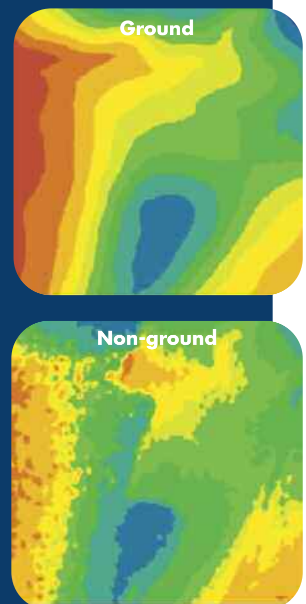
The cooperative seeks to track the latest developments in remote sensing technologies and the cost-effectiveness of these while quantifying and validating the precision achievable with different remote sensing technologies. It also seeks to determine the strategic role that remote sensing has to play in addressing practical problems encountered by the industry. Three separate research avenues were identified, namely the link between wood quality and foliar chemistry; net primary productivity (NPP); and structural assessment.

These have become the focus of research over the past three years and include both process-based and empirical modelling activities. The three-pronged approach includes analysing the relationship between foliar chemistry and wood lignin concentrations.

The relationship is important as mapping wood lignin concentrations using remote sensing provides insight into

High resolution aerial photography and LiDAR (light detection and ranging) top of canopy model





wood quality and aids in planning cost-effective harvesting schedules. The quantification of NPP leads to a better understanding of growth and productivity on different sites. NPP is measured with the aid of remote sensing data and a process based-model called 3-PG.
An additional important variable that can be measured using NPP is the rate of carbon sequestration.

Recently, commercial plantation forests have been identified as potential carbon sinks, as the fast-growing trees remove more carbon from the atmosphere than slower growing indigenous species. Quantifying rates of sequestration using NPP as a proxy will help in determining the amount of carbon offset by the industry. Following NPP, the third project seeks to quantify timber resources through forest structural inventory. Typically, inventory measures such as tree height, stem width and stand density are collected using manual ground-based methods. The project replicates manual inventory using remote sensing technologies, in order to model/predict merchantable timber volumes using cost-effective methods.

Stakeholders such as Mondi BP benefit from full access to research results and also have access to fully trained remote sensing professionals who can distribute their capacity either through interactions with industry partners or through full-time employment.

Model development requires accurate characterisation of the system, which is mostly complex with any number of input variables acting on the object being modelled. The remote sensing cooperative has sought to characterise the plantation forest system through empirical observations during regular field trips. Destructive and non-destructive sampling of timber plantations provides researchers with the necessary data to understand the underlying dynamics of the plantation system.

The foliar chemistry and NPP studies both use destructive sampling techniques to collect leaves and branches for analyses in the FFP labs. The foliar chemistry determines concentrations of nitrogen, chlorophyll, lignin as well as leaf area index. Leaf level measurements are then compared to wood samples using linear regression analysis, determining the strength and significance of the relationships, leading to a better understanding of the system. Following this, hyperspectral imagery derives a relationship between various indices and leaf level measurements. The empirical modelling shows that strong relationships exist between reflected light (coming from the canopy) and selected wood properties. The resulting maps are useful in determining timber wood quality without actually performing any field surveys. The same technique is also used to characterise tree height and width and stand density. The empirical models are used to gain a better understanding of the dynamic relationships that exist within a timber plantation and to determine if remote sensing is indeed a suitable support tool.

The second step in developing a suitable model is to make assumptions regarding the system based on the initial empirical evidence. Following this, the third step focuses on developing either statistical or mathematical models that are able to characterise the system in question. Determining the accuracy and precision of a model involves validating the results against a control data set. Simulation and validation make up steps four and five of model development. If, following these two steps, the results from the model simulation are within an acceptable error range, the model can be applied operationally. The remote sensing cooperative is developing models using this approach. Currently empirical relationships between image spectra and field enumerated foliar and structural data are being investigated.

Statistical models based on the observed empirical relationships will then be used to run several simulations and determine the accuracy of the models. Models that include climatological data such as 3-PG also provide the opportunity to investigate the impact that climate change may have on timber growth and productivity.

The driving force behind all modelling activities is the development of tools that will allow the South African timber industry to remain competitive amidst increasing competition from both Asian and South American competitors. Mitigating and planning for future changes resulting from global warming and climate change are also central issues that will be explored in future.

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Modelling for better ports

by Hans Moes

Stability tests underway on the head of the main Khalifa Port breakwater, with the new (blue) Wallingford wave generators in the background

Senior CSIR researcher Hans Moes

IN MANY COUNTRIES, a significant component of the national economy depends on maritime trade. This is also the case in South Africa, where more than 90% of the country's international trade goes through its ports. In addition, ports are becoming hubs of industrial development, especially for importing basic materials and exporting manufactured products.

In South Africa, Transnet is responsible for large components of the country's national transportation system, including ports. This also relates to port planning, operation and expansion. Ports are exposed to many complex interactions of their physical environment, like tides, currents, waves and wind, and their effects on port structures like breakwaters and quays, on shipping and loading, unloading and storage. In most cases, such interactions have to be quantified accurately as part of the design of a port. This is done by using numerical and small-scale physical models and by prototype monitoring.

The coastal engineering and port infrastructure group of CSIR Built Environment in Stellenbosch operates such small-scale models in its hydraulics laboratory.

Khalifa Port's main breakwater model under construction in the CSIR's hydraulics laboratory in Stellenbosch

Only a few such laboratories exist in the world, usually operating as a national facility. The laboratory in Stellenbosch ranks as one of the 10 largest in the world. It is used for research and training in coastal and port engineering, in cooperation with Stellenbosch University, the Delft University of Technology (TU Delft) in the Netherlands and local consultants such as Murray & Roberts and WSP Coastal Africa, under the umbrella of the Centre for Port Research and Training (C-PoRT). The centre is co-funded by the CSIR, Transnet National Ports Authority (TNPA) and the Department of Science and Technology.

Research focuses to a large extent on waves and monitoring prototype coastal structures and moored ships. This work is done in cooperation with European academic and research institutes and through exchange of research teaching staff and students. The CSIR also undertakes a significant amount of external contract studies. These support South African port developments, in close cooperation with local coastal and port engineering consultants, with the NPA as the ultimate client. In many cases, model studies are carried out for international clients.

Extensive model studies were carried out for the design of the new ports of Richards Bay and of Ngqura (Coega) and for the extension of the ports of Durban and of Cape Town. The largest (in South African rand terms) model investigation ever to be carried out by the CSIR is a study of the design of the Khalifa Port in the United Arab Emirates, undertaken for the Abu Dhabi Ports Company, under contract with Halcrow, an international consultant, and with participation of other laboratories such as Delft Hydraulics. The present value of the contract is about R10 million and it is anticipated that more work will be awarded as the study results become available. The study focuses on the design of the extensive breakwaters to protect the port against waves and on the mooring conditions of container vessels and bulk carriers in the port.

This prestigious contract was obtained in competition with international laboratories and is an indication that the hydraulics laboratory in Stellenbosch is considered a world-class facility. The laboratory was upgraded recently with new Wallingford wave generators, comprising a new wave measurement system with new wave probes and software, and an improvement of the keogram video monitoring system for moored ship dynamics. With a shortage of local coastal engineers, the CSIR has been fortunate in recruiting two engineers from the TU Delft, one of them a postdoctoral researcher, while active technology support is provided by a number of specialist sub-consultants.

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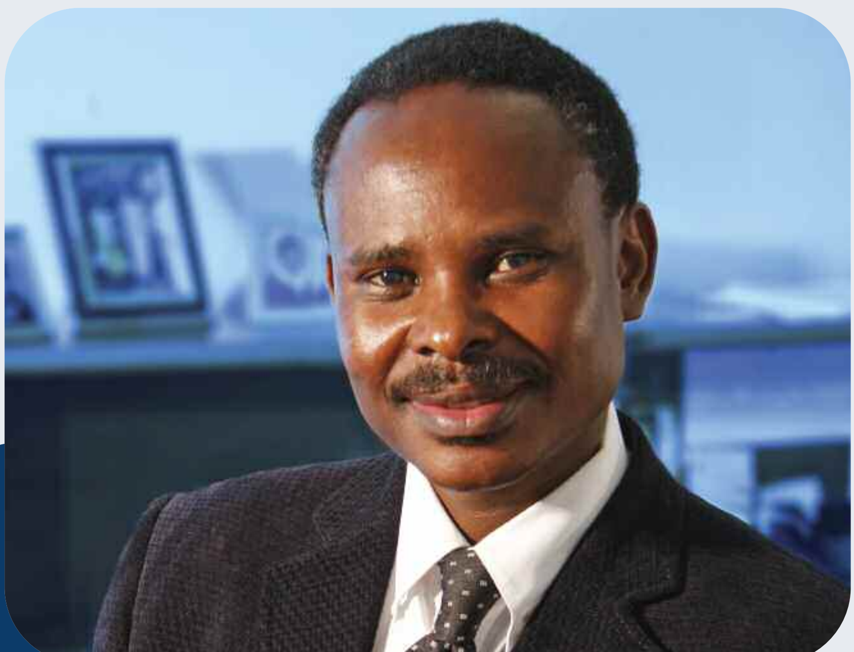
Simulation could aid implementation of legislation

by Dr Jackie Phahlamohlaka



THE UBIQUITY of the internet and associated web-based information and communication technologies enabled by it, continue to prompt scientists, engineers and technologists to experiment with the potential use of computer-based support systems in areas previously unimagined. An example of this is a computer-based modelling and simulation of the implementation of an Act of Parliament within a South African e-government context.

The requirements of South Africa's Promotion of Administrative Justice Act – PAJA (Act 3 of 2000) and the government's Batho Pele policy directive that puts the interests of the people of South Africa first, provided the CSIR with an opportunity for initiating a research project, the design of which involves the creation of a simulation framework in support of the implementation of PAJA. In terms of this Act, South Africans have a constitutional right to lawful, reasonable and procedurally fair administrative action, and to be given reasons for administrative action. The Act sets out procedures that government officials must follow before and after taking a decision. The procedures, which apply to all organs of state, and the rubrics thereof, are documented in the Code of Good Administrative Conduct.

The rubrics align closely with decision-support systems in computer science, operations research and information systems. Our research is conducted within informatics, specifically within decision theory and group decision-support systems. We explore innovative ways in which web-based group support systems (GSS) tools can be used to enable ordinary South African citizens to effectively engage with one another, government administrators and managers. The study also aims to identify and harness opportunities for sustained collaboration and interaction by communities who would use web-based GSS tools within the e-government context. To support innovative engagement, sustained collaboration and effective interaction, collaboration engineering through the notion of a thinkLet and participation in its creation and packaging, is adopted and used.

The main research question focuses on the features needed in web-based collaboration tools and how interfaces should be designed to enable citizens to interact effectively with government and public bodies in South Africa.

The six-year study, which is currently in its fourth year, is partially funded by the National Research Foundation with several postgraduate students and co-investigators researching different topics. It is conducted in partnership with informatics researchers from the University of Pretoria (UP). Several research outputs have already emerged, including three Master's dissertations, two Honours papers, five refereed conference proceedings, an invited book chapter and a journal publication. The study has received support from participants, municipalities and organisations from North West, Mpumalanga, Limpopo and Gauteng.

One may ask what contribution this study makes to the life of ordinary South Africans. From an academic point of view, it could be argued that the answer is clear for all to see. But this study is not meant to satisfy only academic and research requirements, but also to contribute to the betterment of people's quality of life.

State of the public service in 2006

The state of the public service report by the Public Service Commission refers to the importance of PAJA 19 times and identifies it with the Promotion of Access to Information Act 2 of 2000 (PAIA) as the cornerstones of good governance and transparency. The report points out that despite this, the public service is as yet to abide by the Act, indicating that work still needs to be done to enable compliance. According to the report, the capacity to establish mechanisms for explaining administrative actions and redress as envisaged in PAJA is lacking in the public service. The report contends that departments that cannot provide reasons for their administrative actions and comply with the provisions of the Act are less likely to conduct themselves in a manner that is fair and impartial, and argues that at management level, most decisions should comply with the requirements of PAJA.

A possible solution

Of interest to the CSIR is an observation in the report that it would have been easier if decisions were plotted against the procedures for PAJA, as gaps and deviations would be easily identifiable.

Our aim is to show that computer-based technology can help in these processes. Three field locations were selected to carry out the simulation exercises: Siyabuswa in Mpumalanga (hosted by SEIDET), Lebotloane in North West (hosted by Leretlabetse Thusong Service Center) and several civil society organisations (hosted by the UP) in Gauteng. The choice of these locations was influenced by the availability of networked computers, the distance of these from the UP and the CSIR, as well as the willingness of the leaders from these institutions to participate in the research project.

While neither all the features needed in web-based collaboration tools could yet be described, nor how the interfaces could be designed to enable citizens to interact effectively with government and public bodies in South Africa, we are encouraged by the emergence of the thinkLet that was created by the CSIR. We believe a mechanism has been established to do this research on a larger scale, using a repeatable and predictable process that has the potential to be transferred to participating communities and government departments to run on their own, following the principles of collaboration engineering. It is possible that the various thinkLets that are expected to emerge from subsequent simulations could be automated and used within a web environment in support of the PAJA implementation.

In an exploratory study such as this where the value of technology is to be demonstrated, there can't be a better way of achieving this than through simulation.

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THE SOUTH AFRICAN National Defence Force (SANDF) is responsible for enabling stability in Africa. This implies that peace support and counter terror operations will need to be carried out across the continent. The strategy is for rapid response of a highly mobile force based on contingencies or as problems develop. It is very difficult to train soldiers for these missions due to the variety and infrequency of scenarios. Training is therefore limited to relatively unrealistic scenarios that either don't include live fire or enemy forces, or have only small teams training simultaneously.

Internationally, large training facilities and simulators have been created to overcome this problem. Unfortunately, these facilities and simulators cost billions of rand, making this approach unaffordable in South Africa.

Computer soldier games have made significant advances in the level of realism, accuracy and multi-player capability due to the high commercial demand. The CSIR therefore focused on moving from a PC game towards a real soldier scenario in an African context. Various games were researched and Swat 4 was used as a technology demonstrator. This is a first person shooter game, where the player sees a view as if he/she is walking inside the game. Multiple players can participate in the same game and carry out tasks as if in a team or as being the opposition.
To make these games useful for

Simulation for peace support and counter terror

by Trevor Kirsten

Simulated urban training facility (above) and real facility (right)

Simulated South African embassy in a foreign country

peace-keeping and hostage-release purposes, the scenes, scenarios and equipment required modification. Two settings were used as demonstration:

a) an urban training facility used for conventional force preparation and
b) a South African embassy in a foreign country. Following this, a four-terminal network was created to assess the value of this simulation in training and operational preparation.

The users' feedback held that the level of realism in creating their own scenarios was good; the user interface was quickly learned by non-PC users, but the results were dependent on PC dexterity; and the demonstration proved valuable. The SANDF then requested that this capability be placed within the context of all other training and simulation aids and facilities. This is a relatively complex process due to the various dimensions of the problem space, including fidelity, simulation reality, and level in systems hierarchy. A space diagram was constructed based on the dominant dimensions and this was populated using the available systems and future requirements.

The off-the-shelf first person shooter (FPS) games, like Swat 4, are shown in the figures as a low fidelity virtual simulation. After the tailoring of the FPS games to consider specific scenarios, as described, the fidelity moves to a medium level. This indicates a higher user value associated with using a modified game. The modification does, however, not make any changes in the virtual nature of the game. A space diagram will therefore be used to help make decisions, as off-the-shelf games have a low value but tailored games have a much higher user value. What could also be extracted from the diagram is that it would be even better if the tailored FPS game could be moved into the live area by, for example, allowing larger team simulation, possibly linked to physical training facilities.

The CSIR is continously reviewing simulation software available for this application, for example Virtual Battefield Simulation from Australia. The objective is to select the most appropriate tools with the highest impact to cost ratio. In parallel with this, the CSIR aims to move the virtual world as close to the reality as possible.

In summary, this project aims to deliver maximum impact via simulation support to the SANDF's training and operational preparation for missions that are aimed at uplifting the African continent.

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Dr Adam Goliger (left) and Ters van Wyk in one of the CSIR's wind tunnels

Wind engineering improves design of built environment

by Dr Adam Goliger

WIND ENGINEERING is a fairly new discipline of engineering sciences, developed over the past 50 years or so with the aim to research and quantify the interaction between wind and the built environment. A recent example of its value is the CSIR's testing of three large sports stadia, conducted in 2007 at the request of the development teams involved in the 2010 FIFA event.

The progress of wind engineering was driven by the rapid advancement of the built environment and the constant pursuit of better, cheaper and lighter materials and structures. This, in turn, created a specific demand from the engineering profession, which realised that the traditional approach to wind loadings, based on the assumption of uniform flow (adopted in other applications of aerodynamics such as planes or vehicles) is not valid in real-life situations. The modern approach to structural loading, which takes into account the turbulent nature of wind, has enabled people to design and develop a new generation of super-tall buildings and long-span cable-stayed bridges.

Due to its nature, the science of wind engineering overlaps with (and includes inputs from) several other sciences, including weather and climatology, mechanical and structural engineering, environmental sciences and statistics. While wind engineering activities at the CSIR have been carried out for the past

30 years, full-scale measurements of wind flow or structural behaviour are difficult and costly. The modern approach to wind engineering, like in many other sciences, is therefore largely based on:

- Researching and optimising relevant and adequate modelling techniques
- Undertaking comprehensive testing processes
- Developing appropriate methodologies of full-scale application of the information obtained from model-testing
- Developing prediction models to be implemented in design manuals.

The modelling activities currently performed by the CSIR can be grouped broadly into wind-tunnel modelling of structural response; modelling of environmental wind impact; statistical analysis of wind climate and prediction of extreme wind speeds; risk modelling of wind damage and disaster; and development of manuals/codes of practice for structural design of the built environment.

A substantial part of the CSIR's activities involves the boundary-layer wind-tunnel laboratory. This facility and the related expertise are unique in South Africa (and on the African continent). One of its crucial aspects, distinctive from other wind tunnels at the CSIR, is its ability to recreate the complexity of the turbulent nature of wind and its flow correlation characteristics, which are critical for adequate representation of the full-scale situation and economical design.

The results of research studies undertaken in the wind tunnel form specific inputs to design manuals and codes. Examples include comprehensive testing of industrial light fittings, which formed the basis for the development of the SABS South African National Standards loading code of lighting masts, and the findings of the CSIR's investigation into wind erosion within large social housing developments in the Western Cape, which were applied to town planning directives for the Cape Flats.

The wind tunnel is a design tool and most of the modelling is undertaken at the request of engineers, architects or developers of large, modern developments. An example mentioned earlier is the CSIR's testing of three large sports stadia for the 2010 FIFA event. In addition, the results of the CSIR's wind-tunnel research on topographical influences (undertaken in the past) formed the initial inputs to the design of another sport stadium.

The specific design inputs obtained from wind-tunnel modelling of the stadia include:

- Optimisation process of selected architectural principles affecting wind conditions at areas envisaged for spectators (e.g. galleries, passages)
- Wind conditions over the pitch affecting the spectacle and fairness of the game
- Environmental wind impact of the stadia
- Optimisation of the form and extent of the roofs
- The determination of the design wind loadings and structural response of the grandstand roofs, which are significant (for areas of 20 000 to 30 000 m^2, wind uplifts greater than 1 000 tonnes).

The CSIR has also undertaken several studies of new building developments in South Africa, such as the Table Bay Hotel, Cape Town Convention Centre and the San Raphael building in Durban. These studies investigated the distribution of the design wind pressures, overall forces (e.g. overturning moments) as well as the environmental wind impact. Wind-tunnel modelling is largely applicable to buildings and structures of an unusual shape or size, or those to be placed in the vicinity of other large structures. It is also relevant in view of the complexity of wind-flow within the built environment, largely determined by the neighbouring buildings and structures and is impossible to predict by any other means, including computational fluid dynamics. This explains why wind-tunnel testing of new developments involves comprehensive modelling of the surrounding environment.

The analysis and modelling of wind climate forms an important input to the design process. Some 10 years ago the CSIR and the (then) South African Weather Bureau co-authored a book on South African tornadoes. More recently, the CSIR also developed a geographical model of zones of strong wind occurrence in South Africa. A joint project with Stellenbosch University focused on the collection and statistical analysis of historical data on wind damage and related loss of life. This study formed the basis for the development of a comprehensive risk model of wind damage and disaster for South Africa.

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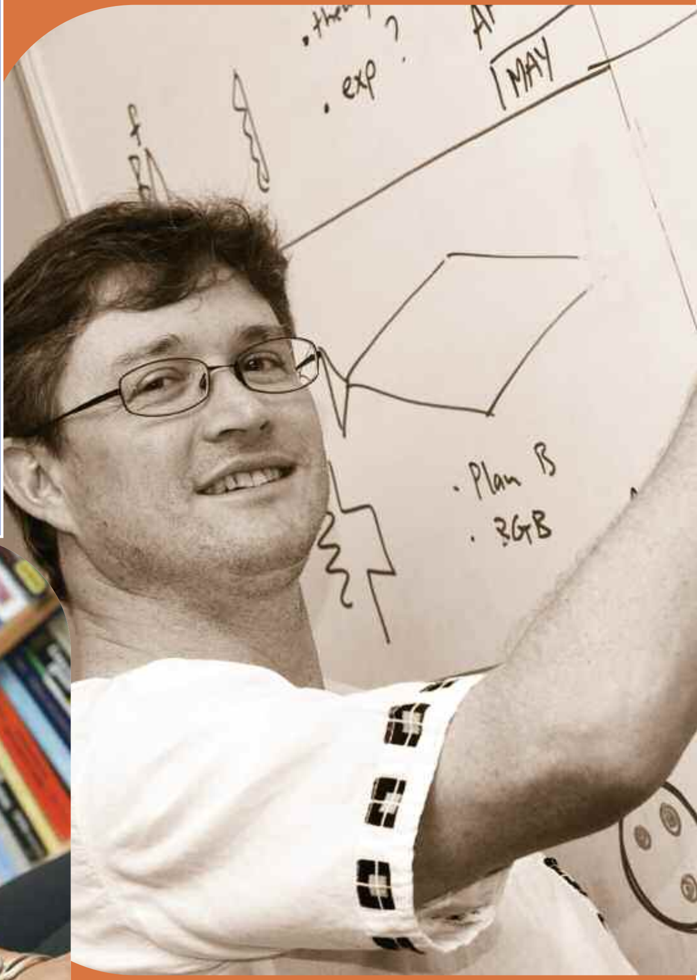
Mathematical modelling

A MATHEMATICAL MODEL involves an abstract structure that uses a mathematical language to describe a system. This abstract structure sometimes depends on the preference and expertise of the modeller and includes, but is not limited to, dynamical systems, statistical models or differential equations. The process of mathematical modelling usually begins with the desire to describe a situation in the real world. In mathematical modelling the goal is to express the real-world problem in symbolic terms that lead to a set of variables and a set of equations that establishes the relationship between the variables. The simple structure allows the modeller to gain insight and clarity about the system because the model is usually designed to describe some aspects accurately, while omitting less relevant details. **– Dr Rebecca Maserumule**

Dr Rebecca Maserumule's research interests involve the use of partial differential equations and numerical computing with and emphasis on inverse modelling in geoscience.



Porro-prism laser enigma
unravelled through mathematical optics

by Dr Andrew Forbes

AN ENIGMA FOR 30 YEARS, a problem in Porro-prism lasers has now been solved by CSIR researchers by applying basic arguments of mathematical symmetry, together with new physical insight into intra-cavity Porro prisms.

The mathematical optics team at the CSIR National Laser Centre concentrates on solving problems in the realms of optics and lasers by approaching problems with mathematical rigour, while recognising the importance of experimental verification. Topics currently studied include creating novel laser beams for biological trapping and tweezing (the technique of using a focused laser beam as an atom trap), propagation of laser beams through a turbulent atmosphere to improve telecommunications signals and creating new laser systems based on micro-optical elements.

This article outlines the approach taken in the recent success of the team, comprising research group leader Dr Andrew Forbes, Igor Litvin (PhD student) and Liesl Burger (MSc student and staff member), and illustrates the power of coupling mathematical, physical and computational tools to solve seemingly intractable problems.

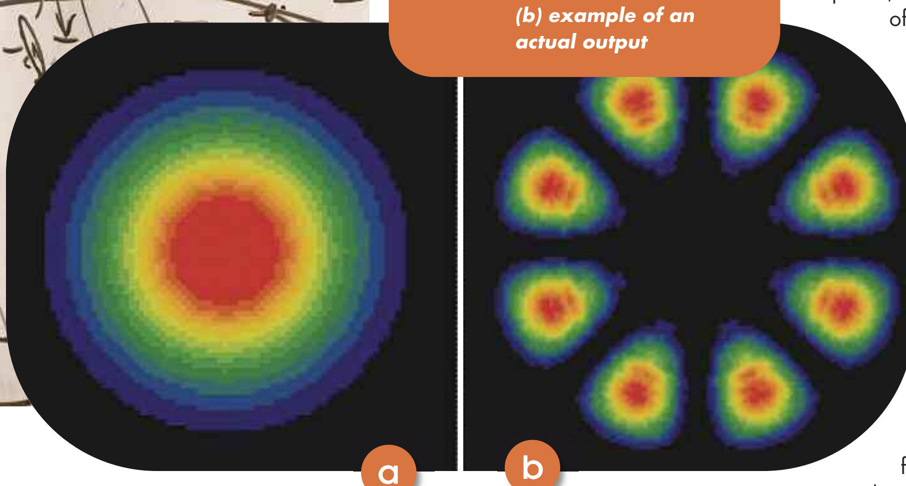


***Figure 1** (a) Example of an expected laser output (Gaussian beam) (b) example of an actual output*

Getting to the bottom of 'temperamental' Porro-prism lasers

Porro prisms (right angle prisms) have the property that all incident rays on the prism are reflected back parallel to the initial propagation direction, independent of the angle of incidence, thus making these insensitive to misalignment. In a Porro-prism laser the traditional end mirrors are replaced by Porro prisms. Such lasers have been exploited for their ruggedness, and used where a laser beam is required at a large distance from the source and where the source is not a stable platform; for example, range finding and laser designators. Despite the ubiquitous nature of these lasers, resonators with internal Porro prisms have not been well understood for nearly 30 years. One would expect an output beam similar to that shown in Figure 1(a), whereas in some lasers the observed output beam was radically different, as illustrated in Figure 1(b), exhibiting petal-like patterns of varying numbers of petals. There seemed no logical reason for these petals, and more bizarrely, the number of petals would vary from laser to laser. Sometimes these lasers would even not work at all, for no apparent reason! Unsurprisingly, the answer was in how one viewed the prisms.

In early attempts to model such lasers, the prisms were treated as though they were perfect mirrors – any incoming ray is returned out, except for an inversion about the reflecting point. This approach was followed and adopted over time as the preferred model for intra-cavity prisms. Since it wasn't working, the question begged: If prisms could not be treated like mirrors, how should they be described?

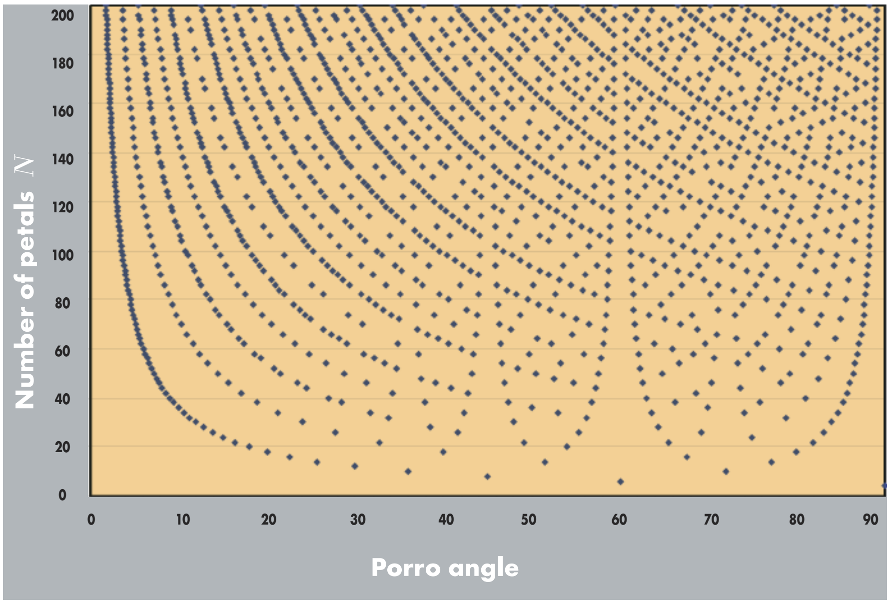


***Figure 2** Plot of the discrete set of angles that gives rise to a petal pattern, with the corresponding number of petals to be observed. Data calculated for $m \in$ [1,100] and $i \in$ [1,50]*

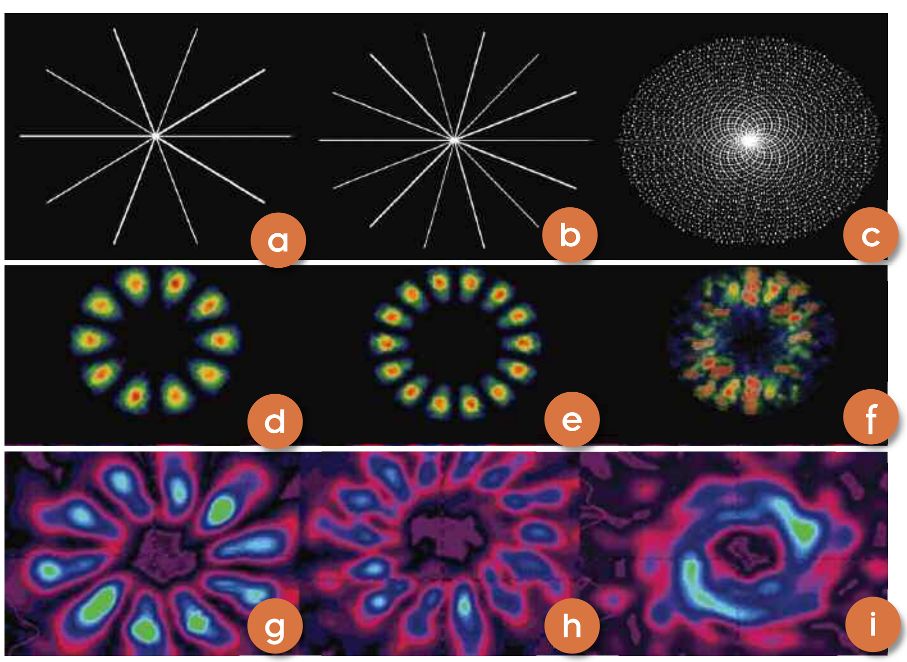


***Figure 3** The analytical model depiction of finitely sub-divided fields in (a) and (b), and an infinitely sub-divided field in (c). Numerically this results in a pattern with (d) 10 petals, (e) 14 petals and (f) no petals. The corresponding experimentally-observed output is shown in (g) – (i)*

Mathematics of symmetries

The researchers approached the problem from a fundamental basis, realising that without a model for the prism, the laser could never be described completely. Two new concepts were introduced – firstly, the prism edges would lead to high diffraction losses and would appear as linear loss lines across the resonating optical field.

Secondly, these linear loss lines would appear to the optical field inside the resonator to be rotating in space, due to the inversion properties of the prisms. To convert these statements into a mathematical expression required consideration of the mathematics of symmetries.

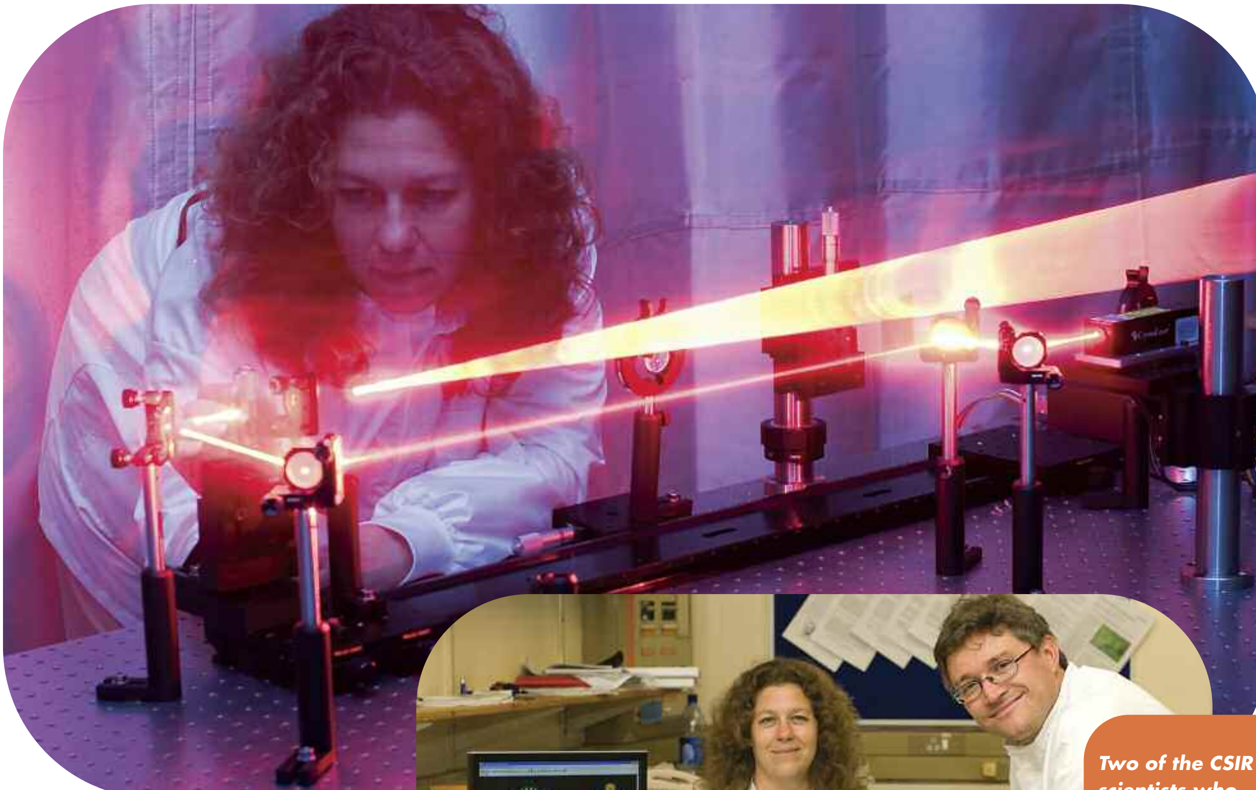
The initial positions of the two prism edges act as mirror image planes – they result in symmetry about each plane after each reflection. These two symmetry planes result in very complex inversions of the loss lines after each pass in the resonator, with the loss lines appearing to rotate in space. Laser scientists asked the question: Will these loss lines ever cycle into a repeating pattern? They were able to derive a simple expression for very specific angles at which this would happen:

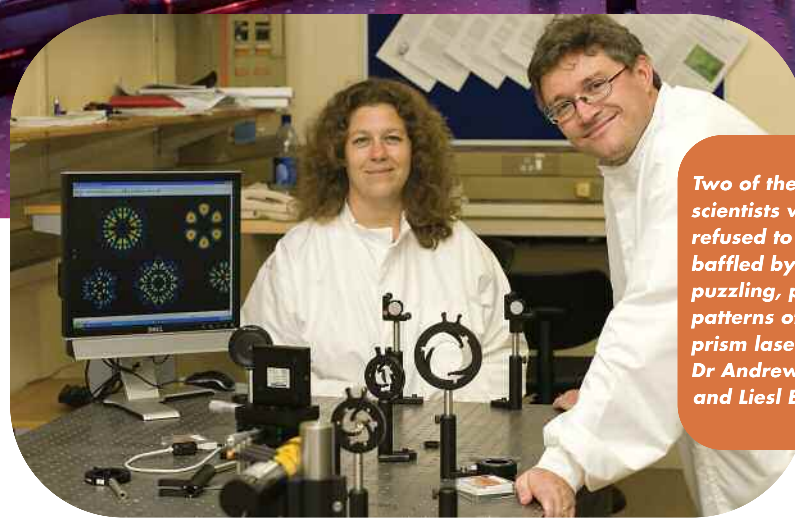
$$\alpha = \frac{i\pi}{m} \quad (1)$$

for positive integers i and m. From this they could also derive the number of subdivisions or petals to be expected:

$$N = \frac{j\,2\pi}{\alpha} \quad (2)$$

for certain integers j. The implication of this is startling:





Two of the CSIR scientists who refused to be baffled by the puzzling, petal-like patterns of porro-prism lasers, Dr Andrew Forbes and Liesl Burger

Only at very specific angles will the field be finitely sub-divided, thus leading to some regions with low loss for lasing to take place. In addition, since the position of these sub-divisions remains stable after a certain number of round trips, the modal pattern that oscillates inside such a resonator will give rise to a petal-like pattern. At other Porro angles the high loss apexes will continuously rotate to new positions, thus resulting in high losses across the entire field. For example, at 30° a laser beam with 18 petals is predicted, at 36° a laser beam with 10 petals is expected, while at 30,5° no stable laser beam is expected. The complete set of calculated stable angles with associated number of petals is shown in Figure 2.

From mathematics to experiment

With this new mathematical model the researchers were able to put together a physical optics computational model of the laser resonator to determine the output laser beam. Having a prediction of the laser beam is crucial for experimental verification of the model. The complete transition from mathematics to experiment is shown in Figure 3. Physical insight, expressed in the language of mathematics and enhanced with computational techniques, allowed a new model to be created of Porro-prism lasers that correctly predicts the observed output. It can now, for the first time, be explained why the so-called petal patterns sometimes seen from such lasers exist, say when these will exist, and predict how many petals will be seen. This new mathematical model also explains why such lasers sometimes do not work, even though very little would appear to have changed in the laser – perhaps only a 0,5° offset in the prism orientations – and opens the way to the restraints on future designs of Porro-prism lasers.

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Movies and further information: www.csir.co.za/lasers/mathematical_optics.html

Operations research: The real art and science of mathematical modelling and simulation

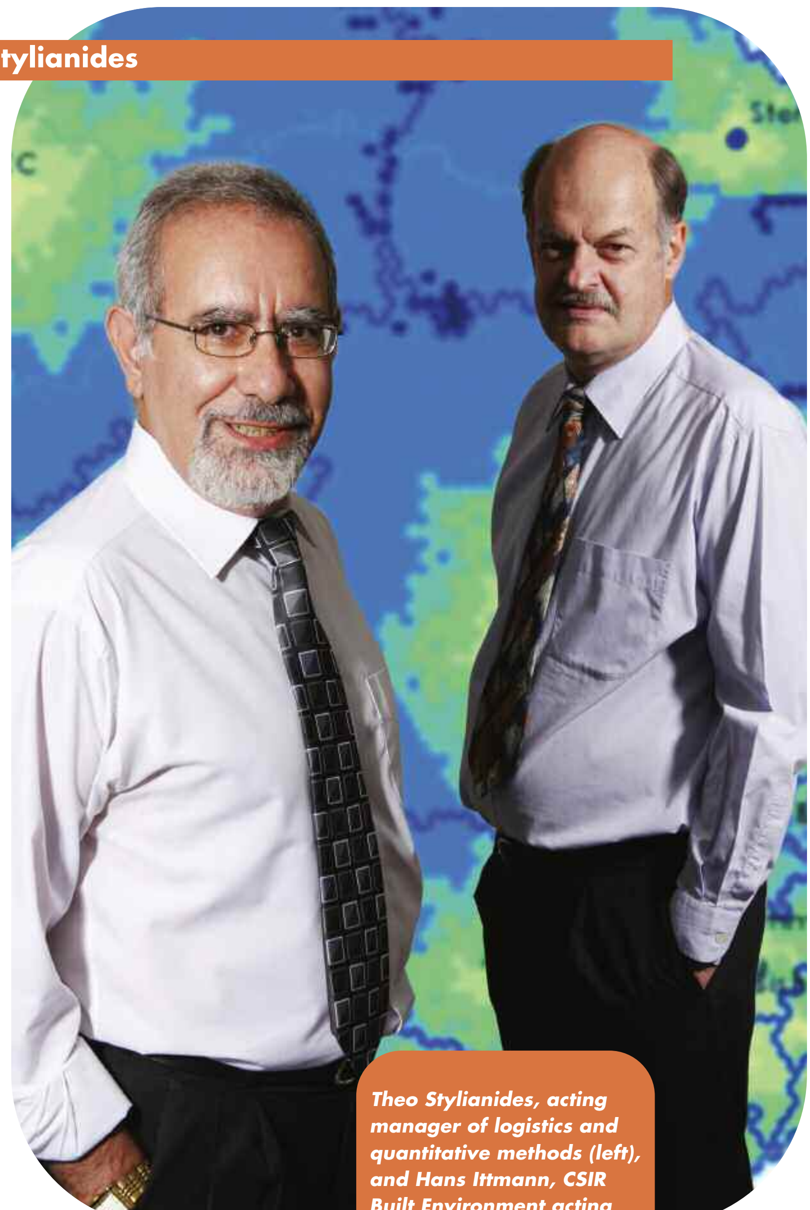
by Hans Ittmann and Theo Stylianides

OPERATIONS RESEARCH (OR) is an interdisciplinary branch of mathematics that uses the scientific approach to problem-solving in any decision-making environment. The emphasis is on the term scientific, implying the use of a mathematical (or statistical) model to represent the problem investigated, and considering the quantitative effects of a range of possible decisions during the analysis.

The modern field of OR arose during World War II, when scientists, mainly in the United Kingdom but also in the United States, investigated ways to make better decisions in areas such as logistics and training schedules. After the war, scientists started applying OR to problems in industry and government. The emphasis was on the mathematical foundation of most of the work being done.

By means of an example, a salesman needs to visit a number of cities but needs to construct the route so as to minimise the distance travelled, the total travel costs or the total time taken to visit all the cities. No city should be visited twice, while avoiding traversing a route more than once. This problem can be solved by formulating (modelling) it mathematically and obtaining an optimal solution. Mathematics is thus used to model a real-life situation to get a solution.

OR is directed towards problems facing the management of organisations in a complex and dynamic world. While it cannot provide solutions to all such



Theo Stylianides, acting manager of logistics and quantitative methods (left), and Hans Ittmann, CSIR Built Environment acting executive director problems, it has been remarkably successful in certain areas. The success of OR has been the result of, amongst others, the following methodology (with feedback between the various steps):

- Understand and formulate the problem
- Develop a conceptual model of the system
- Collect, capture, prepare and analyse the data
- Select a solution technique and build the model
- Test and validate the model
- Communicate and implement the solution.

Due to the complexity of the models and the quantity of data that must often be handled, researchers use computers and sophisticated mathematical models. A mathematical model can be described as an abstract representation of the all-important aspects of a system that uses mathematics to describe the behaviour of the system. Mathematical models are used particularly in natural sciences and engineering disciplines but also in social sciences. Examples include statistical models, differential equations, queuing theoretical models, graph theoretical models, game theoretical models, simulation models, optimisation models and systems dynamic models.

OR has been practised and used within the CSIR by various groups for more than 40 years. Current research focuses on solving complex problems, using mainly quantitative methods. This is achieved through the analysis and interpretation of data and information, the formulation of mathematical models and proposing ways to improve performance, optimise results and guide business decisions.

Operations researchers have a penchant for complex studies and excel in areas such as integration of operations control systems, business modelling studies, logistics and supply chain management solutions, location/allocation problems, forecasting of election results and energy studies. In addition, the achievements of the team in crime pattern modelling, analysis and mapping, in particular, have ensured international recognition.

Successfully completed CSIR projects with a strong mathematical modelling component include:

- **Development of an operations control system for South African Airways**
- **Development of an optimal distribution model for Engen**
- **Development of various resource allocation models for the South African Police Service and the Directorate of Special Operations (Scorpions)**
- **Development of a transmission load forecasting model for Eskom**
- **Development of a vehicle scheduling system for South African Breweries**
- **Optimal location of depots for Omnia Fertilizer**
- **Optimal introduction of kilns within a given planning horizon for Blue Circle Cement**
- **Development of a simulation model for Spoornet**
- **Development of complex simulation models for Sasol**
- **Development of models to forecast South African election results**
- **Development of accessibility models for the location of facilities of the Department of Home Affairs**
- **Development of a large optimisation model for the forestry industry**
- **Development of electricity demand forecasting models for both government and industry**
- **Development of an optimal distribution model for the Swaziland sugar industry.**

Operations researchers at the CSIR have been involved with the local Operations Research Society of South Africa and have served in various capacities in the society. The Tom Rozwadowski award, the society's annual award for the best paper published by a member in a specific year, has been presented to CSIR researchers on nine out of 33 occasions.

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Complexity science:
Solving non-linear and indeterminate problems in an integrative way

by Dr Jan Greben and Dr Bob Scholes

Complexity aspects are included in a number of CSIR research projects, such as the urban dynamics laboratory

Dr Jan Greben (left) and Dr Bob Scholes use complexity science to solve linear and indeterminate problems

IN THE PAST FEW DECADES it has become obvious that many phenomena in nature and in social systems result from the non-linear processes and interactions that often occur in such systems. The main characteristics of these complex systems are interconnectivity, microdiversity, indeterminism and co-evolution. Research on these phenomena has become known as 'complexity science'. Many fields are closely linked to complexity science, including non-linear science, system dynamics, systems theory, chaos theory, spontaneous self-organisation, cellular automata and complex adaptive systems.

This is a multidisciplinary field, which makes the CSIR the ideal place to pursue the development of complexity science. Many projects in the CSIR now have complexity aspects to them, including the sustainability science research theme, a range of poverty alleviation projects and the urban dynamics laboratory. While the roots of this field lie in mathematics and physics (e.g. chaos theory, first developed by the mathematician Ruelle; and non-equilibrium thermodynamics, developed by Prigogine, a theoretical physicist who received a Nobel Prize for this work), the field has since become attractive to both the biological and social sciences. The reasons for this popularity are clear: Many social and ecological problems are non-linear and indeterminate.

A problem currently under study is in the field of changes in the urban landscape. This problem is a mixture of factual data (population, transport system and economic data) and general tendencies (e.g. human behaviour and evolutionary trends). Hence, it is a good area to combine the development of new methods in a rigorous setting with the uncertainties of the social context. The problem is of great relevance to South Africa: The population movements between different areas under the influence of crime is an example of an application.

A statement often made by social scientists is that the behaviour of humans is too unpredictable and the social situations too complex to permit the use of deterministic methods. However, even very complex situations usually depend, at their root, on a comparatively small number of fairly simple relationships. The task of science is to discover the regularities and simplicity in any problem it is considering. While the actions of humans often look very unpredictable, these are actually much more controlled than most people would like to acknowledge. The somewhat random, but in aggregate predictable behaviour of agents in a model is quite a good representation of humans in large populations, just as it works well for elementary constituents of atomic systems. Hence, even for complex systems, deterministic methods with their testable predictions can be of great value.

Rather than ignoring proven techniques because of the perceived complexities of social or ecological systems, it would be better to find phenomena that are common to these and the better-understood physical systems. Emergent phenomena, in other words properties of the system that are not represented in its constituent parts, are typical of complex systems and appear in both contexts. In the case of urban dynamics we can think of individual housing complexes as emergent phenomena. The 'emergence' of these complexes, e.g. gated communities, are the result of the movement (dynamics) of people from less secure to more secure areas. Similarly, the movement of people to the centre of cities is a consequence of the availability of cheap (high-density) housing and work. In such a model the individual complexes are treated as non-linear systems, where boundary conditions play an important role, whereas the interactions between different communities are modelled within systems dynamics software by means of linear interactions. The prospect of modelling different aspects of the system with different techniques is typical of the hybrid approach employed in complexity problems.

This new science is attempting to describe many other phenomena, such as the hierarchy and self-organisation of systems; the understanding of living organisms; new theories of evolution; punctuated equilibrium; the chaotic nature of the weather; and the description of scaling laws in biological systems.

The purpose of complexity modelling is not just to achieve a better description of certain systems. It also forces the modeller to characterise these in a systematic way, thereby identifying the important aspects of the system. The understanding that comes with such a model is often more important than the actual success of the model in reproducing reality. The particular advantage of complexity modelling in this regard is the identification of discrete modes (attractors) of the system. Complex systems tend not to change in a smooth way when placed under pressure – they resist change, and then lurch suddenly (and often irreversibly) into a new state.

It is often more important to know that such alternate states exist than to know how the system will behave to a small nudge in the immediate neighbourhood where it currently exists. In this regard it is important to understand the thresholds that characterise the transition between one state and another. The CSIR currently investigates numerical techniques to quantify such transitions. The emphasis on distinct states rather than continuous linear processes is a characteristic shared with other modelling tools that are currently popular, such as scenario analysis. However, complexity science tries to analyse problems in an integrative way, by providing a consistent methodology that both incorporates the standard linear processes as well as accounts for the more complex non-linear mechanisms.

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Optronic simulations for real-world scenes

by Nelis Willers

PHYSICS-BASED IMAGE simulation of optronic systems provides the user with accurate images of a world scene in any spectral band, from visual to infrared. Such images support research into a wide range of areas, including atmospheric effects, sensor performance optimisation and image processing algorithm development.

Modelling and computer-based rendering of the optical energy in a real-world scene for image simulation purposes require a deep understanding of the underlying physics principles and mathematical constructs. These principles are initially compiled as a set of physics equations that describe the real-world phenomena. These equations are then implemented in a comprehensive computer simulation to calculate the correct optical energy levels, providing images that accurately represent the real-world scene.

A number of phenomena are involved when an image is built in the infrared spectrum, all at the same time, including:

- Self radiation – all objects radiate electromagnetic infrared energy
- Reflected sunlight – direct reflection of the impinging sunlight
- Reflected ambient radiation – both thermal radiation and scattered sky light
- Transmitted background energy, in the case of partially transparent objects such as gas plumes
- Atmospheric transmittance
- Atmospheric path radiance – thermal radiation of the atmosphere as well as sunlight scattered by the atmosphere.

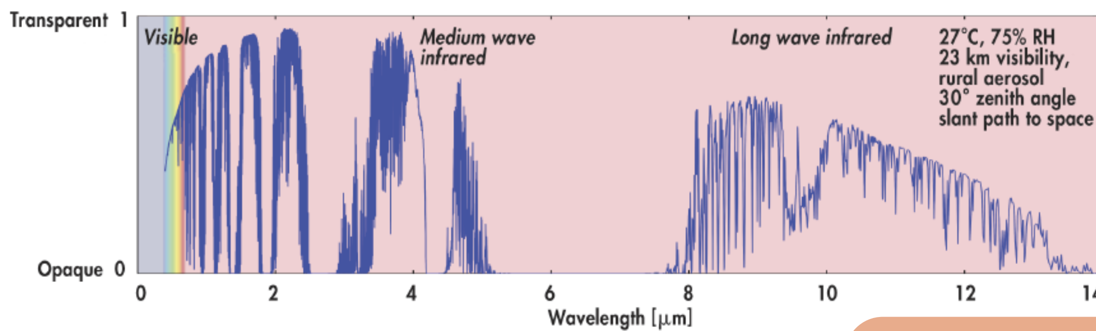
The optronics scene simulator (OSSIM), developed jointly by the CSIR and Denel Dynamics, accounts for all the phenomena listed here. At the root of this activity lies radiometry (the theory and techniques to calculate optical energy). The radiometry of non-trivial scenes requires recognition of the spatial distribution of radiated energy across an object's surface, as well as the spectral variation of radiated energy. This comprehensive radiometry theory was implemented in a computer code, as part of the larger OSSIM simulation system. OSSIM also includes accurate modelling of sensor image formation, mechanical system kinematics and signal/image processing.

Radiometric image simulation requires prior work to build the simulation models. These models include terrain, trees, aircraft, roads and other objects. All the objects required in the synthetic world scene must be constructed and verified. These models are based on theoretical analysis, supported by field measurements. Models comprise a geometrical complex hull description, over which the radiometric properties – such as temperature, emissivity, transmittance and texture – are 'draped'. In some cases, e.g. hot plumes, these radiometric properties are spectral in nature.

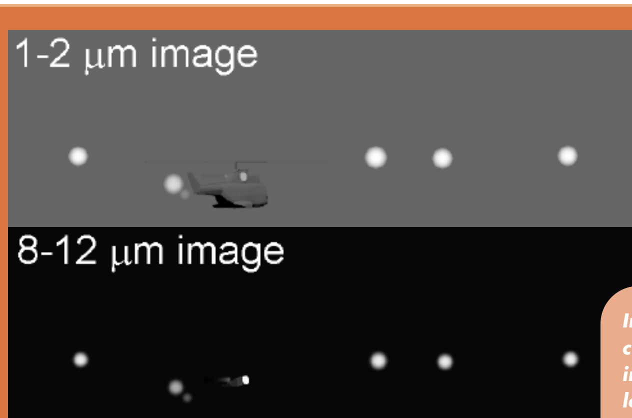
Spectral radiators' energy spectrum varies significantly with wavelength, requiring that all calculations, including atmospheric transmittance, account for such variation. Using the appropriate climatic parameters, the spectral atmospheric transmittance and path radiance are calculated with the acclaimed US-developed MODTRAN atmospheric code. In each sensor spectral band, the radiometric calculations are performed at several hundred finer spectral samples, and the results are integrated together to obtain the total in-band energy.

All these calculations require significant computer time, with the result that the calculation rate can be slower than some applications require. CSIR Defence, Peace, Safety and Security is currently developing techniques to implement at least some of these equations on fast graphical processing units (GPU) processors, in order to reach execution speeds fit for real-time use, in hardware-in-the-loop (HIL) simulators.

The application of the simulator also requires accurate modelling of the behaviour of moving and flying objects. To understand and model the control, kinematic and aerodynamic models of these objects, the laws governing these behaviours are also studied and implemented in computer models. Some of these models require deep specialist knowledge and are developed by collaborators inside or outside the CSIR.

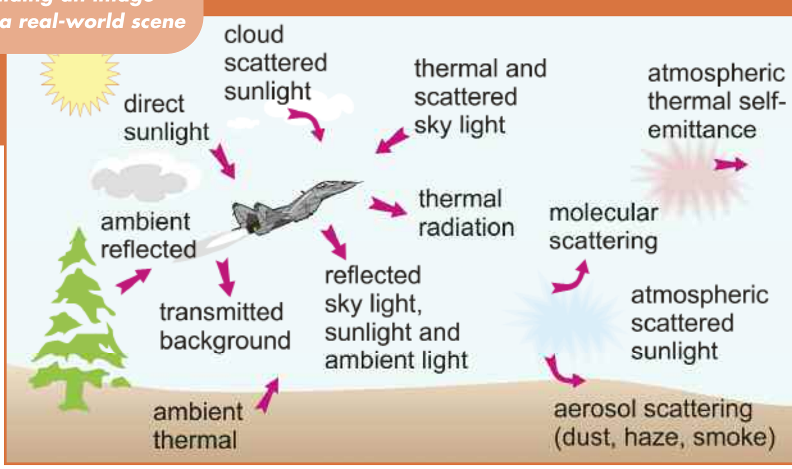


Atmospheric transmittance – note the fine spectral detail attributable to molecular absorption



Images of a helicopter ejecting counter-measure flares in the near infrared (1-2 µm, top picture) and long wave infrared (8-12 µm, bottom picture) spectral bands

Radiometric components taken into account when building an image of a real-world scene



Control systems and aerodynamic and kinematic behaviour are implemented in an embedded finite differences library originally developed by control system specialists in Denel Dynamics, but extended for OSSIM. Alternatively, some models are also implemented in Matlab. These techniques provide the simulation with a precise means to model the behaviour of objects in the scene.

Since results obtained from non-validated simulations may well be in error, it is essential that the models and implementation be verified and validated.

Verification and validation of such a large simulation system are not trivial tasks. The OSSIM models, the simulation and the results are verified and validated against measurements of real-world objects, independent first-order physics calculations, comparison with simulations in other organisations, specialist reviews and extensive regression testing.

The simulation is applied to:

- Develop aircraft self-protection systems
- Predict optronic system performance
- Design and optimise optronic systems
- Implement real-time HIL applications
- Investigate atmospheric or environmental effects on system behaviour
- Develop image processing algorithms
- Perform research on image simulation and synthetic image generation.

A spin-off benefit of the image simulation system development is a novel form of knowledge management. Since all the theory, models and techniques are captured in the simulation code and associated documentation, the knowledge is accumulated for sustained institutional growth.

The optronic image simulation environment provides a powerful tool supporting research and development in the optronics domain. The physics-based approach ensures sustainable knowledge growth and utilisation in a variety of applications.

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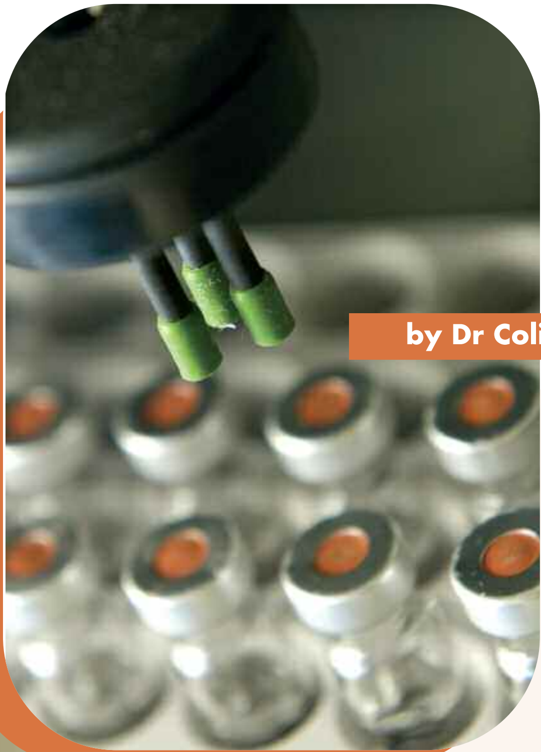


Computational design for targets against disease

by Dr Colin Kenyon, Uli Horn and Dr Chris Parkinson

Dr Chris Parkinson and Sabata Maduna (an intern) use the robotics synthesiser for rapid generation of a collection of molecules predicted to be active by computational studies

THE CSIR IS CURRENTLY working on a number of rational drug design projects. The rational drug design is carried out using the Accelrys Inc suite of protein molecular modelling and rational drug design software. Most of the computational work is therefore applications based, and these computational techniques are absolutely necessary for the rational drug design initiative.

The Cerius2 and Catalyst suites and the new DS modeller within the Accelrys software suite allow for both ligand and target-based rational design of inhibitors through pharmacophore generation. It must be stressed that the theoretical modelling is applications based with the prime objective to use the modelling techniques to manage research projects to solve specific biological problems. The computational work runs parallel with the associated molecular biology, biochemistry, microbiology and organic chemistry.

A number of rational drug design initiatives are currently under investigation. One major project, funded by the Innovation Fund, is aimed at producing novel inhibitors for the treatment of tuberculosis (TB) representation of the active site cavity of the biological target. This can be used to select potentially inhibitory small molecules. The structures of a number of ligands have also been defined using molecular spectroscopy techniques. A significant amount of structural data indicating potential transition state intermediate structures have been obtained from the molecular spectroscopy data, thus allowing ligand-based drug design to be used. Inhibitor/activity data exist for a range of effector molecules acting on the target molecule. Quantitative structure activity relationships (QSARs) are therefore being used in the rational drug design programme.

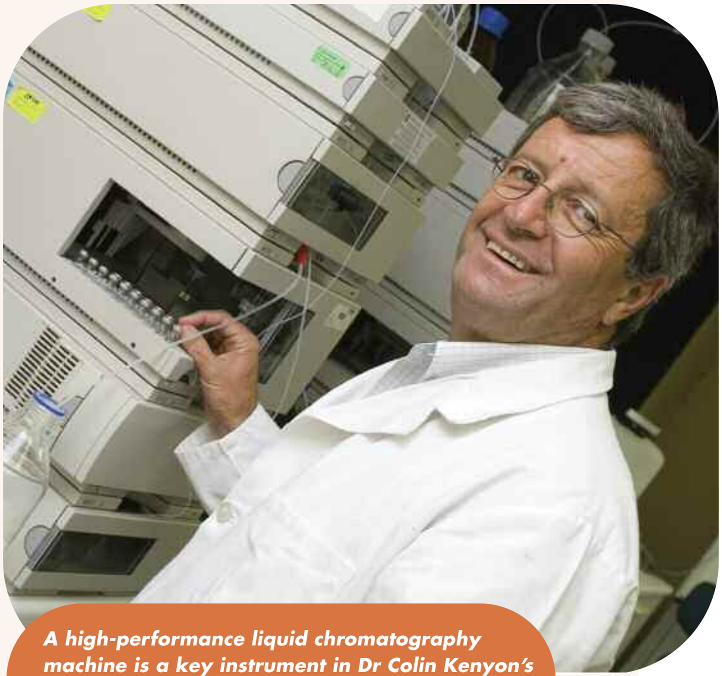
As a result of the homology modelling, key amino acid side-chains have been identified in the protein targets. An extensive site directed mutagenesis programme was therefore undertaken to try to define the role of these amino acid side-chains in the reaction mechanism. In conjunction with the molecular spectroscopy, modelling and molecular biology have contributed to understanding the reaction mechanisms involved. Organic chemists are currently trying to produce molecules that not only inhibit the protein targets by competition with the substrates, but also disrupt the reaction mechanism.

CSIR Biosciences recently acquired computer hardware dedicated to molecular modelling and bioinformatics. The computer hardware consists of:

- Eight Sun Ultra 40 workstations, equipped with two single core 2,8 GHz AMD Opteron Model 254 processors and 4 GB RAM. Due to the visualisation requirement, the workstations were fitted with high-end nVidia Quadro FX3450 graphics cards
- 16 Sun Fire X4100 servers, equipped with two dual core 2,2 GHz AMD Opteron Model 275 processors, 4 GB RAM and service processor
- A 48 port Gigabit Ethernet Extreme switch capable of transmitting traffic at wire speeds
- A dedicated inter-building fibre link using 3 com Gigabit Ethernet switches to connect workstations to the server rack
- The Sun StorEdge 1,2 Terabyte storage unit required to house bioinformatics and other databases.

Due to the often restrictive nature of commercial software licences and the increasing demand for computational modelling, a need arose to marry the strengths of proprietary commercial modelling software and open source software, some applications of which are considered to be the *de facto* industry standard.

Accelrys, a commercial software application, is known for its ease of use, its integrated approach and its wide range of niched modules.



A high-performance liquid chromatography machine is a key instrument in Dr Colin Kenyon's research aimed at clarifying the reaction mechanisms of glutamine synthetase (GS). GS catalyses the conversion of ammonia and glutamate to glutamine. GS is the detoxification of brain ammonia

In contrast, some open source applications have become the industry workhorses in the server environment, often being able to deal with very large computational problems. Of particular interest are the applications making use of a clustered computer environment to handle large problems. Some examples pertaining to biosciences on the bioinformatics side are ClustalW (a multiple sequence alignment application), BLAST (a sequence searching application), Phylip (phylogeny application) and Biopython (general purpose bioinformatics modules that can be programmatically called to solve more specialised needs). Although these exist as single processor applications, they have been extended to run in a clustered environment making use of the industry standard MPI (message passing protocol) libraries. Applications that are particularly suited to the cluster architecture, are the so-called 'embarrasingly parallel' applications where, as the number of nodes dedicated to the application is increased, the resulting wall clock time taken to solve the problem is inversly decreased. ClustalW is a good example of such an application. Open source applications making use of clusters to solve molecular modelling tasks such as structure minimisation or dynamics also exist, Namd being an example.

The standard cluster architecture consists of a head node through which communications with the cluster takes place, and which distributes and collates the job fragments to and from the various nodes, respectively. The traditional bottleneck in cluster computing is the switching backbone, that is the network connections between the nodes that make up the cluster. To overcome this hurdle at reasonable cost, an Extreme 48 port Gigabit Ethernet switch has been employed that is able to transfer internode traffic at wire speeds.

The workstations are all dual boot WindowsXP and RedHat Linux WS3 machines in order to run either Accelrys or open source Linux software.

The server machines have been divided into those dedicated to Accelrys server applications currently running on Windows 2003 Server (32 bit) operating systems and ones reserved for cluster applications running on Centos 4.3 64 bit operating systems, although the nature of the servers are such that they are suited to function in a reconfigurable environment, should such a need arise in future.

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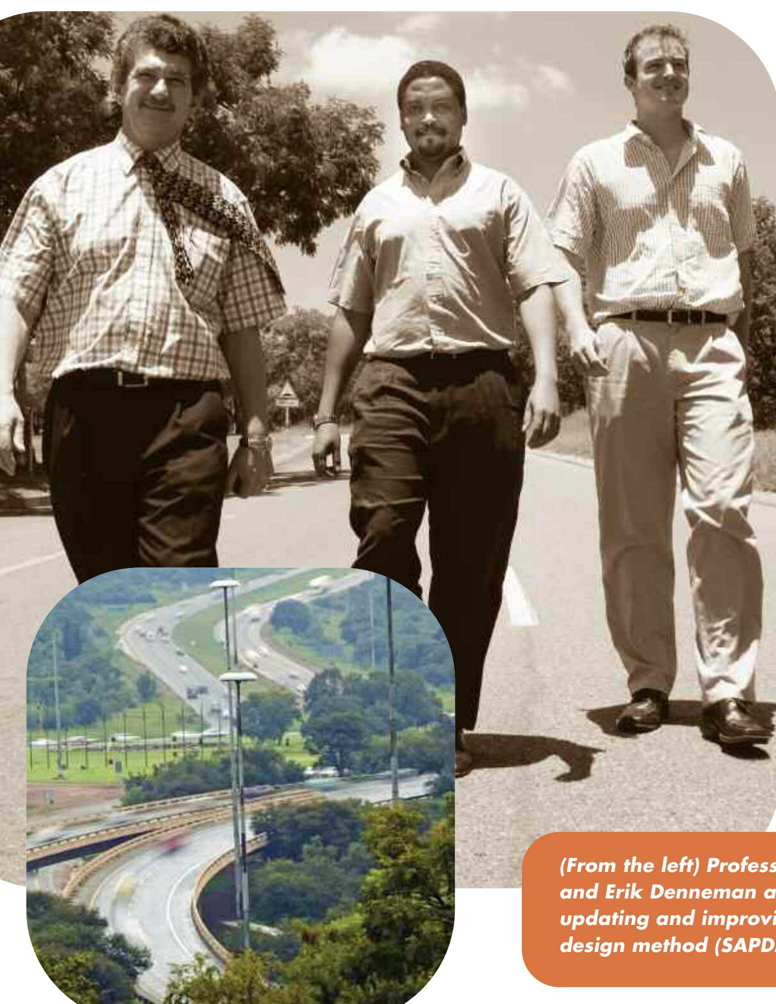
An improved system for modelling and designing road pavements

by Dr James Maina, Professor Morris de Beer and Erik Denneman

CSIR PAVEMENT ENGINEERS have developed a software tool, soon to be released to industry, that simulates actual road pavement behaviour.

A sound road network is an essential ingredient of a country's socio-economic well-being. Once constructed or structurally rehabilitated, however, a road will gradually deteriorate as a result of the combined effects of traffic loading and environmental forces (e.g. rainfall, ultraviolet radiation, temperature). The rate of deterioration depends on the ability of the pavement structure to resist these forces. As road conditions worsen, not only do journeys take longer, but fuel is wasted, vehicles are damaged and the number of accidents increases. The costs to the economy of this invisible tax are huge.



(From the left) Professor Morris de Beer, Dr James Maina and Erik Denneman are involved in the project aimed at updating and improving the South African pavement design method (SAPDM) for road pavements

South Africa has a world-class primary road network and a proud history in road pavement engineering. Maintaining this standard in the face of increasing traffic demands will need an improved system for modelling and designing of road pavements.

The South African pavement design method (SAPDM) for road pavements, in the development of which the CSIR played a key role, has formed the backbone of design methods used in South Africa and could compete with the best in the world. The new traffic realities have, however, rendered important parts of the method obsolete and in dire need of serious revision.

A process was initiated at the South African Road Pavement Forum meeting in 2005, after which a framework identifying research and development (R&D) topics and needs for reviewing the SAPDM was tabled. Based on this framework, more than 20 project proposals were submitted to the South African National Roads Agency Ltd (SANRAL). The proposed projects are aimed at improving the South African method for road pavement design and it is anticipated that the project outputs will be adopted nationwide as primary tools for road pavement design.

The key to proper design of road pavements and subsequent maintenance is the ability to understand the macroscopic behaviour of materials when subjected to traffic loading under varying environmental conditions. The core part of the new SAPDM will involve numerical modelling and simulation of road pavement resilient responses.

Development of analytical methods for resilient response of pavements can be traced back to the early 1940s. Since then, numerous researchers have extended the method to cater for multiple numbers of layers and loads. While these methods are mathematically exact, they have shortcomings based on assumptions that are far removed from actual properties and behaviour of pavement materials subjected to varying environmental conditions and vehicular loading. Since pavement structures with complex loading, boundary conditions and/or material behaviours cannot be handled accurately, results that make practical sense may not be achieved. This is why numerical methods are recommended.

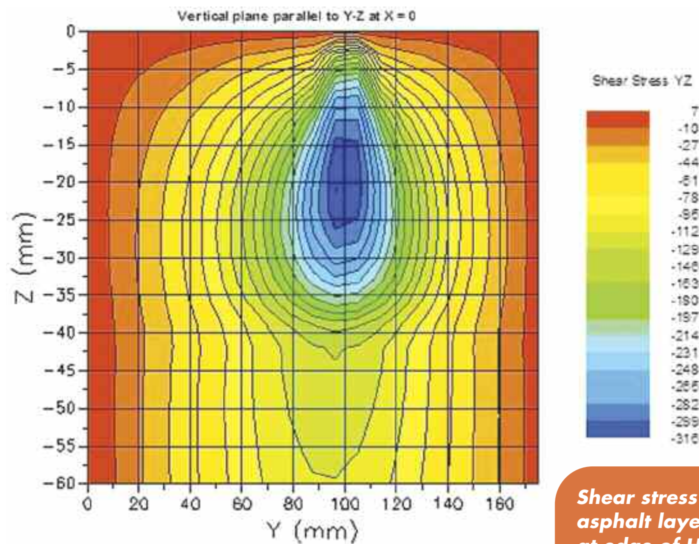
One of the methods used for numerical analysis is known as the matrix method. The well known finite element method (FEM) falls in this category and is based on discrete-element idealisation. In the finite element analysis for road pavement application, pavement layers are considered to be a solid continuum and the domain of the problem is divided into sub-domains.

The complex system geometry of these sub-domains are modelled by discretising into a network of finite-sized and arbitrary-shaped elements that have analytical closed-form solutions. Finite elements are subsequently interconnected by nodes at common edges and assembly of all these elements will represent the problem for general analysis. It is important to note that FEM can be used to solve multi-layered pavement problems with non-linear material (constitutive) engineering properties, non-uniform loading distributions as well as dynamic effects of vehicle/pavement interaction. Assumptions of modelling the tyre loading as circular uniform patterns of stress are not necessary with FEM.

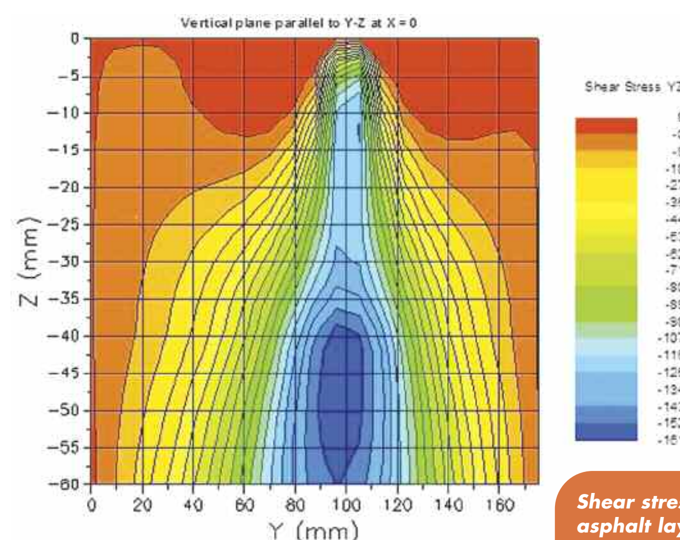
Since the early 1990s the CSIR has invested in advanced measuring systems to capture rolling tyre/road interface data to gain improved understanding of this complex mechanism. This technology, referred to as stress-in-motion (SIM), supplies information on the main characteristics of tyre/road interaction, and roads practitioners are now in a position to utilise this information better in the design, rehabilitation and maintenance of roads. For this to be realised, new modelling and simulation techniques based on FEM are urgently needed to improve and enhance the structural road pavement design based on the non-uniform 3D tyre road stress inputs from the SIM technology.

Researchers at CSIR Built Environment are developing a finite element method for pavement analysis (FEMPA) to improve accuracy of pavement structural analysis by taking into consideration:

- Characteristics of real-life pavement loadings
- Geometry of pavement systems
- Mechanical properties and behaviour of pavement materials
- Responses of pavement systems to vehicular loading.



Shear stress in asphalt layer at edge of HVS tyre at 25 °C



Shear stress in asphalt layer at edge of HVS tyre at 60 °C

To ensure that results obtained from FEMPA are reliable, output was compared against results from a range of available software packages worldwide. Preliminary results from FEMPA have shown a high degree of accuracy and efficiency for analysis of static loading cases.

It is expected that successful development of this software will provide pavement engineers with a tool that closely simulates actual pavement behaviour. Through this tool, proper road pavement design using a range of available materials (conventional and non-conventional), performance evaluation as well as timely identification of potential failures in the pavement systems may be performed. FEMPA is capable of analysing 2D (plane strain, plane stress, axi-symmetric) as well as 3D element shapes and will soon be released to the industry for adoption and use.

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Using isotopes in groundwater modelling for sustainability

by Dr Rebecca Maserumule

WHEN FARMERS pump groundwater from a borehole for irrigation, they may ask: What is the quality of water pumped from the underground reservoir, or how much more water is available in the near future? The farmer will rarely ask what the age of the water is.

The water resource manager at the Department of Water Affairs and Forestry, who is interested in determining the sustainable supply of water in South Africa, and the mathematician, who assists by quantifying the sustainable supply, know the answer to the latter question may be one of the keys to managing this sustainable resource.

As per the South African Water Act of 1998, government is required to quantify the total volume of our water resources and then set aside the basic needs of both humans and the aquatic ecosystems from this total volume.

Groundwater recharge is a fundamental component of a groundwater system and an important factor when determining the long-term safe yield of an underground water reserve. The process of water soaking into the ground to become groundwater is known as groundwater recharge. When precipitation falls to the earth, it ends up as run-off, evaporation and transpiration with a very small fraction that ends up as groundwater recharge. Given the scarcity of water in South Africa it is important to model and quantify the addition of water to groundwater reserves.

The Stampriet Artesian, located in the southwest of Namibia, is about 65 000 km^2. The Stampriet Artesian Basin (SAB) was chosen as a research site because it is the largest groundwater basin in Namibia and responsible for supplying water to many towns and commercial farmers. While regulations were put in place by the South African Water Act of 1998 to control the abstraction of groundwater from the SAB, groundwater levels have declined continuously since 1980.

Over the past 20 years major breakthroughs have been made in the use and development of deterministic and computer simulation models to analyse the flow of groundwater and the transport of solutes in groundwater systems. Similarly, groundwater hydrology has seen the technological growth of isotopic methodologies to analyse groundwater flow paths, ages and recharge areas. Unfortunately, recharge investigations are typically inhibited by the scarcity of quality meteorological and hydrological data and as a consequence numerical models employed to simulate and quantify groundwater recharge, can be inaccurate.

In the Stampriet recharge study, a numerical flow and solute-transport model was developed and calibrated using both water level and radiocarbon data. The solute-transport model was used to simulate the 14C data while the numerical flow model was used to simulate the groundwater. The calibration of recharge using both water level and radiocarbon data is necessary because groundwater models that use only water levels are sensitive to the ratios of recharge and hydraulic conductivity. Model calibration is the process of modifying input parameters to a groundwater model until the output from the model matches an observed set of data.

Amid the first round of simulations, the solute-transport model was linked to a steady-state simulation of the groundwater flow model to determine the behaviour of the simulated 14C activities. During the steady state simulation the recharge rate over the past 30 000 years has been kept constant. The groundwater model was also linked to a transient model to see whether the fit between the simulated and observed values for radiocarbon improved. When comparing Figure 2 and Figure 3, it is evident that assuming a transient recharge rate over the 30 000-year simulation improves the fit of the simulated 14C activities to the observed values. Results from the transient simulation show that recharge rates were greater 15 000 years ago than at present, while recharge rates were lower 10 000 years ago than at present. The greater recharge rates correspond to the last glacial maximum, which has a wetter climate. The lower recharge rates are before the beginning of the current period of the Holocene, which began 10 000 years ago.

By highlighting the use of isotopes in groundwater modelling, CSIR researchers have shown that the measurements of 14C that give insight into groundwater ages bring both the water resource manager and the mathematician closer to answering the question of water availability and sustainability in the SAB.

The Chinese philosopher Confucius said "Study the past if you would divine the future". The future of sustainable water resources in southern Africa lies in understanding the past, which can be measured in isotopes.

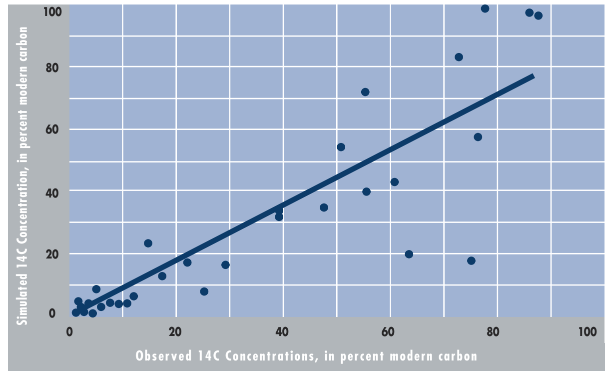

Figure 2 Observed versus simulated 14C activities for steady-state simulation

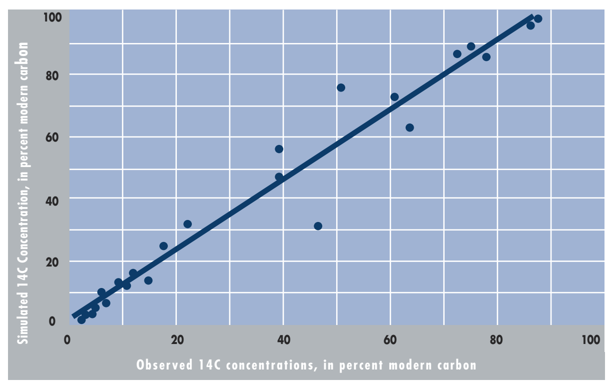

Figure 3 Observed versus simulated 14C activities for transient simulation

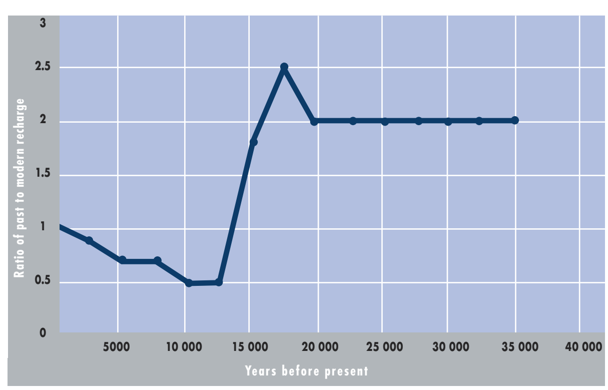

Figure 4 Paleorecharge estimates from transient groundwater simulation based on 14C activity data

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Language and mathematics

by Professor Etienne Barnard

THE DIVIDE BETWEEN the 'two cultures' – one humanist and language-oriented, the other scientific, with mathematics as its basic tool – has always been suspect to many. Great scientists often display a strong love of language (Einstein and Gell-Mann are examples), whereas JM Coetzee is one of a long line of famous writers who underwent advanced training in the mathematical sciences. In fact, research is casting doubt on the very basis of this division, as the linkages between language and mathematics become increasingly clear. As a case in point, CSIR researchers in human language technologies (HLT) are using mathematical models to come to terms with spoken and written language.

In a joint project with the University of the Witwatersrand, a team of researchers from the Meraka Institute of the CSIR are deriving mathematical descriptors for the expression of tone in languages such as Northern Sotho. In these languages, the prosody (or 'melody') of a spoken phrase conveys information on many factors, ranging from stress and emotion, to semantics (meaning).

This poses a puzzle: How do listeners know what the purpose of a particular tonal pattern is? We analyse recordings from several speakers, saying carefully selected phrases, and are starting to understand that tonal 'gestures' correspond to speakers' intent in highly predictable ways. Interestingly, these tonal patterns are quite different from those found in other tonal languages such as Mandarin Chinese. Whereas 'level tones' (where the pitch takes on a certain steady value) and 'contour tones' (where the pitch changes in a particular pattern) are quite distinct in Mandarin, speakers of Northern Sotho apparently use levels and contours interchangeably to indicate a certain tonal value. Tone also spreads across adjacent syllables in the African languages according to a definite set of rules that have no counterparts in the better-researched tone languages.

Another application of mathematical modelling in HLT relates to the durations of the basic units of speech (known as 'phonemes'). Although we rarely think of this when speaking, the durations of these units are highly meaningful. Factors such as word and sentence stress, emphasis and emotion clearly all play a role in the determination of phoneme durations, but how do these interact? And are the effects (and their interactions) different for different types of phonemes?

HLT Master's student Charl van Heerden is building sophisticated models that make it possible to answer questions of this nature. He has found that phoneme durations vary in subtle ways between speakers – to such an extent that these durations are actually useful in determining who the speaker was – and also that the broad classes of phonemes (e.g. vowels and consonants) behave in systematically different ways. Van Heerden's models have to address one of the fundamental challenges to many mathematical models in the domain of language technology: Since the range of phenomena that occur in a particular language is very large, it is not feasible to measure all the combinations of factors that may occur in practice. He therefore develops models that are able to generalise to unseen circumstances. Mathematical models with the ability to

converge to provide insight

generalise also play a key role in one of the fundamental tools used in HLT development, namely pronunciation modelling. Pronunciation models allow computer systems to predict the acoustic properties of words based on how they are written and are crucial in applications such as speech recognition. Dr Marelie Davel, HLT research group leader, has developed a succession of increasingly accurate methods for learning pronunciation models from a limited set of example pronunciations in a given language. Her models are now widely used in speech-processing systems for many different languages, and have been shown to be more accurate than alternative approaches when generalising from small data sets.

Alta de Waal, senior HLT researcher, uses the conceptual framework known as Bayesian statistics to create mathematical models of written documents. The internet has stimulated an explosive growth in the number of documents available for reading – a deluge that would be impossible to navigate if we did not have automated tools to process the contents of these documents.

Search engines and PC tools generally base their findings on specific words in a document, but more sophisticated techniques that delve more deeply into the content of a document are a growing trend.

The most successful techniques are still far short from human understanding: The main successes to date rely on mathematical models that discover underlying topics in documents through the repeated usage of key words related to the topic.

These HLT research projects illustrate that mathematics and language are deeply related – mathematical models, along with careful linguistic analysis, provide deep insights along with practical applications.

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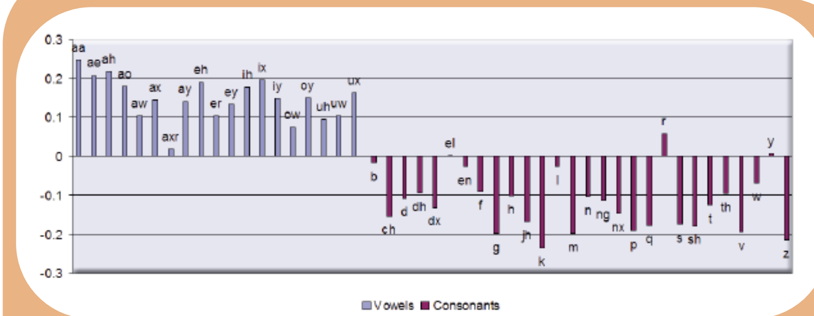
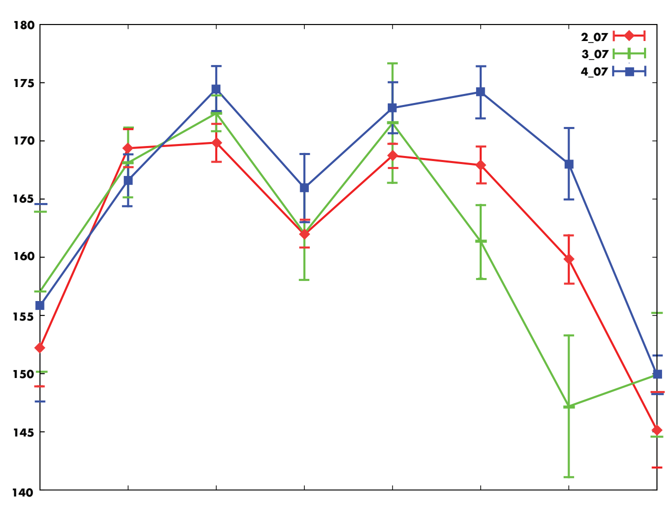


When analysing the durations of phonemes, one finds that the vowels and consonants behave in quite distinct ways – but 'r' and 'y' are, from this perspective, similar to vowels

Nicholas Zulu and Alta de Waal demonstrate the process of gathering data for the modelling of phoneme duration



By analysing measurements (such as these tracks of pitch frequency during a series of spoken phrases), researchers are able to create mathematical models of the underlying structure of speech

Design, modelling and simulation in mechatronics engineering

by Dr Nkgatho Tlale and Ahmed Shaik

THE AUTOMOBILE has come a long way since the Flintstones and is one invention that always seems to have just one more predecessor. The earliest steam-powered car known was finished as early as 1769 by French inventor, Nicolas Cugnot.

When it comes to internal combustion, Carl Benz usually gets the credit. But Benz wasn't first. Another French inventor, de Rochas, built an auto, and an engine to drive it, in 1862. At the time considered revolutionary – and in the early 1900s a marvel – since it was composed of only mechanical sub-systems, the car is an excellent example of the impact of mechatronics on modern engineering systems.

Today, cars are complex mechatronics systems, comprising engine management systems, central management systems, anti-lock braking systems (ABS), collision-detection systems, cruise control, to name but a few, and all connected via an advanced communications technology called controller area network (CAN). Mechatronics refers to the synergistic use of mechanical, electronic, software and IT systems and principles in the development of systems that are superior to the individual sub-systems. Mechatronics has been responsible for the achievement of complex engineering systems, such as robotic systems, machine tools and ABS.

The manufacturing science and technology area of the CSIR focuses on the development and implementation of advanced control principles in mechatronics systems. Research activities include novel mechanical system design, kinematics and dynamics modelling, controller development, algorithm development and implementation, testing and optimisation. Research centres on industrial robots, parallel kinematics machines (PKMs), reconfigurable machine tools and autonomous systems.

Modelling

Modelling of robotic mechatronic systems deals mainly with mechanical modelling for control system design. Mechanical system modelling is a pre-requisite for any mechatronic/robotic system simulation, and is preceded by individual mechanical component modelling. The aim of control system design is to safely and optimally control a mechatronics system. It is closely tied to electronic design as the algorithms created for control are implemented in electronic hardware.

Conceptual design

Conceptual design is the first step in the iterative design procedure for mechatronics applications. The design represents a rough idea of what the mechanical architecture of the machine would look like and function. The PKM that was designed was a four-armed pick-and-place machine for use in the food processing and packaging industries. The conceptual design is presented in Figure 1.

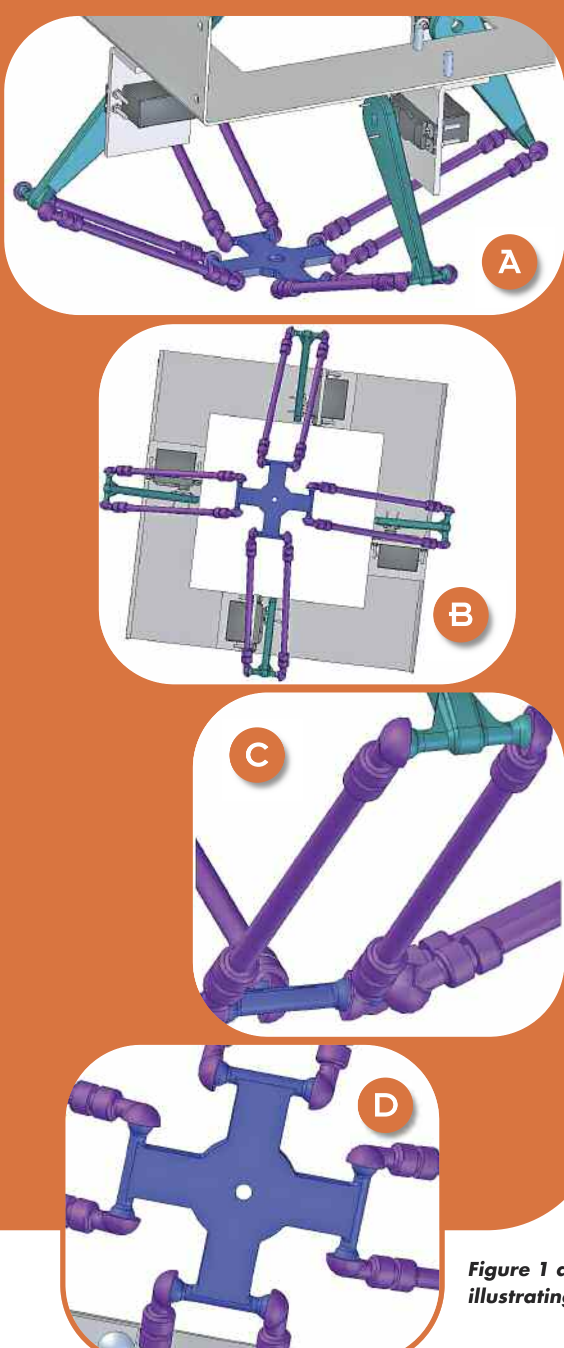


Figure 1 a. All movable parts of 4-armed PKM machine b. Bottom view c. Lower leg components illustrating 'knee' and 'ankle' joints d. Close-up view of the robot hand (end-effector)

Mechanical component modelling

From the conceptual design, each mechanical component is modelled in a simplistic way to maintain functionality in the system, but removing unnecessary information. For initial kinematics analysis (forward and inverse positioning of the machine), volumetric and mass information are unnecessary so single lines can replace 3D components, maintaining distance relationships between joints, and rules are established in the model to maintain constraints of motion (planer, rotational, linear). In a dynamic analysis masses are needed and the system is modified to include the mass of the component, all concentrated at its centre of mass as represented on the component model (Figure 2b, c).

System modelling

Each component, comprising the design with its motion constraints, is then collated to establish the system model, with appropriate labelling and information required to perform the kinematics analysis. In the model each link was collapsed to a single line attaching respective joints maintaining distance relationships. Joints T_i are purely rotational one degree of freedom (DOF), whereas joints A_i and K_i are spherical (three DOF). Also due to the lower arm parallelograms, the end-effector remains perfectly parallel (horizontal) with regard to the base. This is maintained by ensuring that in the kinematics model joints A_i are planer, joints T_i are planer and both planes are always parallel. The parallelograms of the lower arm are then collapsed to single lines, these are shown as lines joining A_i to K_i (Figure 2). Algebraic analysis is then used to develop equations that represent the geometry of motion of the developed PKM.

System simulation

The simulation of the system requires a full kinematics analysis, both forward and inverse kinematics. From these, the total workspace and singularities within it can be found. At a singular point, the PKM will gain one or more DOF, thus rendering the system unpredictable.

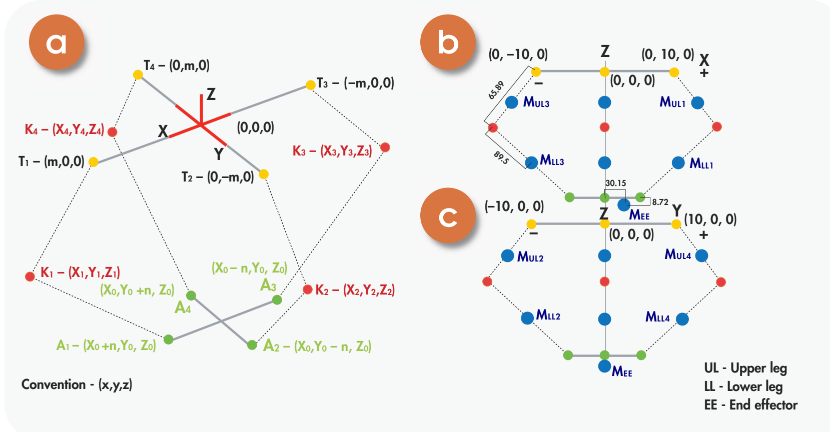


Figure 2 Simplified system model derived from conceptual design a. Simplified geometric model of machine b. Simplified geometric model incorporating component masses (XZ plane) c. Simplified geometric model incorporating component masses (YZ plane)

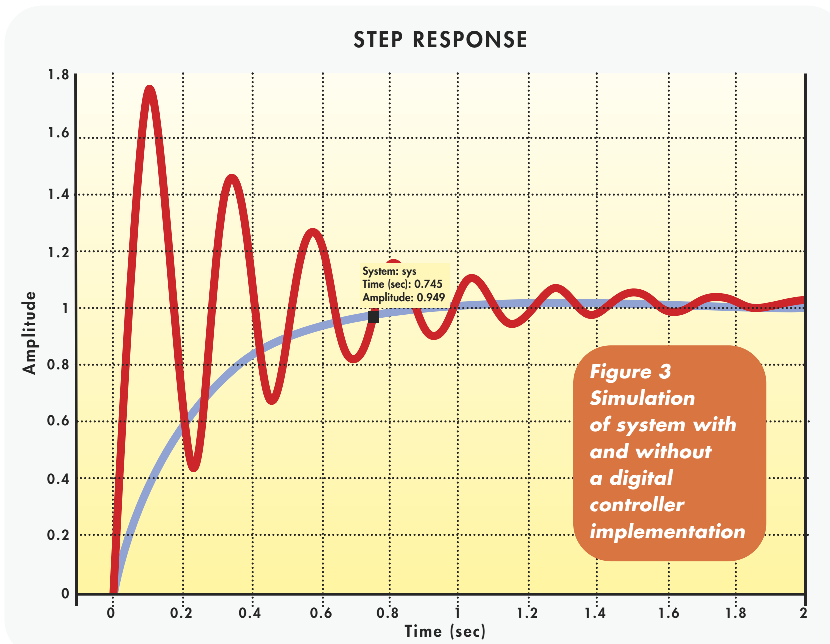


Figure 3 Simulation of system with and without a digital controller implementation

Control system

To create a control system, the dynamic model of the system, incorporating masses, must be analysed. For robotic-arm applications the angle of actuation must have a first order response. Anything more will result in overshoot and oscillation of the end effector, which are unacceptable for robotic positioning (Figure 3). Advanced control techniques (except the common proportional, integral and derivative control (PID)), such as Kalman filter and cost functions can additionally be used to improve controllability.

The definition of step change for the mechanical simulation was moving the end-effector in the geometric model from an initial position to a final position (but pure vertical motion only. The graph illustrates a timeline of the normalised angular values of the driving motor for one arm of the robot. This model incorporated the dynamics of the system and torque ratings of the motors. The red second order curve illustrates the concept of overshoot. Due to the speed and masses of each component, the motor torque was not sufficient to stop the motion of the arm once it had reached its intended position.

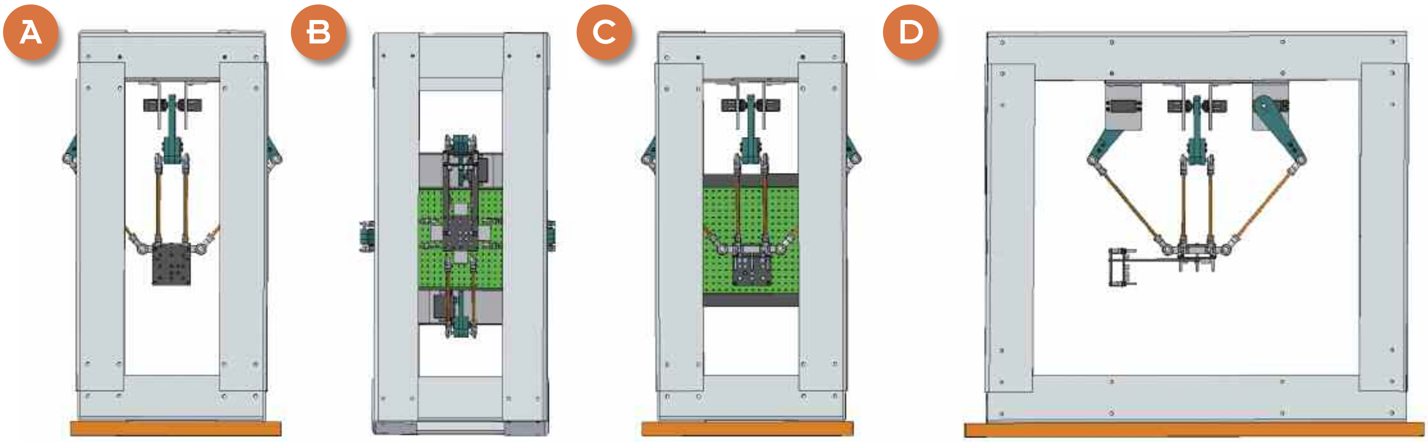


***Figure 4** Final design incorporating real component models. a. Front view b. Bottom view (with base removed) c. Back view d. Left-side view*

It took a finite time for the motor to stop oscillating. The blue curve, however, is of first order and represents the same system with a digital controller in place. It displays a smooth transition from initial to final position.

Finalising the design

Once the control system has been designed and verified, the final system design may be completed. Further 3D simulations are then tested to ensure that all parts move as specified, and a collision detection algorithm is implemented to ensure that components do not collide with each other during routine motions.

A major obstacle facing mechatronic engineers is the lack of a complete mechatronic design and simulation computer-aided design (CAD) package. CAD software design tools exist for each of the various engineering disciplines that comprise mechatronics, but true integration of these development packages to create a holistic and integrated environment is still not yet a reality.

Imagine being able to create a true virtual product comprising all aspects of design, and being able to verify proof of concept before even creating a single real part. To test the product integration of all parts – mechanical, software, electronic, control – a single software tool would be nothing less than profound since it would reduce numerous problems and costs associated with manufacturing and prototyping. It would be a complete revolution in engineering – a step of such magnitude that could be likened to the giant leap in engineering evolution when CAD replaced paper design.

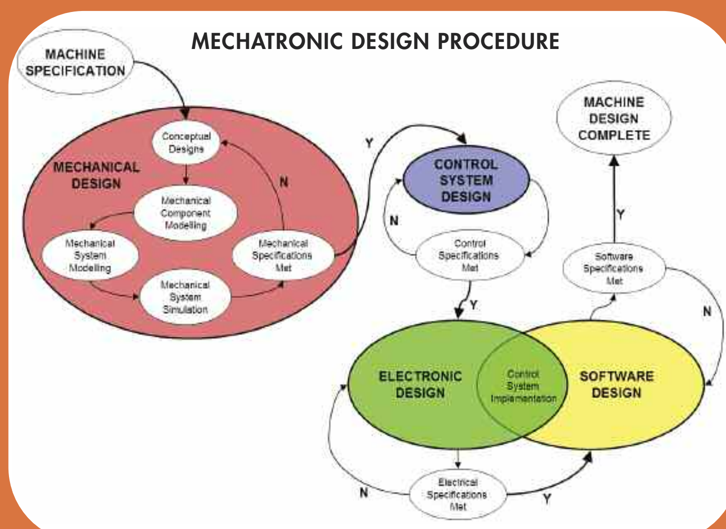


Figure 5

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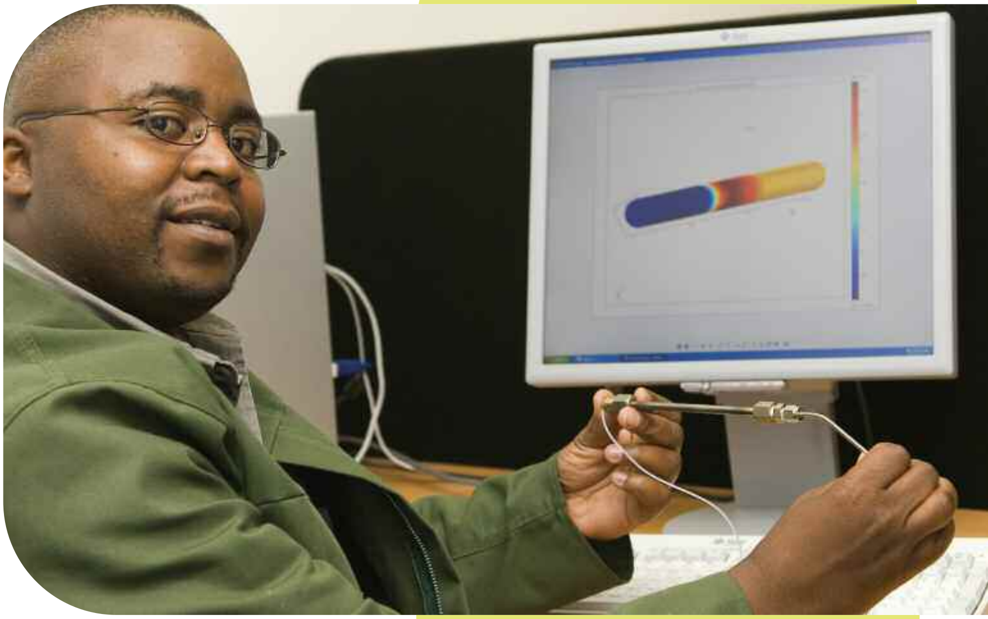
The role of microfluidics in chemical and biological process development

by Dr Njabulo Siyakatshana, Subash Buddoo and Dr Jozef Dudas

MICROFLUIDICS is the science of engineering and manufacturing devices and processes that deal with extremely small volumes of fluid. In diagnostics, miniaturisation permits both increased speed of analysis and minimisation of sample and reagent consumption, in process development, significant improvements of conversions, selectivities, heat and mass transfer lead to a more efficient use of resources such as energy, raw materials and labour. This has enormous benefits for the manufacturing sector for high-value products and also leads to far better control of inherently hazardous or potentially-explosive processes.

Microfluidic components for life sciences can be chips, disks, cartridges, cards for *in vivo* or *in vitro* biological assays (DNA, protein, cells) and microreaction (drug development); dispensing systems for parallel assays; flow controllers, i.e. pressure sensors/valves and fluid diffusion nozzles. Microfluidic devices in chemical process engineering include micromixers, micropumps, heat exchangers and microreactors whereas in the energy sector, extensive research into micro-fuel cells, combustors, steam reformers and microthrusters is ongoing. Some wider industrial applications include flow control sensors and industrial dispensing of lubricants, glue, flavours and scents.

In the biosciences arena, the CSIR has recognised the significance of microfluidics in critical areas such as drug development, biofuels, immuno and genetic assays as well as chemical process development. The ultimate goal of CSIR Biosciences researchers is to formulate indigenous technologies by incorporating microfluidics at world-class level by cooperating with more experienced international role players such as the Institut fur Mikrotechnik Mainz (IMM), Germany and locally with CSIR Materials Science and Manufacturing scientists.



Simulating the real thing … Dr Njabulo Siyakatshana oversees the simulation of microfluidics on a collaborative project

Mathematical modelling and simulation

Computational fluid dynamics (CFD) is a powerful and robust tool for predicting flow in chemical or biochemical processes occurring within an arbitrary geometrical design. CFD uses known equations, derived mainly from the Navier-Stokes equations to simulate physical and (bio)chemical processes. This enables CSIR bioscientists to visualise phenomena in the core of abstruse processes or geometries, which would otherwise be extremely difficult to determine experimentally, thus allowing the efficient and precise design of microfluidic processes and devices from comprehensive computations. Mathematical software such as MATLAB and commercial CFD packages such as COMSOL and FLUENT have found widespread use in industry and research.

Pyrolysis reactions

Linalool is an important flavour and fragrant compound used extensively in perfumes, cosmetics, and household cleaning agents as well as being a key intermediate in vitamin B and E synthesis. Linalool is synthesised in four reaction steps from CST (crude sulfated turpentine) obtained as a waste product of the pulp and paper industry. The key reaction in this sequence is the pyrolysis of 2-pinanol at 600 °C to produce linalool. However, under these harsh conditions, the linalool is just as likely to decompose and form by-products such as hydroxyolefins or plinols. A key factor for optimum linalool selectivity is thus the residence time of the reactants coupled with efficient heat transfer.
To maximise linalool production while limiting by-product formation, an experimental program was undertaken incorporating modelling techniques to simulate this reaction. Reactions were performed first in a tubular minichannel of diameter 4,6 mm and length 15 cm with a 5 cm heated mid-section and secondly in a microreactor (see Figure 3a) with 14 heated channels each of width 500 µm, depth 400 µm and length 25 mm. The modelling was performed in one-dimension (1D) using MATLAB and the simulations in 3D using COMSOL Multiphysics.

The geometrical concentration profiles of the product linalool from some of the simulations at high temperatures and low flow rates are illustrated in Figures 2 and 3. Results from these simulations illustrate some key points:

The concentration profiles demonstrated that the process was improved when using the microreactor, as can be judged by a 25% higher maximum concentration of the product linalool in the reaction chamber. Above all, this was achieved at lower reaction temperatures. The process has to be optimised regarding temperature and/or flow rate, which can be done easily by using the simulation software rather than experimentally. This means that under a given set of conditions, researchers could predict precisely how a system will behave and thus redesign it accordingly.

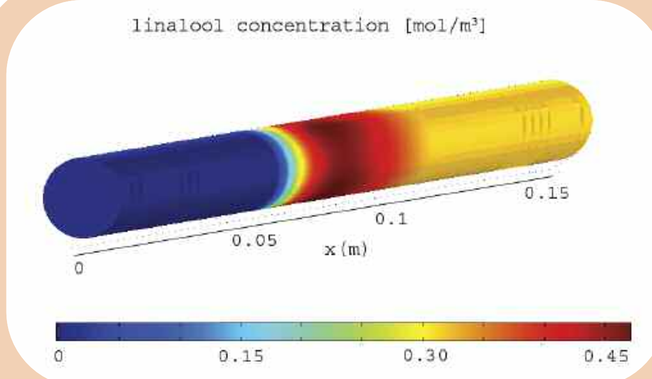


Figure 2
CFD depiction of the concentration of linalool in a tubular mini-channel reactor at low flow rate (50 ml/min) and high temperature (700 °C)

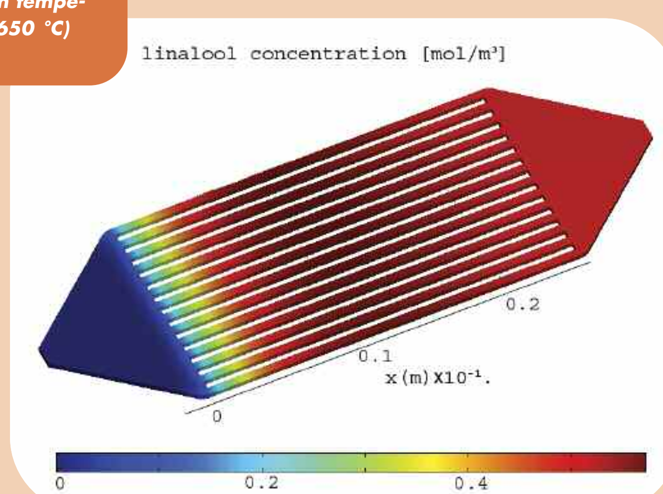


Figure 3
a) Actual microreactor configuration

b) CFD depiction of the concentration of linalool in the multi-channel micro-reactor at low flow rate (10 ml/min) and high temperature (650 °C)

Members of the team with a syringe pump to set microreactor flow rates (from the left) Mesuli Mbanjwa, Subash Buddoo, Kevin Land and Dr Njabulo Siyakatshana

Microreactors are considered to produce results 1 000 or more times faster than batch reactors. A CSIR team hopes to create a cost-effective South African version of these expensive internationally-manufactured assets

These simulations provide insight into the reactor chamber by, among others, analysing a host of parameters such as the internal concentration profiles of a product, assessing the heat transfer characteristics, measuring pressure drop along the channels and predicting the mixing capabilities from the velocity profiles.

The versatility of the CFD and mathematical modelling techniques were illustrated by comparing output parameters such as the conversions and selectivities to experimental results. For the tubular reactor at flow rate 50 ml/min and 650 °C, the team experimentally determined 74% conversion and 70,4% selectivity, whereas the CFD simulations predicted 74,5% conversion and 72,8% selectivity, and the mathematical modeling in MATLAB predicted conversions of 79,5% and 69% selectivity. Deviations with CFD modelling are no more than 2% while mathematical modelling exhibited 5,5% deviation at most.

Generally, there is a good consilience between model, simulation and experimental results, which enhances the researchers' understanding of the fundamental processes and facilitates the use of modelling and simulation techniques in geometrical equipment design and process development.

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Modelling a domain using ontologies

by Dr Tommie Meyer

FOR MANY, LIFE WITHOUT ACCESS to the worldwide web is virtually impossible to imagine. It provides access to amounts of information that would simply have been unthinkable 10 to 15 years ago. Finding meaningful information among the millions of information resources is an entirely different matter, though. The problem is that the current web is, for the most part, aimed at people who determine the relevance of a web page by manually perusing its content. What is needed, is a way to automate the process of determining which pages contain relevant information.

At present the best way to do so is through syntactic searches in which keywords are viewed as patterns of characters, and are matched to strings occurring in web resources. Given these limitations, it is illuminating to bear in mind that Tim Berners-Lee, the founder of the web, originally had a much more ambitious vision. He envisaged a web where machines would have access to the meaning of the available information: A semantic web with information shared and processed both by automated tools, such as search engines, and by human users.

The basic approach to realising this vision is to ensure that information resources on the semantic web will not only contain data, but also metadata, describing what the data are about. This will allow machines and their human users to identify, collect and process suitable information sources by interpreting the semantic metadata based on the task at hand. The crucial part in all of this, the method for describing what the data are about, is provided by the use of ontologies.

Ontology research promises to deliver a means of providing improved data quality in application domains of crucial importance in the South African context

A graphical respresentation of a medical ontology

In computer science the term ontology refers to a designed artefact consisting of a specific shared vocabulary used to describe entities in some domain of interest, and a set of assumptions about the intended meaning of the terms in the vocabulary. An ontology structures information in ways that are appropriate for a specific application domain, and in doing so provides a way to attach meaning to the terms and relationships used in describing the domain.

The vision of the semantic web is still far from being realised, but it forms part of a growing body of work on ontologies, applicable to a much wider variety of application domains. While the use of ontologies, in one form or another, is nothing new, advances in recent years have made it possible to apply this technology in ways that no one would have dreamt of a few years ago. In particular, it is now possible to reason efficiently over large ontologies, where reasoning refers to any procedure that makes explicit facts that are represented implicitly in an ontology. Reasoning is an important component of the construction and maintenance phases of an ontology where it is used to ensure that the ontology is a good representation of the application domain it is intended to model. Once an ontology engineer is satisfied that the ontology correctly represents an application domain, the role of reasoning changes and shifts to the inference or extraction of new facts about the domain that are implicitly represented.

As an example of the power of reasoning, consider the case of SNOMED CT, which is being adopted as the standard medical ontology in a growing number of countries worldwide, including the United States, Australia and a number of countries in Europe. It is a phenomenally large ontology with over 300 000 concepts and more than 1 300 000 relations between concepts. The correct classification of concepts – determining how the different concepts are related to one another – is crucial to the practical utilisation of SNOMED CT. Using state-of-the-art reasoning techniques, it is now possible to classify the whole of SNOMED CT in less than half an hour, a feat that would have been considered impossible 10 years ago.

The knowledge systems group in the Meraka Institute of the CSIR is investigating the use of such recent breakthroughs in ontology research as a means of providing improved data quality in application domains that are of crucial importance in the South African context. At present researchers are focusing on the development of modelling and reasoning tools for the biomedical domain. One of the major benefits of such tools is the long-term applicability of these to a wider range of application domains.

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Atmospheric modelling to predict air quality

by Miles Sowden and Mogesh Naidoo

THE CONSTITUTION of South Africa guarantees, "the right to clean air for all". Proving this requires expensive analysis and often overlooks specific incidents. Atmospheric modelling allows for faster and cheaper estimates of concentrations everywhere and at any time within the modelling domain.

Air pollution is the modification of the natural characteristics of the atmosphere by a chemical, particulate matter or biological agent. Worldwide air pollution is responsible for large numbers of deaths and cases of respiratory disease. While major stationary sources are often identified with air pollution, the greatest source of emissions is actually mobile sources, mainly vehicles. Substances not naturally found in the air, or at greater concentrations are referred to as pollutants. Pollutants can be classified as primary or secondary, with primary ones being substances emitted directly from a process, such as ash from a volcanic eruption or the carbon monoxide gas from a vehicle's exhaust. Secondary pollutants form in the air when primary pollutants react or interact. An important example of a secondary pollutant is ground level ozone, which is a significant contributor to photochemical smog.

Atmospheric dispersion modelling

It is impossible to monitor air pollution both simultaneously and ubiquitously. Atmospheric dispersion modelling is the computer simulation of the mathematical equations of how air pollutants disperse in the ambient atmosphere. The dispersion models are used to estimate the concentration of air pollutants emitted from sources such as industrial plants and vehicular traffic. Such models are important to both government agencies (tasked with protecting and managing ambient air quality) and industry seeking to maximise production within air quality standards. Additionally, the models are often employed to determine whether existing or proposed new industrial facilities are or will be in compliance with the National Ambient Air Quality Standards and to assist in understanding causes of severe air quality impacts and in designing effective control strategies.

The dispersion models require a host of input data, including:

- Meteorological conditions such as wind speed and direction, the amount of atmospheric turbulence, the ambient air temperature and the height of any inversion layers that may be present
- Emissions parameters such as source location and height, stack diameter, exit velocity, exit temperature and mass flow rate
- Terrain elevations over the entire modelling domain
- The location, height and width of any obstructions (such as buildings or other structures) in the path of the emitted gaseous plume.

Many modern, advanced dispersion modelling programs include a preprocessor module for the input of meteorological and other data, and many also include a postprocessor module for graphing the output data and/or plotting the area impacted by the air pollutants on maps.

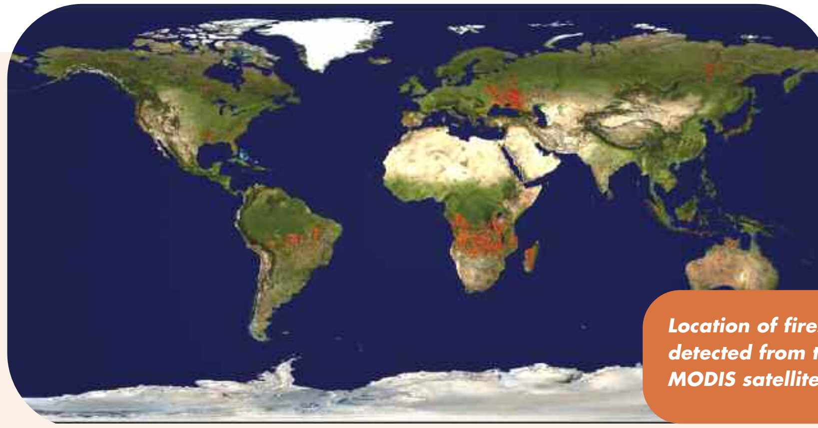
From left to right: Mogesh Naidoo, Miles Sowden, Warren Carter and Atham Raghunandan

Ozone brown haze over Cape Town, note the poor visibility of the mountains in the background

In essence, various components of the models must:

- Take into consideration all emission source types and compute an emission rate typically using air pollutant emission factors, which represent emissions per activity (e.g. grams SO_2 per ton coal burnt)
- Allow the emission to rise either by momentum or buoyancy, usually by using the Briggs plume rise equations
- Generate a 3D wind field over the modelling domain. Using observed data from radiosondes, weather satellites, surface weather observations and coarse gridded data from a global weather prediction model. The data are then assimilated using fundamental equations derived from conservation of mass and energy to compute future weather events
- Disperse the pollution under current meteorological conditions, typically using the Gaussian plume model, which considers the variance in the horizontal and vertical components (z and y) of the wind as a function of the atmospheric stability class and of the downwind distance to the receptor
- Simulate chemical and physical transformations of the pollutant such as photochemical reactions and/or deposition
- Graphically display the results in four dimensions, i.e. space and time (x, y, z, t).

The two most important variables affecting the degree of pollutant emission dispersion obtained are the height of the emission source and the degree of atmospheric turbulence. Turbulence leads to better dispersion and lower concentrations. The resulting calculations for air pollutant concentrations are often expressed as a concentration contour map to show the spatial variation in contaminant levels over a wide area under study. In this way the contour lines can overlay sensitive receptor locations and reveal the spatial relationship of air pollutants to areas of interest.



Location of fires detected from the MODIS satellite

Finding the right model

Various atmospheric dispersion models exist; they differ in the pollutants accommodated (e.g. radioactive, reactive, inert), source types (e.g. stack, vehicle exhaust, wind-blown dust) and whether these use a grid cell approach or a puff approach. Most modern models use a puff approach where the emissions are simulated in small time steps that may vary from seconds to an hour and track each 'release'. This differs from the grid cell approach where each emission is assigned to a cell. Each cell is 'dispersed' as a whole for each time step. The plume approach is mathematically more technically correct but is significantly slower; so many new models compromise by using a 'plume-in-grid' approach and start the emissions as puffs but switch internally once y approaches the grid cell size.

The contributions of all the input data and sub-models used add to the overall accuracy of the model. Typical errors encountered are emission sources that are ignored or incorrectly incorporated into the model (e.g. trans-boundary pollution) and utilising a wind field that is not applicable to a local scale (e.g. where fine topographic features are contributing to the local conditions but are not included in a larger grid domain). To improve the accuracy of models, scientists at the CSIR are combining the new field of remote sensing of pollutants with model results that will allow modellers to refine their input data and improve the model's algorithms.

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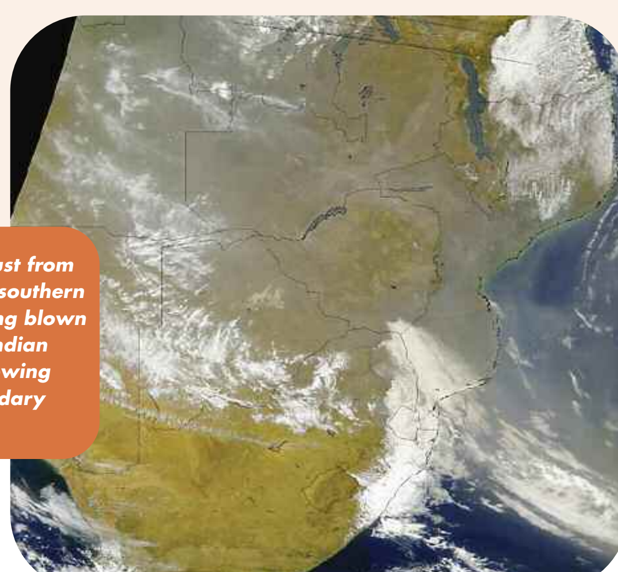


Aerosol dust from fires over southern Africa being blown over the Indian Ocean showing transboundary effects

Numerical modelling in rock engineering

by Dave Roberts

ROCK ENGINEERING involves the design of excavations in rock, including the sequencing, support strategies and design of monitoring and management systems to ensure the stability of the excavation for the duration of its lifespan. In mining, most excavations need to remain serviceable only for short time periods, so excavations are often designed to relatively low safety factors. The nature of the rockmass tends to be variable, so the stability of an already marginal excavation can be compromised further by unexpected changes in conditions.

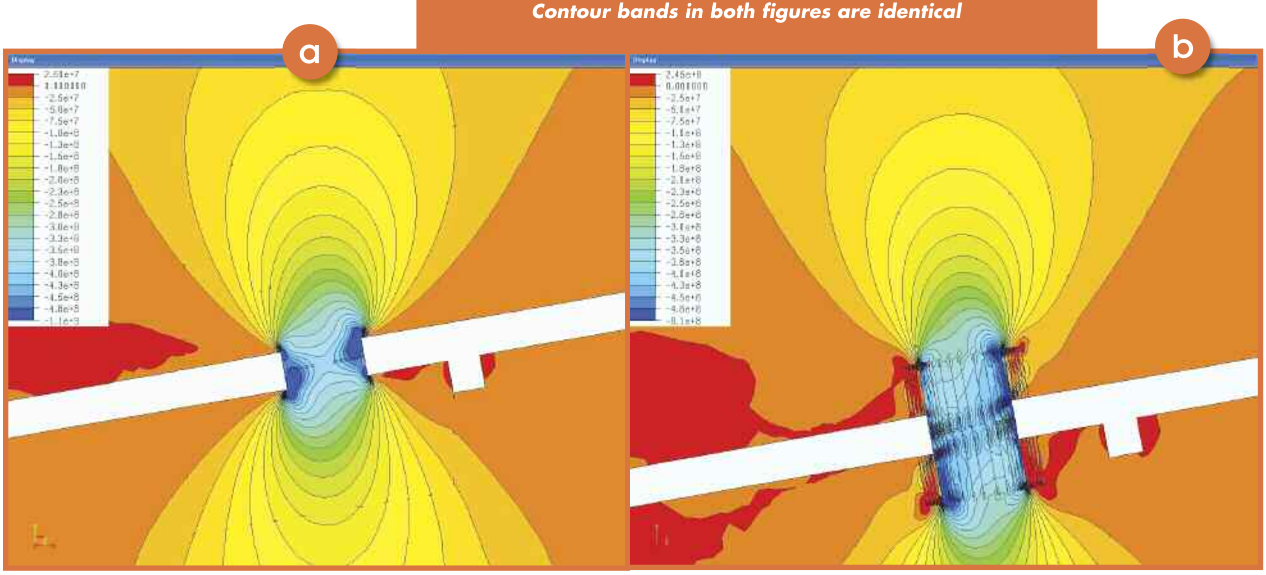
In most situations, established procedures and the experience of the practitioner are sufficient to negotiate these conditions, but often a situation arises for which little or no guidance is available. Numerical modelling is then often the only means of obtaining an indication of how best to design and support the excavation. Numerical modelling is particularly useful in evaluating scenarios, interpreting observed or measured behaviour and in exploring how the rockmass may behave in new commodities or with novel mining methods.

Modelling can improve our interpretation of observed behaviour. For example, a series of stress measurements were conducted over a pillar in a platinum mine. The measurements, when resolved to the same elevation as the pillar, indicated much higher stresses than expected. It was suggested that the presence of sub-vertical jointing and fracturing around the pillar had channelled stresses through the pillar, resulting in increased stresses near the measurement horizon. Comparative models (with and without sub-vertical discontinuities) were constructed to test this idea. The results (Figure 1) show that the hypothesis is correct. Stresses along a line at the top of the continuum pillar are of similar magnitude to stresses along a line at the top of the jointed zone of the fractured pillar. The stress measurements (taken just above the jointed/fractured region) therefore indicate lower stresses in the pillar than assumed from the elastic stress resolution.

Modelling has also been used in an attempt to better understand other aspects of the behaviour of the Bushveld Complex (platinum-bearing) rockmass. Discrete element modelling has shown that the behaviour of the blocky and sometimes stratified hangingwall (roof) is controlled by the evolution of a zone of vertical tension that grows as the excavation span increases. When this tensile zone crosses horizontal layers, an abrupt increase is observed in the closure, layer separation and stress magnitude. Figure 2 shows the distribution of vertical tension.

This work showed that tensile and compressive stress components co-exist within individual blocks to produce beam-like behaviour. This has implications for understanding how these discontinuous beams behave, and more importantly, how they fail. It has been suggested that platinum hangingwall failure can occur by the propagation of mining-induced fractures through intact

***Figure 1** Vertical stress contours around a continuum elastic pillar (a) and around a jointed and fractured pillar (b). Contour bands in both figures are identical*



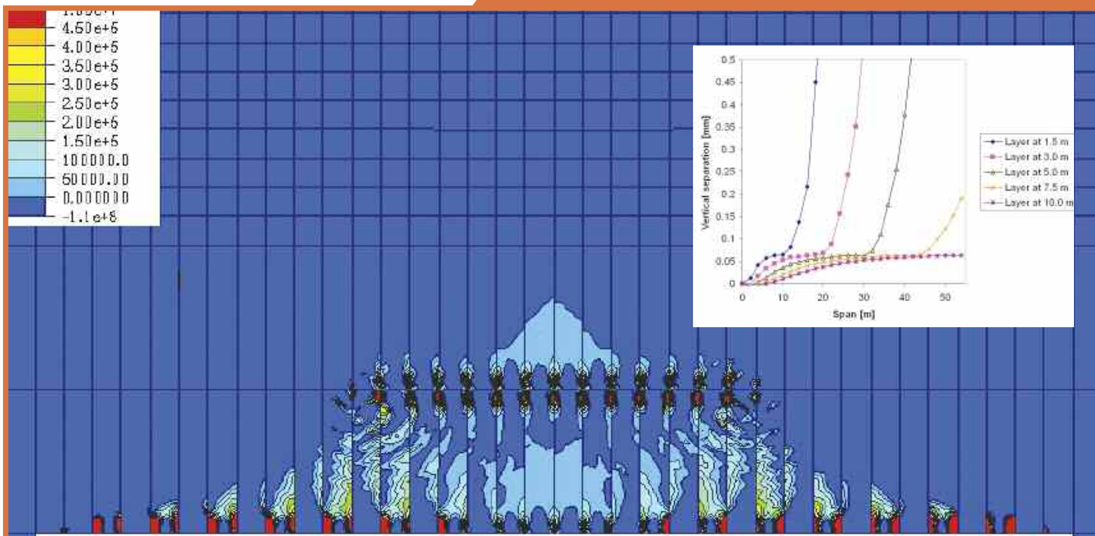
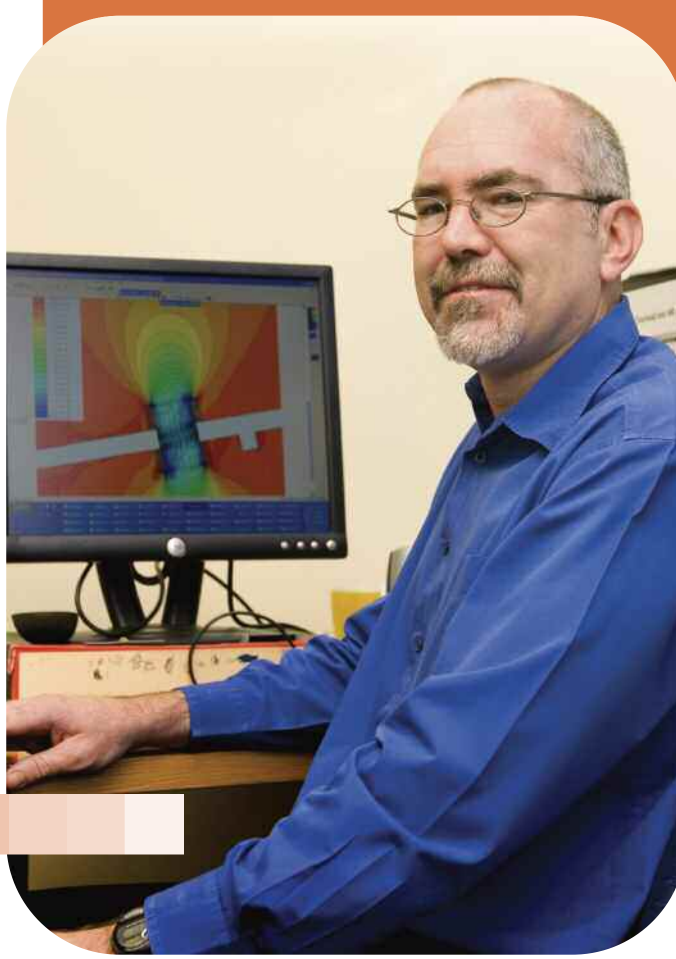


***Figure 2** Vertical tensile stress distribution for a 7,5 m high discontinuity at a span of 54 m. The inset shows the relationship between span and layer separation for various discontinuity heights. The circled point corresponds with the VTZ distribution in the figure*

rock blocks. The presence of large tensile and shear stresses in individual blocks corroborate this hypothesis, allowing researchers to design strategies that can prevent these failures.

Numerical models are also used to model mine workings on a much bigger scale. Mining operations typically cover many square kilometres of simultaneous workings. Models of such operations are analysed using the MINSIM boundary element program, originally developed at the CSIR. The results from these models can show the presence of features associated with seismic events, but results are limited in that they are linear and elastic. MINF, an in-house code similar to MINSIM, has been developed to model the non-linear behaviour of pillars in terms of their potential to release seismic energy. A cap stress and edge-weakening model has already been developed and was used in generating the first pillar strength formula for Bushveld (platinum) mines.



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Modelling the effect of excavations on seismic inversions:

Do stopes act as sources?

THE DEEPEST MINES in the world are found in South Africa, with stoping occurring at depths of almost 4 km. The enormous weight of the overlying rock strata results in high rock stresses at depth, which may cause pre-existing geological features to be reactivated or previously intact rock to rip and tear. The sudden rupture generates seismic waves, which race through the earth at speeds of about 6 000 m/s for P-waves and 3 800 m/s for S-waves. When the waves encounter the excavation surfaces, interference, diffraction and refraction effects may cause violent shaking. Rock fragments are often ejected and stopes and tunnels may collapse, with devastating consequences to men and machines.

The geometry of the underground excavations also affects the type and levels of seismicity. Blocks of the reef horizon are regularly left unmined to help support the excavation. These blocks, known as pillars, may also be left behind if the mining conditions deteriorate or if the ore grade drops below economic levels. Pillars become increasingly stressed as the mining excavations become more extensive. The stress concentrating effect can be compared to the pressure exerted by a stiletto heel – compare being trodden on by a high heel shoe to that of a gym shoe. An extremely detrimental consequence of stress concentrations is rockbursting. Rockbursts remain amongst the greatest challenges facing the South African mining industry and cost the industry about one billion US dollars per year (in terms of ground lost in pillars, local support, difficult mining as well as other factors). Rockbursts pose more of a threat to deep-level gold mining than the shallower platinum mines, whereas pillar bursts are more common in the platinum industry.

Different pillar layouts are used in different mining situations because the load-carrying requirements vary. For example, the deep level gold mines currently favour dip pillar systems, where the pillars consist of strips of unmined reef approximately 30 m wide, aligned down the dip of the reef. In contrast, the shallower platinum mines use so-called 'crush' and 'yield' pillars. These pillars have smaller dimensions than the dip pillars described previously and are designed to fail non-violently.

Non-classical source models

A number of pillars failed violently recently, resulting in localised damage at a platinum mine in the Bushveld Complex. The seismograms recorded by the in-mine network were unusual and showed features not previously described by the seismological community.

The first paper detailing the unusual seismograms was written by Dr Steve Spottiswoode (CSIR), and two peers from Impala Platinum Mine. It showed that the seismic source mechanisms associated with five pillar burst events were not compatible with the classical shear slip model that has been used to explain mining-induced seismicity, worldwide, for the past 25 years. Spottiswoode and his team had made a fundamental observation that required further investigation. To achieve this, two former CSIR researchers, Dr Lindsay Linzer (University of the Witwatersrand) and Dr Mark Hildyard (Liverpool University in the UK) are collaborating with the CSIR and running models on the CSIR's C4 high performance computer. The CSIR's Steve Donovan had the challenging task of 'parallelising' WAVE, a 3D modelling tool written in the early 1990s.

WAVE is used to model seismic wave propagation around a faulting source that 'daylights' into a stope. Synthetic seismograms are calculated using WAVE and compared with the recorded data. A problem with attempting to make these comparisons is that the seismic data is recorded in the 'far-field' (i.e. at hypocentral distances much larger than the source size) whereas small grid sizes are needed to preserve the finer details of the source – modelling the effect of fine structure within large objects requires enormous numerical models. To compound matters, if the effect of multiple model parameters is to be investigated, model execution times can run into thousands of hours of computation time. Such studies become feasible only with the availability of high performance computing infrastructure, such as the C4, where the calendar time required to run the model can be reduced by running many models in parallel.

Most seismic earth models and wave propagation modelling codes assume an infinite, homogeneous medium.

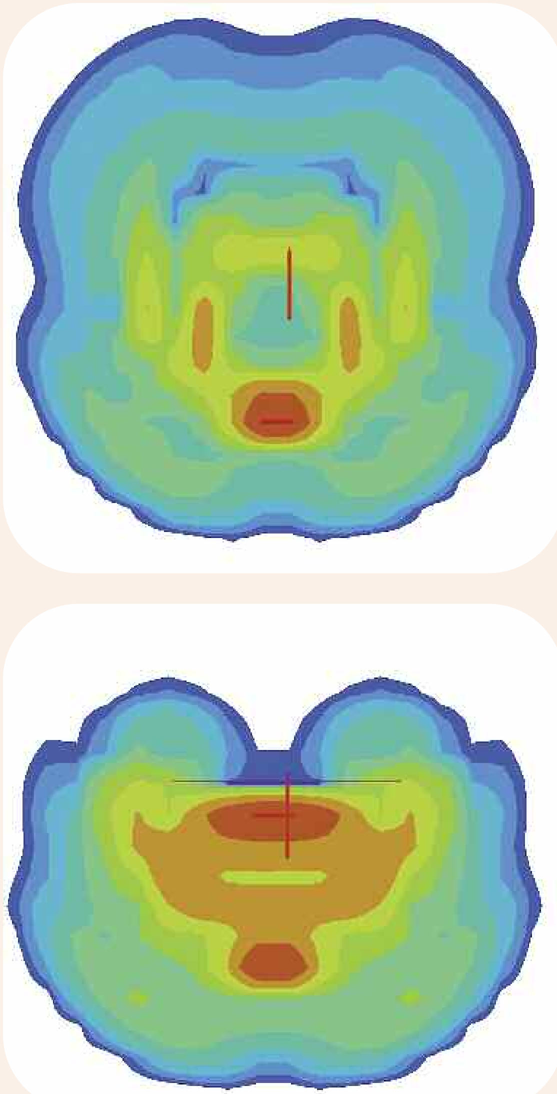

Figure 1 *Vertical cross-section showing the wavefield generated by a vertical shearing source (top) case with no stope (bottom) in the vicinity of a horizontal stope*

However, in South African gold mines, the tabular orebodies are mined extensively and the excavations can extend for many kilometres. Since most mining-induced seismic sources occur within the region of mining, the infinite, homogeneous assumption that the seismic inversions depend on, is badly violated. WAVE is unique in that it is able to model the effect of voids on the seismic wavefield in 3D.

Previous work attempted to investigate the effects of stopes on seismic inversions. However, because of limitations such as computer memory and speed, it was not possible to run large enough models to propagate wave forms at sufficiently large distances. The research was not able to confirm conclusively that the far-field seismic inversions were significantly influenced by the stope.

The main objective is to determine whether the source parameters calculated from recordings (seismograms) of the radiated wavefield are influenced by the presence of the stope. Since the source mechanism is known in detail (because the source is explicitly input into the model) the accuracy of the seismic inversions can be evaluated. Preliminary results are shown in Figure 1.

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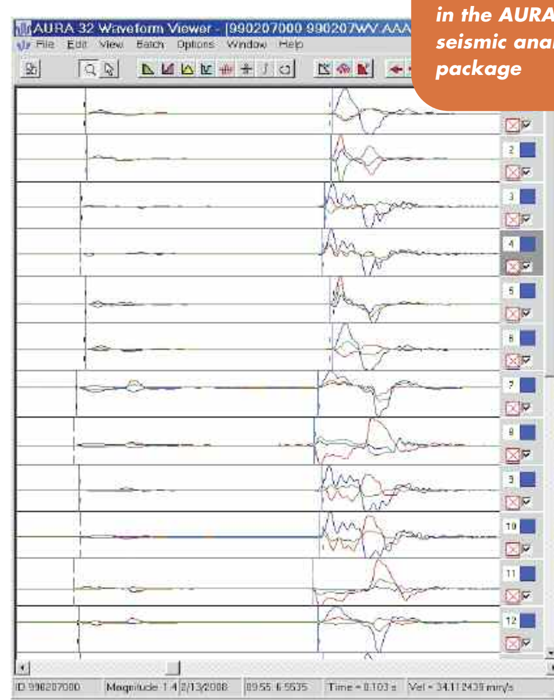

The synthetic seismograms generated by WAVE shown in the AURA seismic analysis package

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Statistical modelling

TRADITIONAL STATISTICAL modelling helps researchers accommodate and understand the level of uncertainty associated with predictions made by models, when compared with empirical data. This is useful when researching complicated systems, that is systems that can be understood well enough to obtain predictions. More recently, however, statistical modelling techniques have been used for dealing with complex, adaptive systems that are often unpredictable and exhibit emergent behaviours.

Complex systems present researchers with wicked problems. New computer-enhanced techniques in multivariate statistics (including agent-based Bayesian belief networks, morphological analysis, social-networking models and genetic algorithms) are being used to help classify and integrate understanding of complex system hierarchies, dynamics, interdependencies (such as feedback) and agent and system level behaviours. In particular, where modelling-based large interdisciplinary research programmes are being conducted, these statistical modelling techniques help to facilitate interdisciplinary interaction and to identify trends and patterns in large, overloaded (or incomplete) data sets and model outputs. The CSIR has invested in this area of research, as it holds promise for future crossdisciplinary work on large-scale human development programmes. – Camaren Peter

Camaren Peter works with local and international research and software development partners to help deal with sustainability challenges brought about by complex socio-ecological system interdependencies.

Statistical modelling: An appropriate methodology to deal with uncertainty

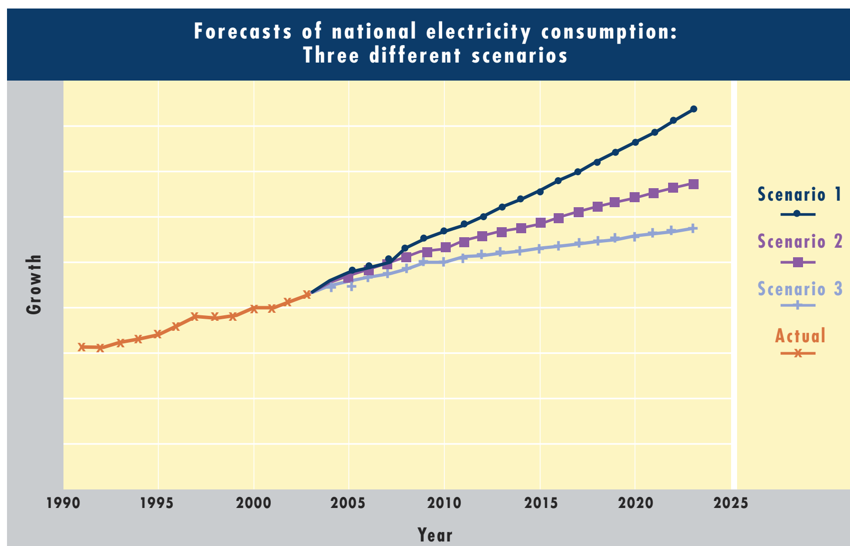
by Dr Chris Elphinstone

IN MANY SITUATIONS 'true' values of phenomena cannot be observed directly, but only values that are modified by uncontrollable random effects. In other situations, uncertainty arises due to the fact that only a sample of measurements can be obtained from which conclusions about a larger population need to be inferred. Uncertainty is also often present in observed data due to measurement variability. Variations between instruments and the skill of users can, for example, result in differences between measurements of the same phenomenon. In other cases, the observed values represent a stochastic process, such as wind speed or wave height, where repeated realisations will result in different values being observed. Statistical modelling takes account of uncertainty in input data and relates this to the uncertainty in projected outcomes. For these and other situations where uncertainty is present, statistical modelling is often an appropriate methodology.

The statistical modelling and analysis research group at CSIR Built Environment specialises in, among others, the application of statistical modelling techniques to a wide variety of situations. Some examples include:

Forecasting long-term energy demand

Planners are often required to make long-term forecasts for electricity demand. Such forecasts need to learn from the past as well as take future uncertainties into account. The first step in the research process is to identify covariate factors that influence electricity demand, such as population, gross domestic product and other industrial indicators. The task is then to determine the statistical relationships between these factors and electricity demand, based on historical data. The next step generates forecasts of electricity, using predicted values of the covariate factors and the relationships of these with electricity demand, using the well known regression and time-series models. The methodology allows planners to incorporate their own belief in future scenarios for the covariate factors.



Election night forecasts

Election night forecasting is the activity whereby, when new voting results are available, forecasts are made of the final results to assist analysis and reporting. The challenge is to compensate for the fact that results become available in a non-random way and early estimates would tend to over-report some areas. Urban and easily accessible districts are, for example, counted quickly. The CSIR developed a model founded on fuzzy clustering to segment the electorate, based on voting patterns observed in previous elections. A feature of fuzzy clustering is that each voting district is represented in each cluster, albeit with unequal weights. The underlying assumption is that the voting patterns within a particular cluster will be the same in the new election, even though these may differ from those of previous elections on which the clusters were defined. As soon as a few results are available, the party support for each cluster can be estimated, and by aggregating these, national and provincial results obtained. The model has been highly successful and new analyses are being added to assist the detailed analysis of future elections.

Supply and demand forecasting

As part of the footprint project carried out for the Department of Justice and Constitutional Development, a model was developed for predicting the demand at various offices and comparing it with existing service delivery. It was found that a model using population size, employment status, gross geographic product and total reported crime could be developed to predict, amongst others, the time required for criminal, civil, family and other court work.

Risk of extreme events as a result of climate change

Climate change is a phenomenon that is cause for major concern. The CSIR is participating in a multidisciplinary project aimed at quantifying certain risks due to climate change. Specifically, one of the objectives is to develop a risk assessment framework for selected sectors of southern Africa. This framework could then be used to forecast the change in risk under various climate change scenarios. As an example, the generalised extreme value distribution could be used to model the probability of wave heights exceeding a specified threshold associated with coastal flooding. This will form the basis of predicting the increased probability of such occurrences resulting from climate change in the future.

Forecasting future outbreak of a disease

The CSIR recently participated in a multidisciplinary team studying outbreaks of cholera in Beira, Mozambique. The statistical relationship between the environmental (climatic) factors and the outbreaks of cholera at different time periods was of particular interest in this study, and the question of whether these relationships could support the hypothesis that climatic conditions drive the proliferation of cholera cases. A second objective was to apply multivariate time series techniques and negative binomial regression techniques, especially suited to this type of 'count' data, to forecast new outbreaks, taking account of environmental variables. The ultimate aim of the project was to create a short-term early warning system for cholera outbreaks in Beira, which could also be used in other high-risk areas.

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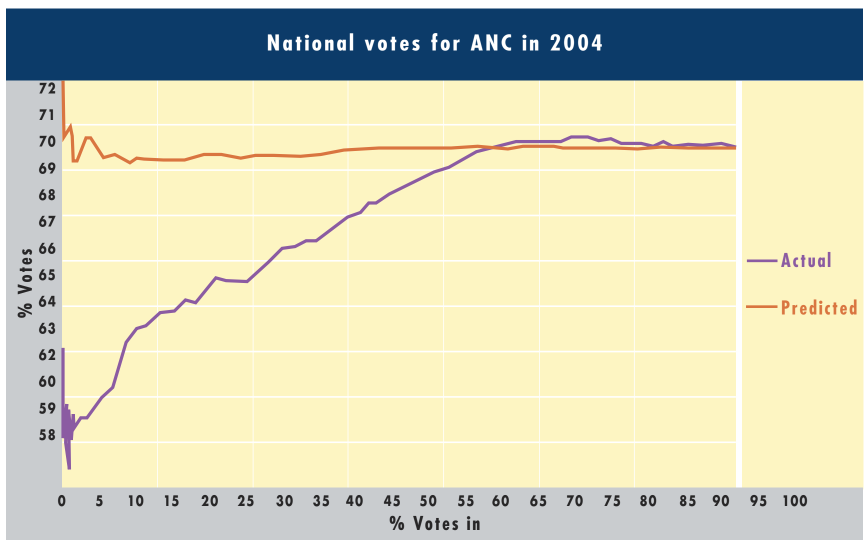
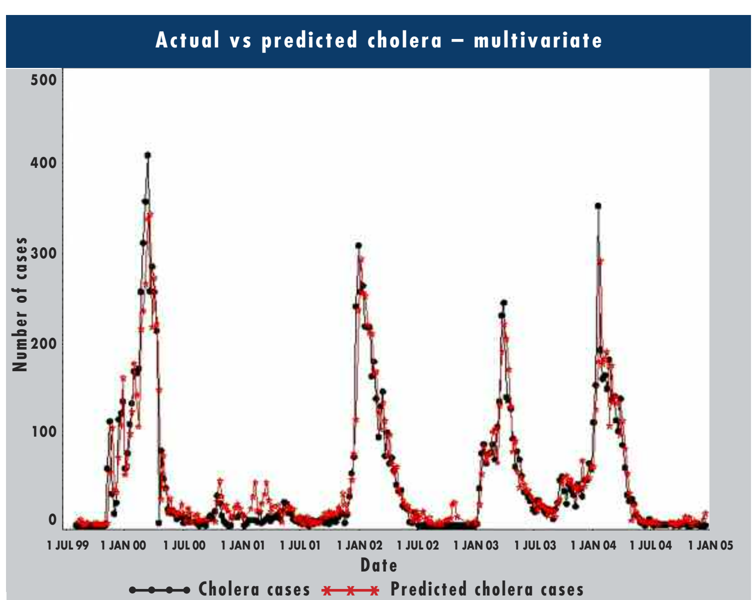
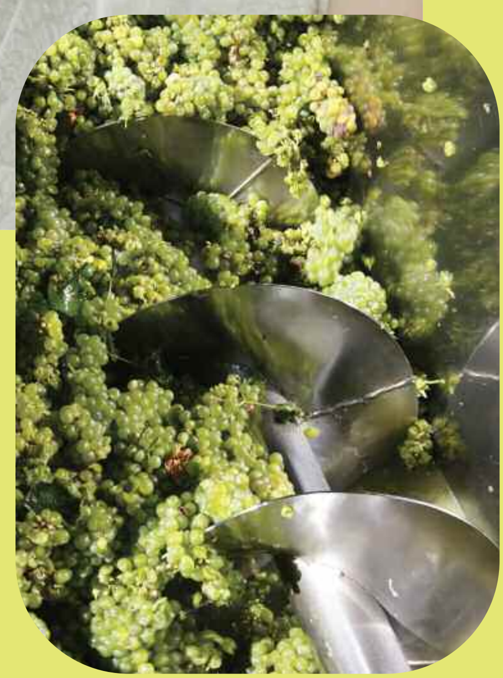
Dr Chris Elphinstone leads the statistical modelling and analysis research group





Modelling agricultural supply chains

by Dr Esbeth van Dyk and Dr Gert Engelbrecht



Dr Esbeth van Dyk has been involved in the modelling of supply chains in the fresh fruit and wine industries

VARIOUS AGRICULTURAL supply chains have been analysed by the CSIR in the recent past. Some of these, or components thereof, including supply chains in the fresh fruit, wine and sugar industries, have been modelled mathematically.

Fresh fruit supply chain

The CSIR was commissioned to analyse the logistics infrastructure capacity for the fresh fruit export industry in order to make recommendations for its utilisation and the possible need for investment in infrastructure.

The study comprised four phases and covered a large variety of activities. The following modelling components are of particular relevance:

- Simulation models were developed for fresh produce terminals in Cape Town and Durban to analyse the flow of produce through these terminals in detail
- A maximum flow optimisation model of the infrastructure network was developed to determine the maximum volume of produce that can be handled by certain sections of the network
- An Excel model was developed to determine the then current and potential future utilisation of the various conventional and container terminals that load fruit for export.

These models were used to determine whether investment in logistics infrastructure would be required in the foreseeable future. All the models showed there was no immediate need for investment in additional infrastructure other than at the container terminals, which were operating too close to capacity, resulting in congestion and delays.

These needs had already been identified by the relevant parties and capacity expansion plans were in progress. The congestion and delays experienced at the conventional terminals in Durban during the peak citrus season were identified to be largely due to the inability of the cold stores and transport management system in the greater Durban area to provide the terminals with a continuous supply of the right fruit at the right time and not due to insufficient capacity at the terminals, as was perceived by many producers and exporters.

This problem could be addressed through upgrading some of the cold stores and investing in IT infrastructure and software, both for cold store management and transport management. The simulation model of the Durban fruit terminal therefore identified

Dr Gert Engelbrecht led the research project aimed at modelling the supply chain of the Swaziland Sugar Association

the true cause of congestion and prevented the fruit industry from making costly investments in additional terminal infrastructure that would not have resolved the problem.

Wine supply chain

This project aims to lend decision support to management at wine cellars, with a specific winery being a special case study. The decision-support system is to be delivered in the form of Excel spreadsheet models and currently focuses on three features. The first is to assist in the scheduling process of assigning grapes from different suppliers to different tipping bins by suggesting rapidly and in an automated fashion, a possible schedule based on the information currently considered when making such decisions. The second is to assist the viticulturist in the sometimes difficult rescheduling decisions when the agreed-upon amount of grapes cannot be delivered to the cellar due to unforeseen technical or operational problems. The last feature of the decision-support system is to assist in solving a layout problem concerning the floor plan and pipelines for a cellar. This feature should be able to evaluate the current layout of a cellar and therefore also assist in the design of a floor plan for new facilities or the renovation of current facilities.

The research project forms part of the larger global drive to establish an international wine industry supply chain research network. The network, which includes the Georgia Institute of Technology in the USA, the Catholic University of Chile, the CSIR, and CSIRO in Australia, will attempt to collaborate on issues in global wine supply chains. Together, the countries involved are responsible for 22,5% of total worldwide wine exports (2004). This project presents a unique opportunity for CSIR researchers to collaborate with top researchers internationally and will also assist the South African wine industry in its quest to compete in the global market.

Sugar supply chain

The Swaziland Sugar Association (SSA) commissioned the CSIR to conduct a study to improve the association's supply chain. This involved two distinct chains: it was necessary to model the SSA sugar cane supply to its mills and secondly the delivery chain of the association's refined, semi-refined and raw sugar products to its customers.

Regarding the sugar cane supply to the mill, research was undertaken and a model designed, based on work done at the University of KwaZulu-Natal that provided metrics to evaluate the quality of the chain, the use of available capacity in the chain and the chain cost per ton of sugar cane delivered to the mills. The sub-processes identified were harvesting operations, loading operations, transportation, mill yard operations and milling operations. The study revealed a number of sub-optimal practices that result in over-capitalisation in the industry. These are currently being addressed by the SSA. The delivery chain was modelled as a transshipment problem and an optimal strategy for distribution derived. In the process, certain pricing anomalies were discovered, which, if rectified, could lead to significant savings to the industry.

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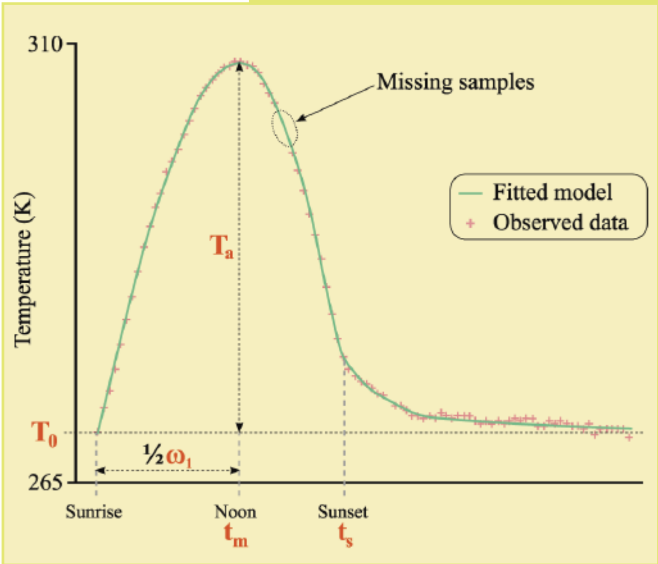
Optimising the constraints of a diurnal temperature cycle model

by Dr Frans van den Bergh

EARTH OBSERVING SATELLITES allow us to collect a wealth of information about the earth's surface properties. In particular, the Meteosat Second Generation (MSG) satellite, a geostationary weather satellite, transmits a snapshot of the observed brightness temperature over Africa and Europe at 15-minute intervals. The Advanced Fire Information System (AFIS) employs this satellite to detect active fires in near real-time by looking for areas that have unusually high temperatures compared to the immediate surroundings.

With the MSG satellite it is also possible to detect fires by looking for sudden changes in temperature through time, rather than space; this requires a model of the temperature changes throughout the day. Figure 1 illustrates a parametric model that describes these changes – called the diurnal temperature cycle (DTC) – with a high degree of accuracy. Scientists describe the DTC using a cosine function during the period from sunrise to sunset, and an exponential decay function (according to Newton's cooling law) to model the period from sunset to the next sunrise. The smallest area that the satellite can observe is called a pixel; researchers model the data observed through time at each pixel in the satellite image independent of other pixels.

Figure 1



Dr Frans van den Bergh

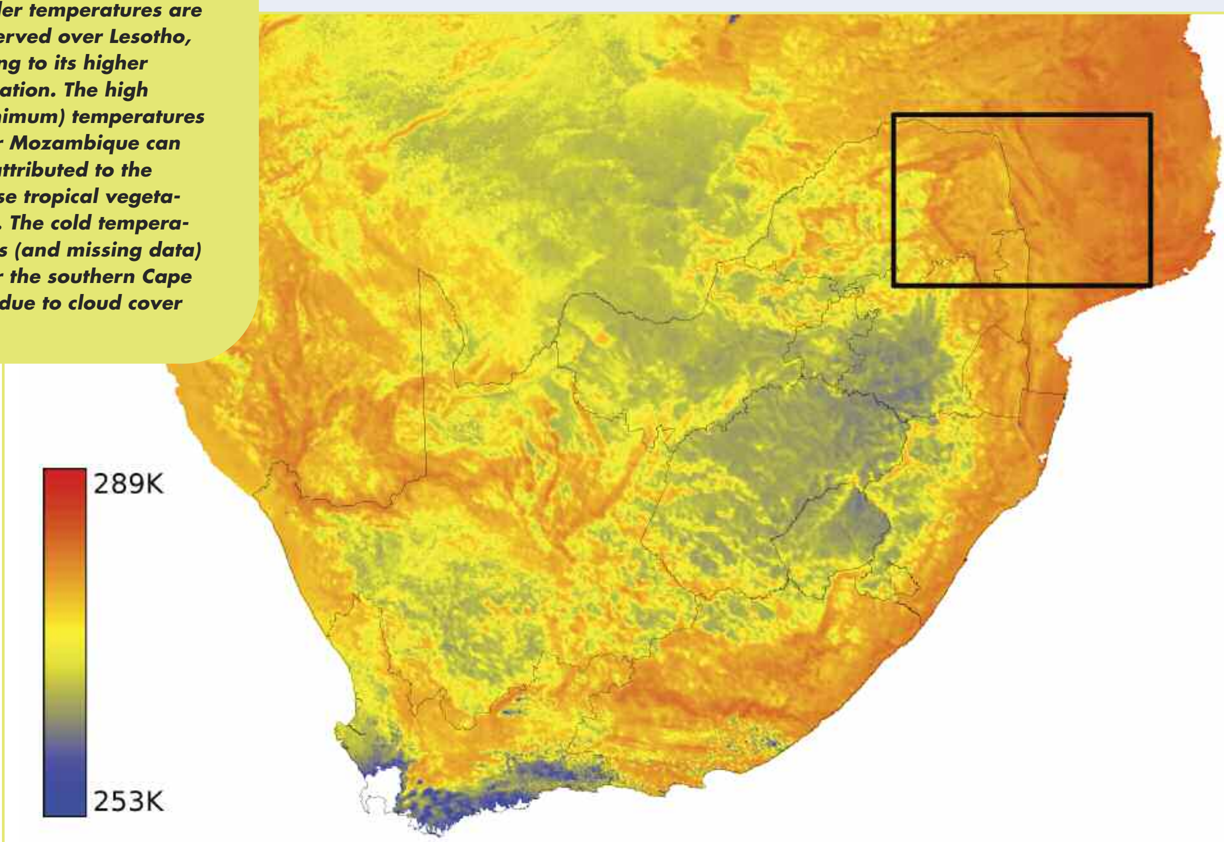


Figure 2
A map of the T_0 parameter on 2004/07/22 over southern Africa. Cooler temperatures are observed over Lesotho, owing to its higher elevation. The high (minimum) temperatures over Mozambique can be attributed to the dense tropical vegetation. The cold temperatures (and missing data) over the southern Cape are due to cloud cover

Some of the model parameters have a natural interpretation, for example, the T_0 parameter approximates the minimum temperature observed at a given pixel on a given day. The values of these parameters can be visualised spatially to produce a map like Figure 2.

The process of model fitting involves adjusting the parameters of the DTC model so that the temperatures predicted by the model are as close to the observed temperatures as possible; this process is automated using a robust optimisation algorithm. The first implementation produced the results shown in Figure 3a, which clearly illustrates large, unwanted variations in the fitted model parameter T_0, which manifests as 'blotches' and 'grainy' regions. Scientists discovered that the parameters determined by the model fitting procedure were sensitive to small measurement errors present in the data, which caused the parameters of two very similar data sets (e.g. two neighbouring pixels) to differ significantly.

Requiring another approach, scientists applied some constraints to the model parameters, producing the output shown in Figure 3b. The parameters obtained with the constrained model fitting procedure are much smoother, and reflect the true surface properties more accurately.

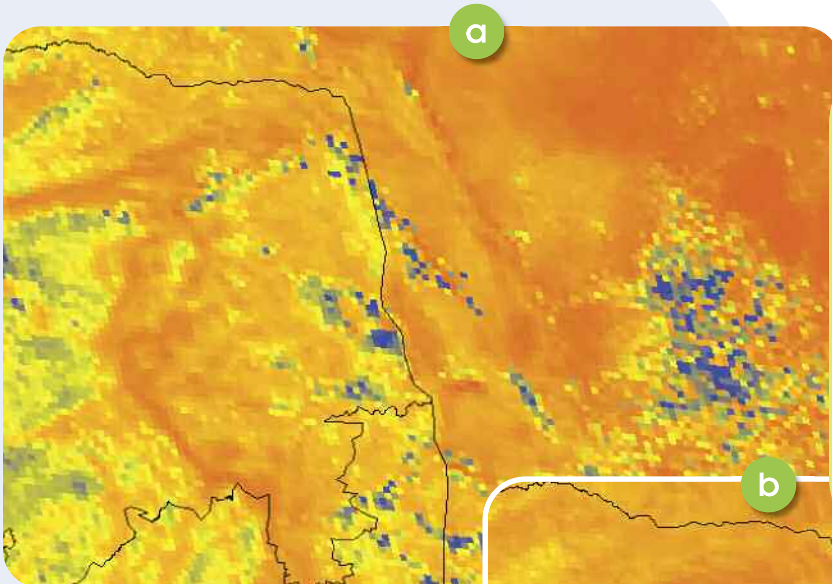
How do these constraints work?

The values of some parameters in the model can be estimated, such as the length of a day (ω_1), without using the observed data. These estimates are used in the model fitting procedure to 'punish' proposed parameter values that stray too far by adding a penalty proportional to the deviation. Scientists use a combination of Monte Carlo simulation and optimisation to compute optimal weights for these penalty terms, which increases the reliability of the model fitting procedure dramatically. This optimisation process is computationally intensive and took 20 hours to complete using 42 processors (in parallel) on the CSIR Cluster Computing Centre's Opteron facility. On a PC, this would take 35 days!

Applications

The fitted diurnal temperature cycle model is used to perform a variety of tasks, including temperature interpolation to obtain missing values caused by transmission errors or cloud cover, as well as driving a temperature tracking algorithm used to detect fires. The temperature tracking algorithm is expected to be able to detect smaller fires than what is currently possible using the existing spatial fire detection algorithms.

This new algorithm, a collaborative effort involving the French National Institute for Research in Computer Science and Control (INRIA) and the Tshwane University of Technology, is still under development, but initial results are very promising.



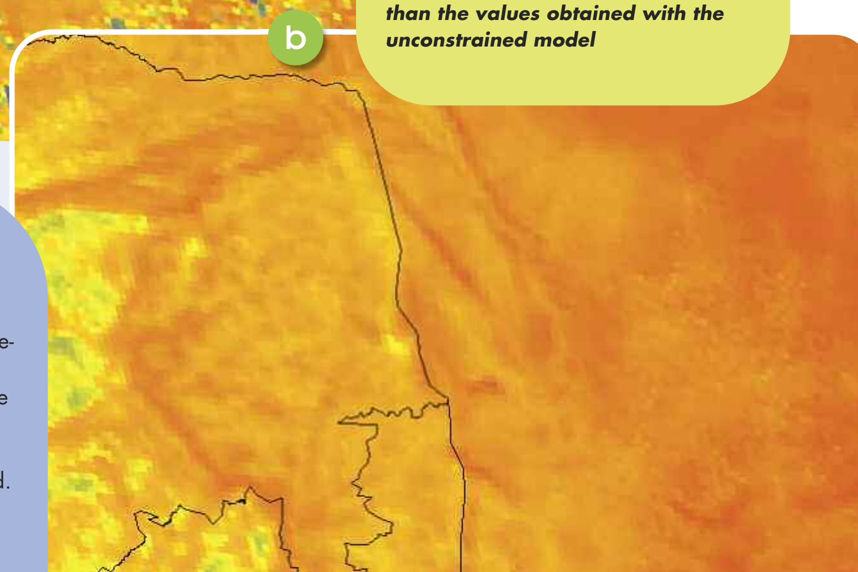


Figure 3
(a) An enlarged view of the T_0 parameter over Mozambique and the Limpopo province, obtained using the unconstrained model. The image appears grainy and there are several blue patches (cool temperatures) that are inconsistent with reality

(b) An enlarged view of the T_0 parameter over the same region, obtained using the optimised constrained model. The image is noticeably smoother and more consistent than the values obtained with the unconstrained model

Monte Carlo simulation

IF 10 PEOPLE MEASURE the width of a desk with the same ruler, 10 slightly different measurements are likely. The differences between these measurements and the true width of the desk are called measurement errors. If we calculate the average of all 10 measurements, we hope the effect of the measurement errors will be reduced. If a different group of 10 people measure the width of the desk, the average measurement is expected to be similar to that of the first experiment. If this experiment is repeated with 20 groups of people, one would be able to say whether this method of measuring the width of a desk is reliable, that is, if the different groups all gave consistent measurements.

The problem is that this method can be applied only to situations where repeated observations are possible, which unfortunately does not apply to satellite imagery, since things may change between observations.

Monte Carlo simulations are a way in which the reliability of fitted model parameters can be measured without having access to repeated measurements. The solution, developed by researchers at the Los Alamos National Laboratory in the 1940s, is to generate synthetic data sets based on a single observation. These synthetic data sets are treated as additional observations, allowing scientists to calculate the sensitivity of their model parameters to the expected measurement errors. This process is illustrated in Figure 4.

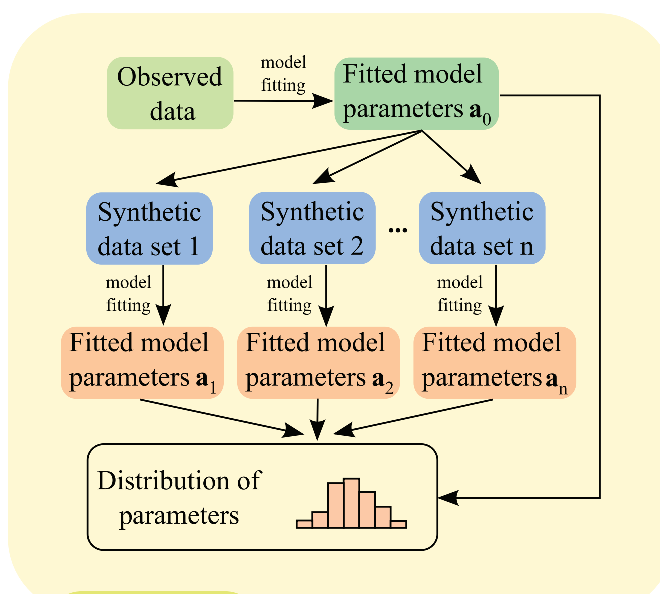


Figure 4

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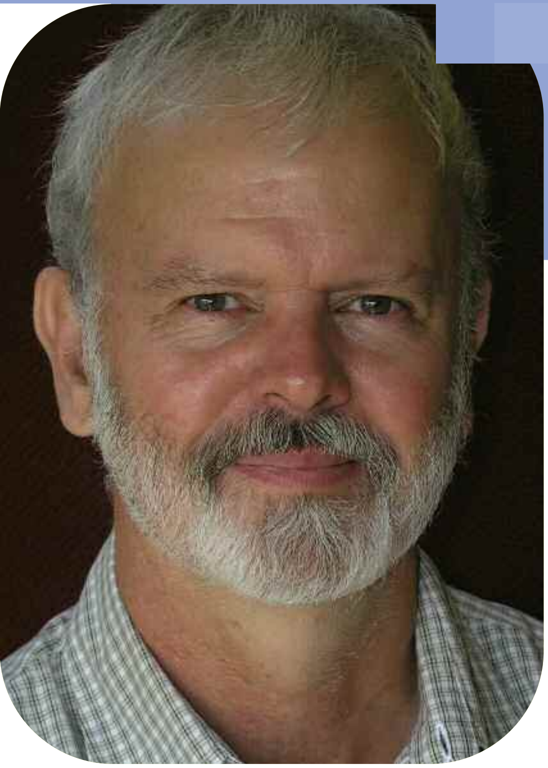
Modelling the growth and water use of South African forest plantations

by Dr Peter Dye



AN IMPORTANT ASPECT of forest plantation management in South Africa is the need to monitor tree growth rates and predict suitable harvest dates, final yields and overall profitability. It is generally necessary to plan for an even rate of harvesting from forestry estates to ensure a regular flow of wood to the mill. Profit margins are low and it is thus preferable to try to spread income evenly over time.

Foresters have considerable research information to guide them in decisions such as choice of tree species, planting espacement, fertiliser application, scheduling of thinning and pruning, control of diseases and pests, and the optimal timing of harvesting. These decisions are made for each 'compartment' of trees comprising a block of same-aged trees. Typically, forest estates contain scores of compartments that are delineated to ensure that each occurs on reasonably uniform sites so that the trees can be managed as a uniform block.

Currently, growth prediction involves the use of well-established empirical growth models based on fixed relationships between tree growth, the management of stands and site conditions. These models reflect much knowledge gathered over many years, but are acknowledged to have some limitations:

- They do not take changing weather conditions into account. Rotation periods commonly range from six to 40 years and extremes of rainfall and temperatures over such long periods may have profound effects on tree growth patterns
- They require a site index based on measurements recorded in previous rotations of trees. This is not available if trees of the same species have not been grown on a site previously
- New clones are being introduced constantly, diminishing the value of growth data gained from past rotations
- They cannot take into account long-term influences on tree growth such as climate change, declining site fertility or long-term soil water dynamics
- They do not predict rates of water use by the trees. This point is of particular significance in South Africa. Forestry is a declared streamflow reduction activity. It is therefore important for regulatory authorities to gain realistic information on the water use of forest plantations.

In recent years, 'process-based' models (PBM) have received increasing attention from scientists and forest managers. This class of model simulates the month-by-month growth and water-use of stands of trees (weekly and daily time steps are also used in certain models). Such models numerically follow the changing structure of tree stands over an entire rotation, as well as some of the major physiological processes regulating growth and water use.

Thus, biomass increase is calculated at each monthly time interval by taking into account the total leaf area of the trees, how much sunlight is intercepted, what proportion is photosynthetically active, what amount of carbon is fixed, and how the fixed carbon compounds

are respired or allocated to different parts of the trees. Similarly, these models can track what proportion of rainfall infiltrates the soil, and at what rate it is taken up by the trees and evaporated back into the atmosphere. This rate of transpiration is estimated from the availability of soil water, the leaf area, the diffusion rate through leaves and the current evaporative conditions in the atmosphere. Earlier models of this kind were not useful to the non-scientist because of the complexity. However, recent knowledge of forest physiology has now advanced to a point where it is possible to develop much simpler PBMs that are able to provide a balanced and realistic simulation of tree growth and water use. One of the more successful and practical PBMs is 3-PG (physiological principles in predicting growth).

A CSIR-led research consortium was successful in securing three years of funding from the Innovation Fund to set up 3-PG for use with the major forestry species in South Africa. The research consortium was led by the CSIR and included the Institute for Commercial Forestry Research, the University of KwaZulu-Natal, as well as additional consultant programmers and forestry modellers. The project was aimed at removing two impediments to implementing 3-PG on an operational scale in South Africa:

- Model parameterisation of the most widely grown tree species. Growth and site descriptive data were accessed from an extensive database maintained by three major forestry companies. Three of the most widely planted forestry species (*Eucalyptus grandis, Pinus patula* and *Pinus elliottii*) were parameterised and parameter values were tested against independent data
- Improvement in the ease with which input data can be sourced and entered, and output data can be viewed and assessed.

The final product is easy to use, allowing the user to run 3-PG for any given location and combination of growing conditions. A GIS module permits weather records and site descriptors to be accessed easily from an incorporated database containing 51 years of weather data for many hundreds of weather stations situated around South Africa. By further stipulating the tree species, more detailed site conditions and management activities, a month-by-month simulation of a stand of trees is generated. Such simulations are anticipated to lead to improved predictions of final yields, a better understanding of what is limiting the growth rates of trees, efficient scenario comparisons of different species and management options, and a means of improving assessments of drought risk in forest plantations.

Negotiations are underway to decide on the most appropriate way in which this product can be released to the forestry industry.

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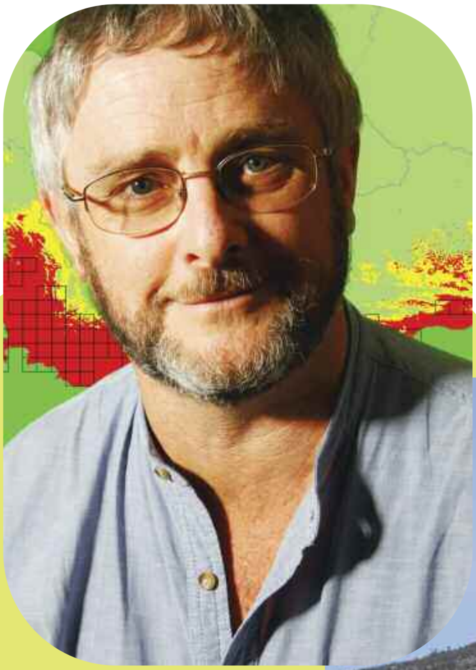
Modelling the potential distributions of invasive plant species

by David C Le Maitre



MODELLERS HAVE TO exercise judgment when deciding what to include in a model and what to leave out, and in assessing the consequences of that decision.

One of the CSIR projects in the natural resources and the environment domain is particularly interested in predicting the potential distributions of introduced plant species (weeds) invading natural ecosystems. The Working for Water programme has made many people aware of the undesirable impacts of invading plants; but few know that most weeds are actively expanding their ranges and many new ones are arriving. Weed managers need to know where these weeds can invade so that they can target control measures.

Modelling of the current and potential distributions of plant species is a very active field of research internationally with more than 300 papers in the past five years covering communities, plant or animal species and diseases. There is much interest in understanding how species will respond to climate change and concern about increasing problems with diseases (e.g. malaria).

Views of a Hakea sericea bush with nuts [follicles] (below), typical invasion showing the tall shrubs (right) and a heavily invaded mountain slope (centre) where the hakeas can be seen as dark green shrubs

Species distributions are determined by combinations of three factors:

- Abiotic (non-living) elements, such as climate and soils
- Biotic (living) elements, such as competition from other species, requirements for other species or diseases
- The kinds and frequencies of natural disturbances that renew species and communities, such as fires.

The multidimensional space defined by the limits that a species will tolerate for each of these factors is called its niche. Tolerances to abiotic factors and disturbances are fairly easy to estimate while biotic factors are not. These require detailed and sometimes long-term studies. Since we have only sufficient data to develop full models for a few species, most studies use abiotic factors and assume that biotic factors and disturbances are relatively unimportant. Most models are based on estimating the limits from data about the sites where it occurs.

A further complication is the fact that most observations tell us only where the species was present; not where it was absent. We cannot assume that every absence is a true absence because there are different reasons for absences. The species may not have reached that place yet, or it may be there but has not been detected yet, or it may be unable to establish a viable population. Only the third one is a true absence, the others are false – but we do not know which of the three is true for a particular place. Simply using all the absences will weaken the models that use methods that require presence and absence data. Some methods need only presence data, but these have no clear advantages over those using absences as well. This specific project has focused on developing a logical and defensible way of filtering absences to see if this produced more accurate models.

Three *Hakea* species were chosen because of very good presence data. The three *Hakea* species are members of the protea family and major invaders of Cape fynbos. A spatial data set for a range of climatic variables for South Africa was compiled and then the climatic variables filtered to select threshold values of two climatic variables, which matched the limits of the presence records in areas where *Hakea* has been present for several decades. All absences with values less than these thresholds were considered true; the rest were false. The presence data were then sub-sampled and two regression models fitted using an equal sub-sample of all the absences and only the true absences.

Models using only true absences fitted the presence data more accurately because these correctly predicted virtually all the presence records. Far fewer presences were also predicted where there were true absences. Filtering of the absences does result in better predictions. An example of a potential distribution is shown in Figure 1. Some ideas exist on more objective ways of identifying the right variables and the limits. It is anticipated that these will be pursued using hierarchical Bayesian approaches and that ways of testing the sensitivity of these models to increase confidence in their outputs will also be investigated.

South Africa is likely to experience marked changes in its climate by 2050 and models like these can be used to predict the potential distributions of invading species as well as indigenous species, communities and diseases. Insights provided by these models can be used to anticipate the impacts of climate change and develop strategies and action plans to mitigate the impacts and safeguard our unique biodiversity. The CSIR is developing ideas for collaborative research on this topic with the South African National Biodiversity Institute, the University of the Witwatersrand), the Laboratoire d'Ecologie Alpine, Université Joseph Fourier in France and the Department of Environment and Conservation in Western Australia.

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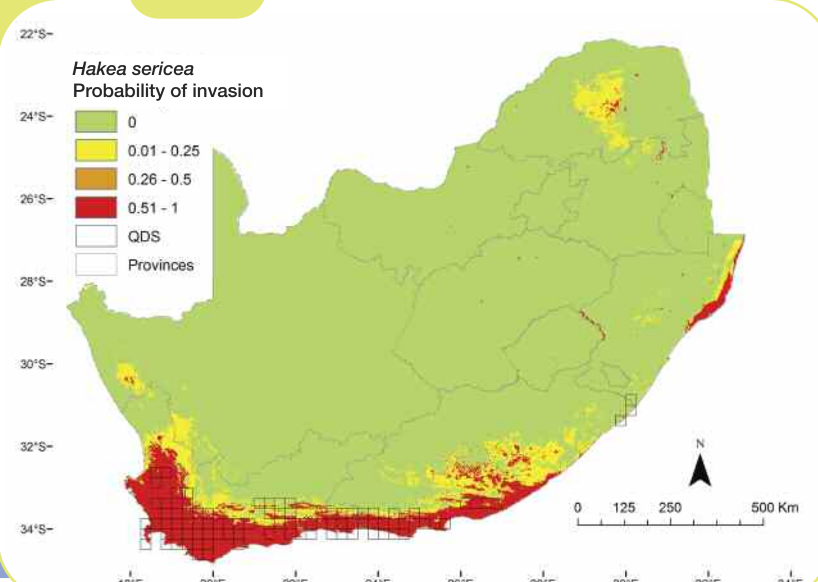
Figure 1



The potential distribution of Hakea sericea in South Africa based on presence records and true absences. The QDS squares are 15′ latitude x 15′ longitude and indicate the areas where the species has been recorded. The areas with a probability of occurrence of less than 0,6 are too limited to be seen at this scale

Modelling vegetation phenology from 20 years' daily satellite data

by Dr Konrad Wessels

The research team members in the field: Dr Konrad Wessels, Sally Archibald, Karen Steenkamp, Graham von Maltitz and Asheer Bachoo (not present)

CSIR RESEARCHERS have used close to 20 years of daily satellite imagery to model vegetation phenology, allowing unique analyses of patterns across the entire southern Africa. Vegetation phenology examines life cycle events such as bud burst, flowering and leaf senescence. The phenology of terrestrial ecosystems reflects the response of the biosphere to proximal climatic factors (e.g. temperature and rainfall). Phenology can thus be used to identify and describe different vegetation types and to monitor vegetation responses to changes in these climatic determinants. Vegetation phenology has already shown clear changes in the northern hemisphere during the past 20 years, with growing season length increasing by up to a month.

Field data on leaf phenology are difficult to obtain, labour intensive, and can give information at only one point in space. Time-series of coarse resolution satellite data, however, contains indispensable information on seasonal vegetation dynamics at regional to global scales, as it provides consistent measures of vegetation greenness and activity (estimated by means of vegetation index or NDVI) at high temporal frequency over extended periods. Models can then be applied to the time-series of satellite data to extract meaningful phenological parameters such as start of growing season, date of peak greenness, onset of greenness decrease and end of the growing season. The regional distribution, inter-annual variability and trends in these phenometrics can then be investigated. The derived phenometrics are also being used to map biomes and vegetation types based on observed functional dynamics rather than traditional mapping efforts that rely on plant species' composition and its relation to abiotic variables, such as rainfall and elevation. These can also be used to identify areas of land use and land cover change, for example cultivation or deforestation, as such human-induced changes radically alter vegetation phenology. Ultimately this data can be related back to important measures of ecosystem health, such as net primary productivity.

South Africa is in the fortunate position of having received, archived and calibrated almost 20 years of daily 1 km AVHRR satellite data since 1985. Ten-daily, near cloud-free composite images for the entire time series were used to fit the phenological curves for each image pixel through

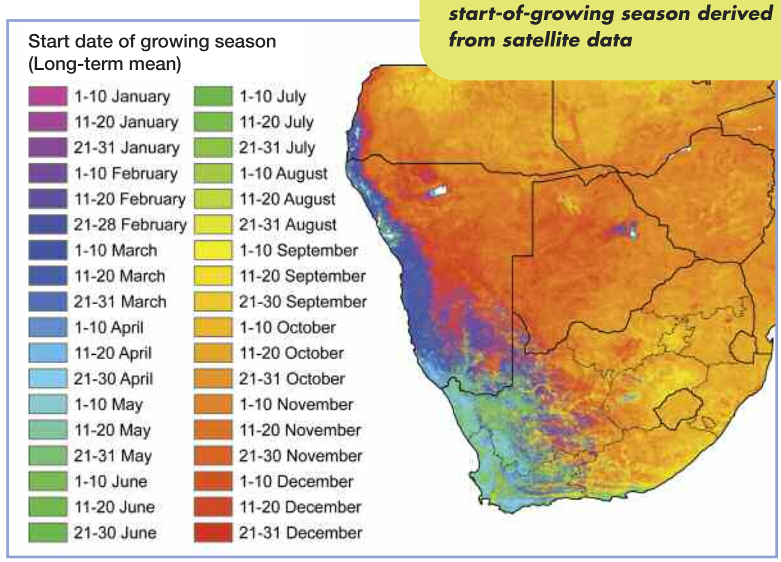


Figure 1 Long-term mean date for start-of-growing season derived from satellite data

time. This unique long-term dataset allowed researchers to determine the mean and inter-annual variability in these phenometrics.

Tremendously insightful maps were produced for the entire southern Africa, showing patterns that would otherwise have been impossible to observe. The mean start-of-season map (Figure 1) clearly shows the winter and summer rainfall regions.

During the growing season higher NDVI values indicate larger amounts of growing vegetation. It therefore follows that the area under the phenological curve of an NDVI graph (referred to as the large integral) gives a reasonable approximation of annual net primary production (Figure 2).

The dark blue in Figure 2 is mostly forest, including exotic plantations, or dense woodlands, whilst the brown areas are the Namib and Kalahari deserts and the Karoo). Grasslands, savannah and the fynbos have intermediate values. The higher biomass of the Okavango delta is also seen clearly. It is well established that in South Africa the variance in between-season rainfall increases as rainfall decreases. Figure 3 considers the variance in the small integral, which represents seasonal change in net primary production. As is expected, the very arid areas of the Karoo, Kalahari and arid Limpopo valley have high variance. The high variance in some forested areas of the Mpumalanga escarpment and the KwaZulu-Natal east coast is probably due to clear cutting of plantations and then gradual regrowth. The high variance in the fynbos is thought to be related to infrequent fires that destroy the accumulated biomass.

By contrast, the grasslands show relatively little variance as rainfall is more predictable. High variance in the lower reaches of the Okavango delta is probably related to shifts in the seasonal flooding patterns known to occur.

Various computational problems needed to be overcome in order to extract useful phenological information across the entire region. Time-series of satellite vegetation index data is notoriously noisy due to cloud and atmospheric contaminations, and varying sun and sensor angles. Thus, robust models have to be developed to distinguish the signal from the noise and reconstruct a clean time-series. Various curve fitting methods were tested including symmetric Gaussian and polynomial functions. However, locally-adaptive Savitzky-Golay filtering proved to be most useful in South Africa's highly variable environment.

All the data products are currently being related to the newly delineated bioregions and agrohydrological model outputs using decision tree analysis and regression analysis, respectively. This will provide new insights into the drivers of regional vegetation dynamics and long-term distribution in the light of climate change.

This research, funded by the CSIR Strategic Research Panel, is a collaborative project between remote sensing researchers of the Meraka Institute and the CSIR's ecosystems, processes and dynamics research group.

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Figure 2 Growth season vegetation production (NPP) as indicated by mean integral of fitted NDVI curves

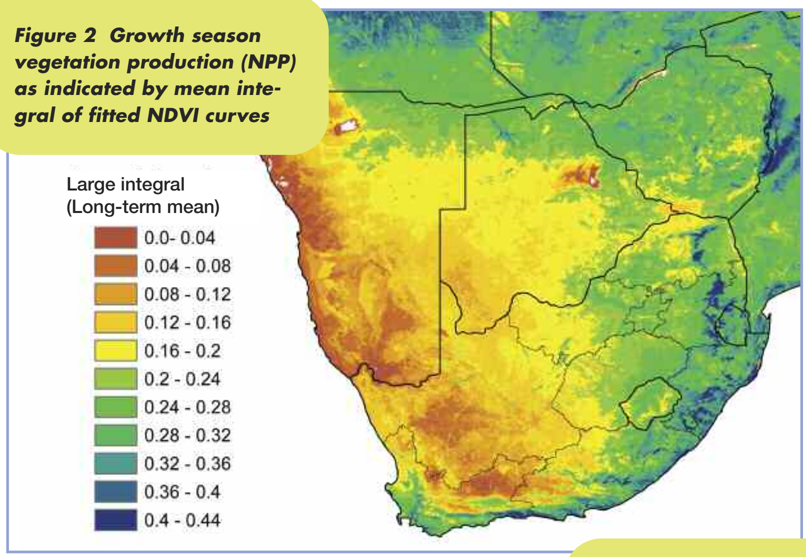
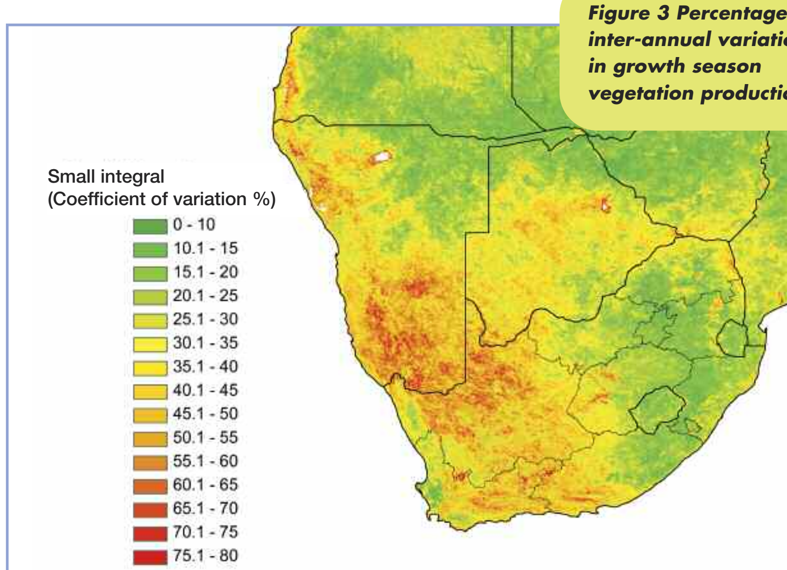
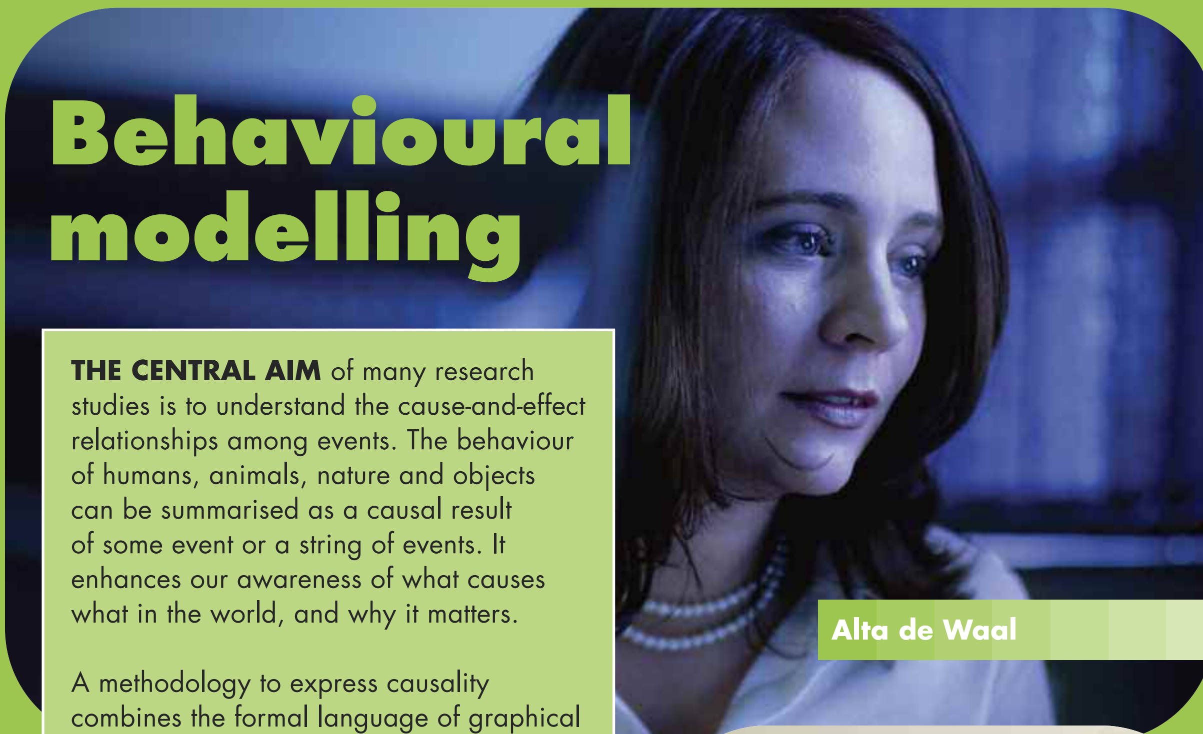


Figure 3 Percentage inter-annual variation in growth season vegetation production



Behavioural modelling



Alta de Waal

THE CENTRAL AIM of many research studies is to understand the cause-and-effect relationships among events. The behaviour of humans, animals, nature and objects can be summarised as a causal result of some event or a string of events. It enhances our awareness of what causes what in the world, and why it matters.

A methodology to express causality combines the formal language of graphical models with probability theory and is called a Bayesian network. It can be used, for example, to model the causal relationships of variables in a system or knowledge domain. Once a Bayesian network is constructed, it is able to respond to changes in the state of one or more variables. Given a scenario or a set of interventions, the behaviour of a system can thus be analysed. This attribute of a Bayesian network leads to a sense of gaining deep understanding of a system: Not merely knowing how things behaved yesterday, but also how things will behave under new hypothetical circumstances[1].

– Alta de Waal

Alta de Waal has been working with this type of modelling approach for almost 10 years and has been astonished by how realistically causality represents complex behaviour of systems. A challenging and exciting part of her work is to discover which events only marginally influence an outcome, and which are the real trigger points of a system.

Reference:

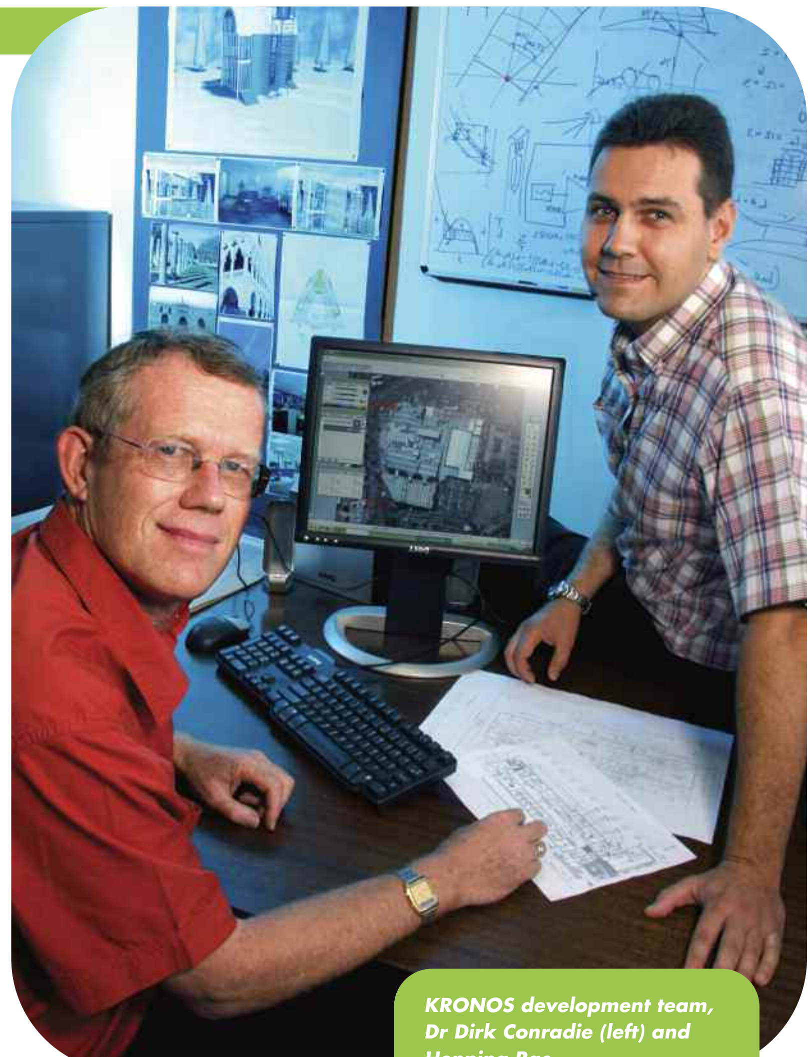
[1] Pearl, J Causality: Models, Reasoning, and Inference. Cambridge University Press, Cambridge, 2000.

Supporting dynamic, space-time related research through building simulation

by Dr Dirk Conradie

THROUGHOUT THE WORLD people are moving into cities. In sub-Saharan Africa this trend is more pronounced and within the southern African region, South Africa is a magnet. Urbanisation brings with it a host of developmental challenges, including stressing available resources and having a profound effect on quality of life. Modern thinking recognises the importance of understanding complexity, interrelatedness and correlation between various systems.

Contemporary computer simulation tools have developed significantly since they were first introduced in the 1960s. They are responding to increasing recognition that architecture and building processes are characteristically the result of incremental adaptation and change. Simulation processes can be a very useful tool to test, predict, visualise and represent the various design options and scenario planning. In this way it can be used to inform strategic planning to test hypotheses about human interaction with the built environment. It is also a useful communication tool.



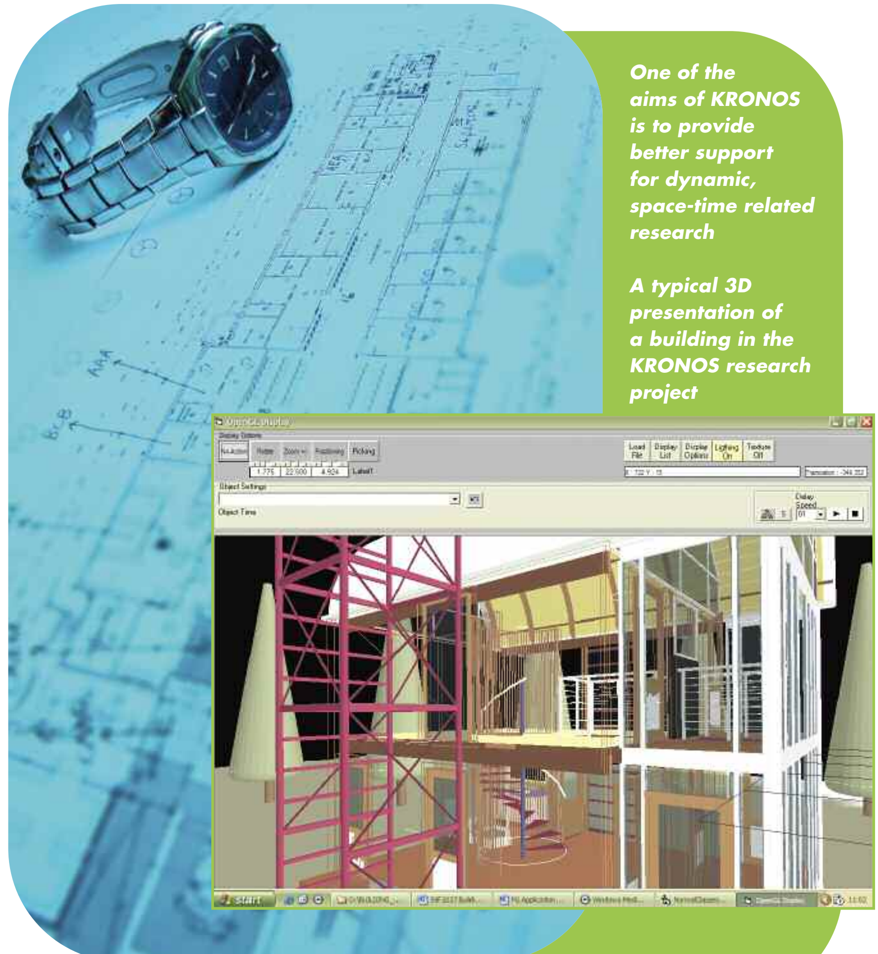
KRONOS development team, Dr Dirk Conradie (left) and Henning Ras

The CSIR's architectural research into complex structures, innovation and modelling (ARCSIM) project is an attempt, by a small team of researchers, to develop a computational building simulation (CBS) tool, termed KRONOS, to advance built environment and architectural research questions such as user behaviour in buildings. The intention is to provide better support for dynamic, space-time related research as well as investigations into static building modelling, simulations such as energy performance, solar movement, position, shading and traffic analysis. The team views the CBS tool as a technical specialisation of building product models (BPM).

A weakness of many existing commercial simulation software packages is that very few are agent-based. The reason for this is that the software, hardware and algorithms only recently became powerful enough to attempt advanced simulations of this nature. As a result most of these experimental systems are still confined to research laboratories and academia. The agent-based simulation approach makes it possible to experiment with whole-systems thinking, complexity theory and sustainability science at building or micro-simulation level. It is believed to be the first attempt to develop this technology for application in the design of buildings and traffic safety assessment in South Africa. An agent is seen as an autonomous entity that can move, such as a human, vehicle or animal. KRONOS also uses entities called props. Props are normally static and are placed in the simulation environment. Props can be 'sensed' by the agents and include entities such as road furniture, trees, buildings or construction elements. The CSIR believes that agent-based simulations will yield better results than traditional simulation methods, such as cellular automata, for the following reasons:

- **Accuracy:** Simulations such as people movement consist of a large number of emergent behaviours. It is the result of the individual decisions of drivers, pedestrians and traffic controllers. Agent technology helps building micro-simulation models with detailed, rich behaviours for individual entities. The architecture for individual agents promotes modularising internal behaviour and decision-making capabilities of an agent and changing behaviour from its interactions with other agents. This is particularly important for human behaviour that changes with locality as well as time.
- **Computational performance:** Agent technology is inherently distributed. In future it would be possible to deploy KRONOS on a network of computers, facilitating the creation of a super-computing capability.
- **Integration with control systems:** KRONOS can be used to visualise data that come from external sources such as the Sensor Web (NyendaWeb). In this mode, data give instructions to KRONOS, which in turn makes the various instructions visible to enable traffic engineers and researchers to study traffic patterns. Alternatively, new scenarios can be configured in KRONOS and tested. Due to the interaction of a large number of parameters or characteristics, emergent behaviours such as traffic congestions and accidents develop.

The KRONOS infrastructure is built on a BPM platform, an integrated digital information structure describing objects making up a building. It captures, *inter alia*, the form, behaviour and relations



One of the aims of KRONOS is to provide better support for dynamic, space-time related research

A typical 3D presentation of a building in the KRONOS research project

of the parts and assemblies within the building. The original purpose of a BPM was to centralise electronic building information with the prime purpose of avoiding translation of information between different software systems.

To build the visual part (model) of the simulation, existing bespoke 3D software such as AutoCAD 3D Studio Max can be used. Systems like the one mentioned offer the creation of photo-realistic 3D models, potentially with dynamic walkthroughs, but no support for the calculation of physical characteristics such as daylight factor, energy usage and isovists, all of which require the support of multiple physics. Once the visual model has been built, additional intelligence can be added depending on the type of research question.

The ultimate aim is to have a generic and virtual experimentation platform going well beyond pure visualisation. With further development KRONOS could also be used for the design of a heliostat field and solar receiver for power generation.

The research findings are at this stage supported by two case studies and the Moloto road feasibility study, which will use KRONOS to model and predict the efficacy of specific road safety interventions. Within this environment, agents and props are placed to dynamically simulate and predict behaviour. This clearly indicates that building performance cannot be predicted through the development of building and environment models alone. It must be understood as a product of both the environment and its users. To study or predict building performance requires both advanced static and dynamic capabilities.

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Evaluating concepts and developing tactical doctrine through modelling and simulation

by Shahen Naidoo

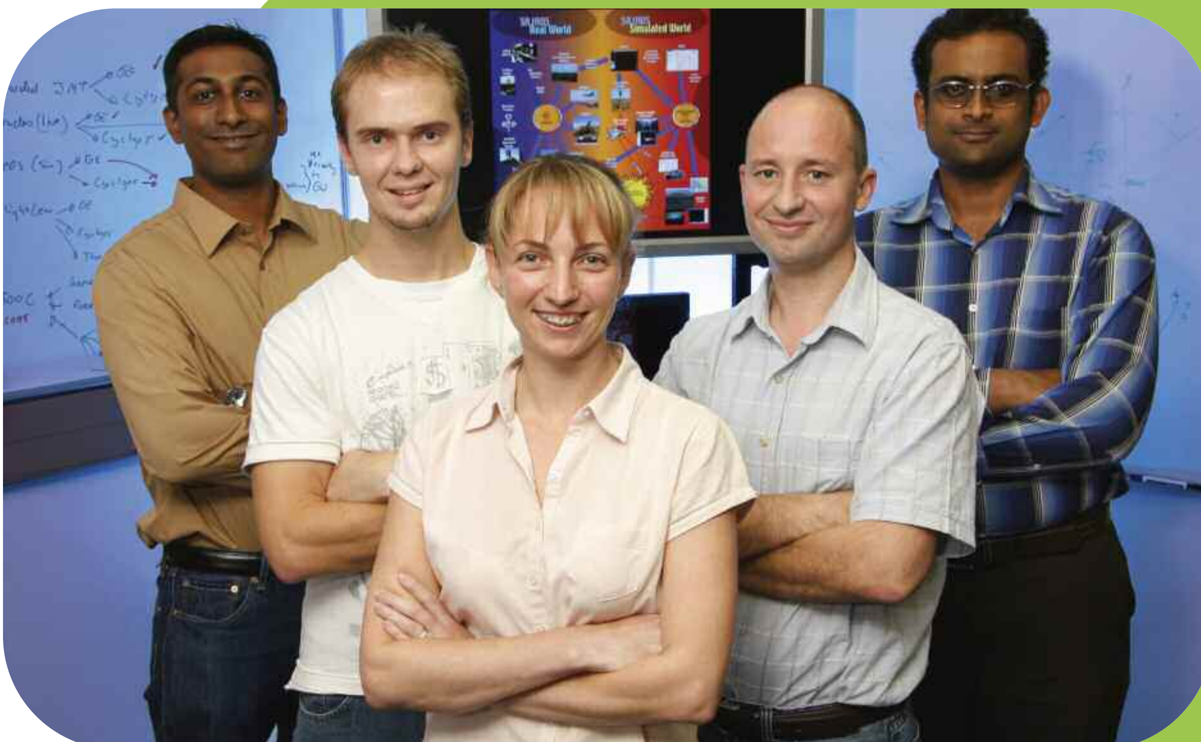
THE GROUND-BASED Air Defence System (GBADS) acquisition program of the South African National Defence Force (SANDF) offered an opportunity to apply modelling and simulation as a support tool. The CSIR's systems modelling and simulation capability is being used to assist in concept evaluation and concurrent tactical doctrine development. The virtual GBADS demonstrator (VGD), developed for this purpose, provides a virtual environment for deploying GBADS entities in a defined scenario to observe the behaviour, as well as interactions between these various entities of a user system, comprising a products system and human operators. Using VGD as a decision-support tool, tactical doctrine is developed to improve the operational effectiveness of the future user system.

Traditionally, the main acquisition focus has been on procuring the 'tangible' product system, often neglecting the impact of the emergent behaviour that results from the interaction of one system on another or the interaction of the operator on the system performance. The change in focus implies a system-of-systems approach, requiring the early development and alignment of tactical doctrine, and the modelling of complex operator and system behaviour. This article explores the contribution modelling and simulation made in support of doctrine development during acquisition.

Virtual GBADS demonstrator

VGD is an in-house suite of software that provides for the deployment, simulation and analysis of virtual entities within a defined scenario to observe the behaviour and interaction between the various operators and their related sub-systems within a GBADS deployment. VGD supports the distributed simulation of many-on-many engagements. The behaviour of equipment and operators is modelled, as well as the interaction between these entities.

VGD can function both as a virtual and a constructive simulator. For virtual simulations, operator-in-the-loop (OIL) consoles allow human operators to interact with real-time simulations to evaluate various doctrinal concepts from within the virtual environment. Constructive simulation is used for statistical analysis and evaluation of emergent behaviour. In real-time mode, VGD supports the integration with operational systems allowing a live air picture to be imported into the simulation, thus allowing tactical doctrine to be tested through the active participation in live exercises.



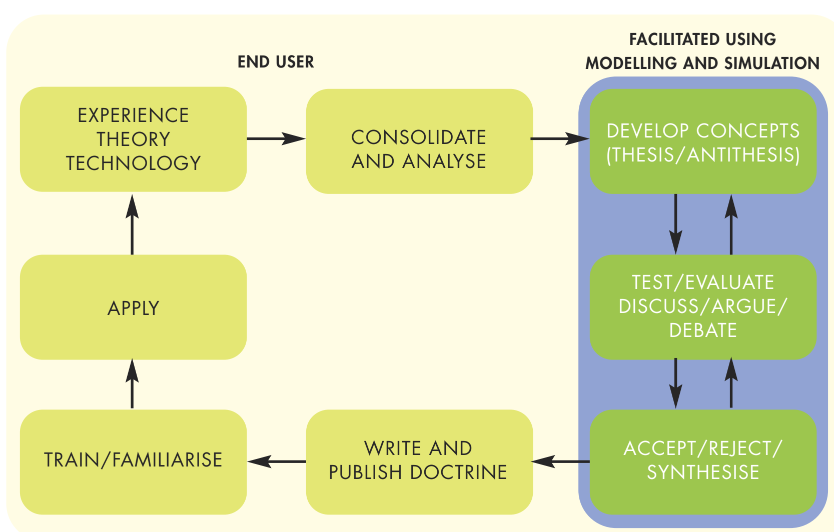
The team from left to right: Shahen Naidoo, Arno Duvenhage, Anita Illes, Herman le Roux and Sanya Rajan

Doctrine development

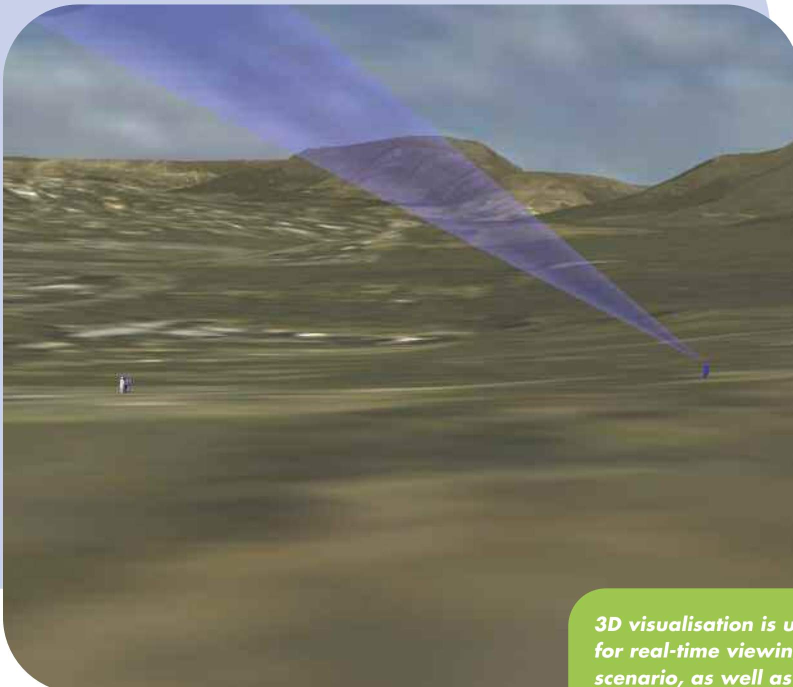
Doctrine refers to the methods employed to achieve an objective and involves the actions of a human. Doctrine is thus inherently part of a user system as it extends the ability of the operator to enhance user system effectiveness. The acquisition of a new product system necessitates the enhancement of existing doctrine or developing new doctrine to accommodate new system characteristics and functions.

Doctrine development proceeds through various phases resulting in promulgated doctrine as a final state. As the development proceeds through each phase, the draft doctrine is evaluated, tested and updated before subsequent phases.

The structured steps of a research project provide a framework for the development of doctrine (DM Drew, 1995). These steps are: devise a research question; devise a research plan; gather the required data; analyse the data; formulate and evaluate potential answers to the research question; identify the best answer; and write and publish the research report. The basic process for doctrine development adopted by the SANDF in the GBADS program follows a similar approach: initial drafting and validation of conceptual doctrine; validation through virtual simulations; and validation through involvement in field exercises. Iteration occurs between concept development, concept evaluation and testing, and concept acceptance/rejection.



SCREENSHOT OF 3D VISUALISATION TOOL



3D visualisation is used for real-time viewing of a scenario, as well as after-action review. 3D visualisation, specifically for complex scenarios, allows for the detailed analysis of events and object interaction

Drafting and validating conceptual doctrine

This is a preparatory stage where current doctrine and system-specific technical information provide the embryo inputs to the doctrine development process. Doctrine is the formalisation of 'common sense'. For doctrine to be developed, an environment needs to be created for the soldier to develop this 'common sense'. During the important initial phase, system characteristics and current doctrine are captured in VGD and through simple demonstrations the 'common sense' is developed.

Existing tactical doctrine, in conjunction with the system characteristics, is critically evaluated and specific focus areas are identified. Areas for analysis are prioritised and sets of experiments are defined to evaluate the existing doctrine, and alternatives, within VGD.

Results are presented to the user and the doctrine may be updated. The cycle continues with the implementation of the updated doctrine within VGD and further experimentation.

Validation through virtual simulations

Virtual simulations make it possible to immerse operators into scenarios to apply procedural doctrine and to optimise roles and responsibilities. The OIL terminals allow actors at different levels of the battery to procedurally control air defence activities. Other entities still function automatically, in predictable ways, allowing for the testing of concepts without requiring large numbers of people. The OIL-based experiments also serve to highlight shortfalls in doctrine.

Validation through involvement in field exercises

The validation of doctrine during a live field exercise is a critical next step in the process. The non-availability of a product system necessitates the use of modelling and simulation during such exercises.

Integrating VGD with the operational system provides the facility to simulate the planned acquisition systems in real time during an exercise. By importing the real-time air picture into the simulation, a trained fire control officer is able to perform fire control on a virtual GBADS battery against real aircraft, exercising the draft doctrine developed.

The data logging facility of VGD was used to record a complete exercise and the exercise was reviewed using the 3D viewing tool. This provided the various SANDF personnel with an opportunity to review and visualise the interaction during an exercise, thereby facilitating discussions among the various subject-matter experts.

Using modelling and simulation together with live exercises allowed the user to evaluate draft doctrine in a representative operational environment concurrently with system acquisition, and to participate in the operational test and evaluation activity with doctrine that had already been verified within that environment.

Whilst modelling and simulation are utilised widely for acquisition decision support, concurrent doctrine development is rarely applied. Clearly, final validation of the doctrine takes place through application. The VGD/MVGD is available as a decision-support tool for doctrine optimisation during the operating phase of the system life cycle once GBADS has been transferred to the end user.

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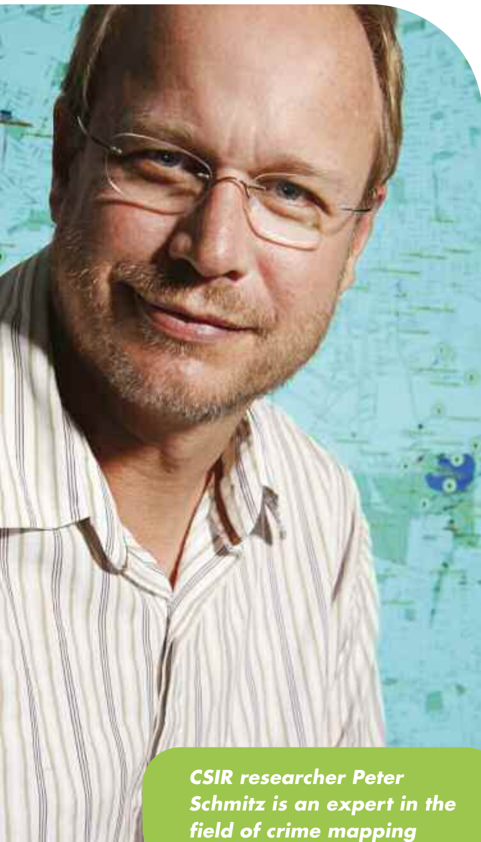


CSIR researcher Peter Schmitz is an expert in the field of crime mapping

Crime mapping proves its worth as crime-fighting tool

by Peter Schmitz and Antony Cooper

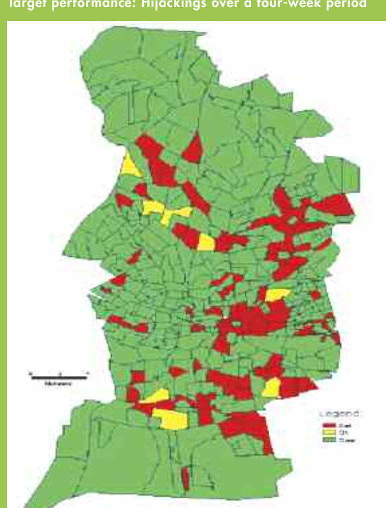
CRIME MAPPING can be used at three levels, namely strategic, operational and tactical. At the strategic level, crime mapping is used to deploy police resources effectively to combat crime. An example could be where high incidents of crime per police station are compared against resources available. If there is some correlation, resources can be transferred from well-resourced police stations to assist low-resourced stations to combat crime. Another application at the strategic level is to plan specific national or provincial crime combating operations based on the mapped crime levels.

At the operational level, crime mapping is used to deploy daily or weekly police patrols for visible policing and to have resources available where needed. In South Africa a police station is divided into several crime administration system (CAS) blocks in which crime incidents are recorded. This allows for targeted interventions by the station commander to combat crime. Over time, a station commander can monitor the displacement of crime that can be attributed to operations within the police station's jurisdiction. This information could be used to predict possible displacements and place officers in those areas where the criminals could move owing to police interventions elsewhere.

Hot-spot analysis and target performance maps are examples of crime maps used for operational purposes.

Target performance maps have been developed by the CSIR, based on the cumulative sum (CUSUM) methodology used in quality control. Using past crime incidents, the methodology calculates an acceptable target as well as an improve-to target with regards to the number of incidents. Maps then show which areas are above, between or below these two values. Areas that are worse than the acceptable target are then prioritised for police operations. Once an improve-to target has been reached consistently, it becomes the acceptable target and a new improve-to target is calculated, with the aim of continuous improvement. The CSIR has also developed crime clocks, which give a picture of the distribution of crime by time of day and/or day of week. This is used to plan when and

Target performance: Hijackings over a four-week period



Crime clocks: Hijacking incidents over a one-year period given in two-hour time slots

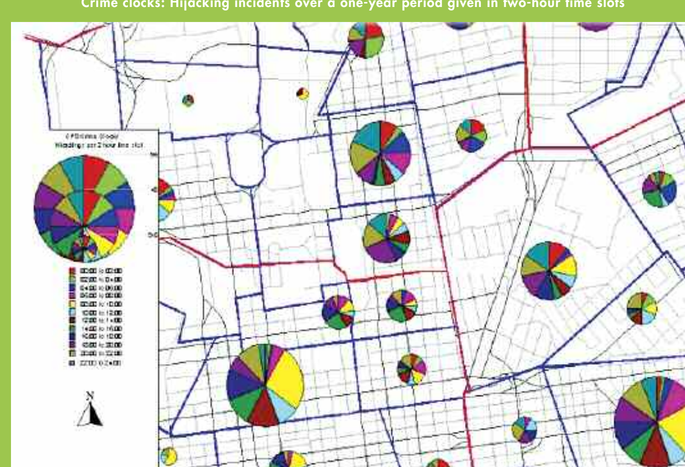


Figure 1 Target performance map and crime clocks

where crime combating operations will take place. Examples of both are shown in Figure 1.

Crime mapping at a tactical level is used in investigations and prosecutions. At this level, data are collected to assist investigators in tracking down and arresting offenders. By mapping the various incidents that are linked to an offender or a gang, it is possible for the investigators to build an understanding of the offender's *modus operandi* such as suburb preference, time of day of incidents and time lag between incidents. According to environmental criminology theory, criminals operate within their comfort zones and are unlikely to commit a crime in an area where they do not feel comfortable. Hence, the offender or offenders will prefer certain suburbs above others. The times of incidents give an indication of when the offender will commit a crime. This information is used to launch an operation with the aim to arrest the offender(s).

Geographic profiling is the most widely used tool to perform tactical crime mapping. It uses various crime theories such as journey-to-crime, rational choice theory and mental maps. Journey-to-crime gives an indication of how far an offender will travel to commit a crime, rational choice theory gives an explanation of the choices the offender makes with regards to the type of crime committed, and mental maps explain the offender's understanding of the area where the crime is committed.

The mental map also indicates the suburb preference of an offender. Geographic profiling is used to determine a possible anchor point from which an offender will commit a serial crime, ranging from rape and murder to house break-ins. Geographic profiling uses various quantitative and qualitative procedures to determine these anchor points and this concept has been tested on several serial murder and rape cases in South Africa. Figure 2 shows the geographic profile of the Wemmerpan serial killer. The serial killer's anchor point (residence) was within the red area as shown by the circle in the figure.

The CSIR has extended alternative geographic profiling theory using cellular telephone data from which possible routes, anchor points, time of criminal activity and criminal activity space can be determined (see Figure 3).

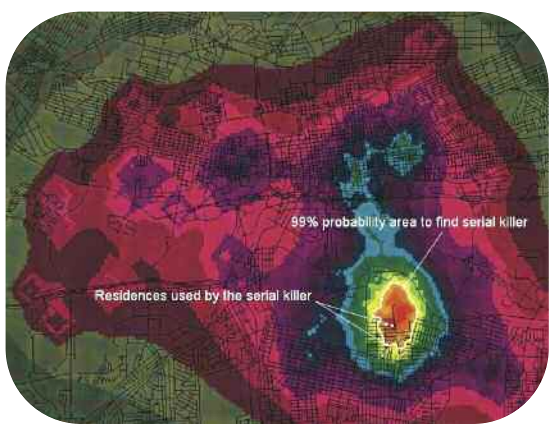


***Figure 2** Wemmerpan serial killer's geographic profile*

Cell phone data provide the place of use (the cells) as well as the time of transactions (calls and messaging) and information of the other party participating in the transaction. This information is used to plan tactical operations such as surveillance, and determine attractions such as night clubs within areas of high cell usage. The movement between cells is used to determine possible routes used by the offender. Time of usage gives an indication of the offender's diurnal and nocturnal patterns. Combining this information with crime incidents, the investigators can plan when and where to arrest the individual. This methodology is used in combating gang activities.

Once the arrest has taken place, information of importance to the case such as crime incidents, proximity to night clubs, shopping centres, and time, day and location of cellular calls as well as vehicle satellite tracking data are mapped for prosecution purposes. The CSIR has had several successes with regard to the prosecution of offenders based on maps created by the organisation, the best known case being the successful prosecution of the so-called New Year's Gang in Cape Town in 1999.

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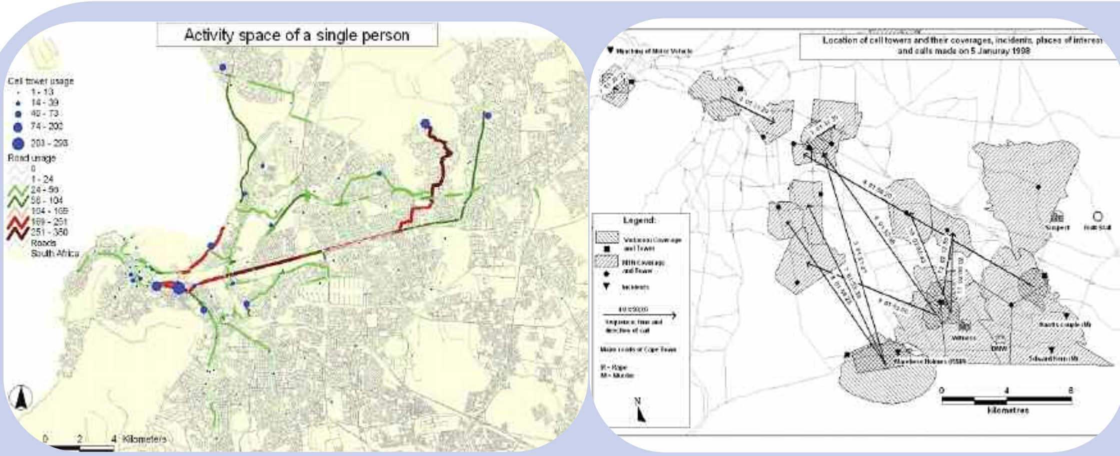
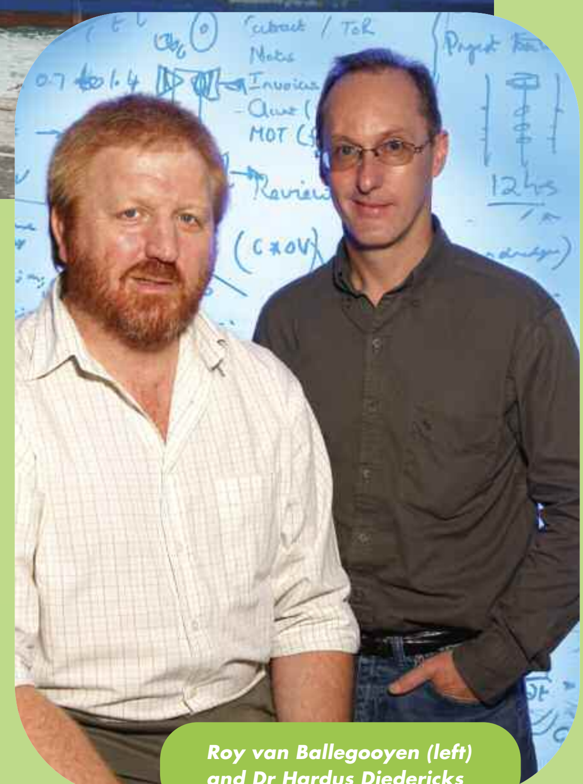


***Figure 3** Mapping activity space and routes using cellular telephone data (far left) and the map used for prosecution purposes (left)*

Protecting the environment during port development

by Dr Hardus Diedericks and Roy van Ballegooyen



Roy van Ballegooyen (left) and Dr Hardus Diedericks

IN MANY PARTS of the world, development and associated economic activities regularly come into conflict with the desire to conserve valuable habitats. South Africa is no exception.

Transnet National Port Authority is in the process of expanding and improving the major ports in the country. These include the Saldanha Bay harbour to extend the iron ore berths; the deepening of the Ben Schoeman dock in the Table Bay harbour; a sizeable development at the Coega harbour; and the widening of the Durban harbour entrance.

An important monitoring instrument that assesses the environmental bearing of these planned expansion activities in advance is an environmental impact assessment (EIA) process. During any port development, dredging is inevitable, be it capital or maintenance dredging. The dredging industry and environmentalists are linked in a somewhat uneasy alliance, both groups striving to find sustainable solutions to environmental questions. The coastal systems research group at the CSIR regional office in Stellenbosch contributes to this relationship by providing specialised predictive solutions to complicated dredging scenarios as part of such EIAs.

Simulating effect of waves, wind and tides

The CSIR participated in the EIA regarding the deepening of the Ben Schoeman dock and is now engaged in the EIA for extending the iron ore berths at the port of Saldanha Bay. In both cases the focus was on predicting the possible consequences of dredging activities and providing advice on how to minimise environmental impacts. To achieve this, scientists used the Delft3D hydrodynamic and water quality software to simulate, among others, the combined effects of waves, wind, tides and water column stratification and the effect of these on processes in the marine environment. Effects include the transportation of sand and/or mud and the resulting changes in the topography of the seabed as well as a range of ecological processes. The quest is thus to predict nature, starting from the fundamental environmental driving forces and incorporating various human interferences to provide predictive simulations on which to base practical decisions.

Modelling Table Bay harbour

The Ben Schoeman dock in the Table Bay harbour is being deepened by the dredger Gefion R from the Danish company, Rohde Nielsen. The CSIR's role in this project was to select appropriate disposal sites for the dredge material and to assess potential environmental impacts associated with the dredging in the harbour and the disposal at the dump sites. For the project, the CSIR set up a model of the whole Table Bay area and simulated the actual hourly wave conditions, sea currents and water column structure for one year.

At the start of the project the CSIR marine laboratory in Stellenbosch characterised the sediments to be dredged in terms of type, composition and possible toxicity when dredged and disposed of off-shore. Using information on the type of dredger and estimates of the overspill and sediment loading at the dredge head, the numerical model was used to predict the turbidity and potential release of toxins in the Ben Schoeman dock and its surroundings as well as at the proposed dredge disposal sites. Marine ecologists from Lwandle Technologies then used this information to assess possible environmental impacts. A high degree of accuracy of the simulations was crucial since there are many users of the harbour, for example, the Two Oceans Aquarium requires an uninterrupted supply of 'clean' sea water, which they abstract from a nearby basin.

In the initial phases of the project two possible offshore dredge disposal sites were identified in water depths of 40 m and 60 m, respectively. Estimates of the rate at which barges would transport the dredge material to the respective dump sites were then used in the numerical model to simulate the concentration of suspended sediments, the movement of the dumped material as well as the deposition thickness of sediment in different areas. A high degree of accuracy was required in the simulations since the dump site that was finally selected, is located near the environmentally sensitive Table Bay National Park Marine Protected Area. An environmental management plan (EMP) was developed for the dredging activities, based on a characterisation of the sediment types and habitats at the proposed dredge disposal site, the modelling results, assessed impacts and proposed mitigations measures.

Accuracy of model predictions

A biomonitoring programme is being conducted to ensure compliance with the EMP. The CSIR will use these biomonitoring measurements to assess the accuracy of the model predictions. The comparison between the numerical results and the measurements from the monitoring will not only improve understanding of dredging processes, but also allow uncertainties in certain process parameters to be minimised. Understanding the processes is vital since there is a huge difference in geological, meteorological, environmental, morphological and physical differences from harbour to harbour. The diverse range of conditions makes it difficult, if not impossible, to set up programmatic standards or develop solutions that apply equally to all sites and situations.

Project contributions such as this one have made significant contributions to the EIA process as well as to the underlying science. This specific project has also strengthened the collaboration between dredging and environmental stakeholders.

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Sustainability modelling aids integrated energy planning

by Dr Alan Brent

THE SOUTH AFRICAN National Research and Development (R&D) Strategy states that for sustainable development to take place, rural and urban communities should have access to innovations that accelerate development and provide new and effective solutions compared to those utilised previously. To this end, the challenge for South Africa and NEPAD, which is captured in the Department of Science and Technology (DST)10-year innovation plan in terms of searching for energy security, is to develop fully the available energy resources and to promote innovative, competitive, equitable and sustainable energy systems for various economic and social sectors across South Africa and the continent.

The response of the South African government to the challenge is the Draft National Energy Bill, which provides for integrated energy planning. It is envisaged that such integrated energy planning must apply the principles of sustainable development, i.e. the optimal use of indigenous and regional resources; consider the balance between supply and demand, and their characteristics; economic viability; and incorporate environment, health and safety impacts associated with energy developments in the southern African region. In terms of sustainable development, the key conditions that must be achieved are:

- Economic growth that is significantly greater than population growth
- Population size and growth that are in harmony with the changing productive potential of eco-systems
- Changes in the exploitation of resources, direction of investments, orientation of technological development and institutions that are consistent with future as well as present needs
- Equitable access to resources so as to enable social progress/improvement.

To achieve these conditions, decision-makers at all levels must understand the linkages between economic (regional, national and international), social, technical and ecological resource systems in a holistic and comprehensive manner. Macro-economic modelling approaches that build on energy-systems models, such as the long range energy alternatives planning (LEAP) system and energy-oriented life cycle analyses, have subsequently been developed to address specific aspects associated with the conditions of sustainable development for energy planning. However, in the South African context, there are still these research challenges to determine:

- How the approaches may be merged to contribute to increased understanding of the relationship between energy-planning scenarios and options, and specific sustainable development objectives
- How to separate decision-makers from the perceived complexity of modelling.

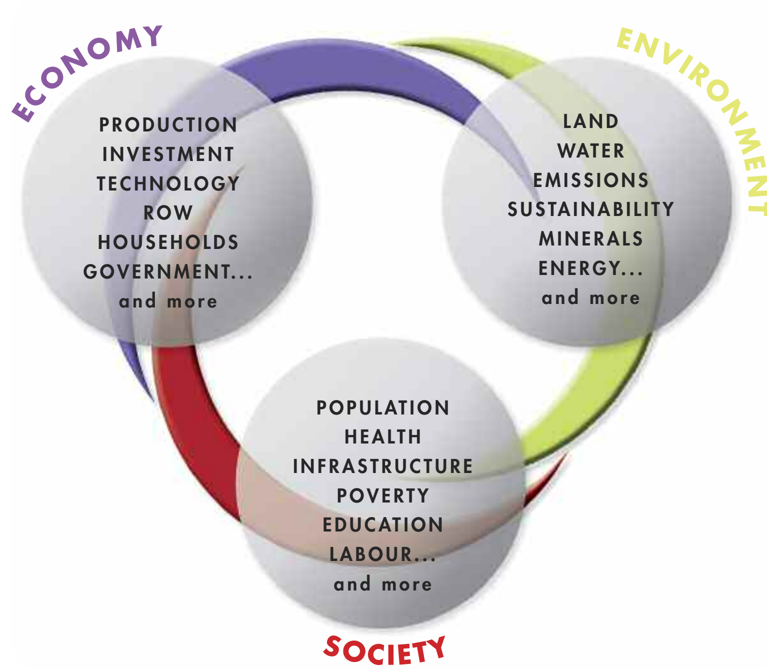
For example, recent and ongoing changes in the political front may lead to a shift in the macro-economic policies of the country, with consequences for developmental priorities. Decision-makers at provincial level need to respond to these changes, whilst maintaining other sustainable development objectives that are specific to provinces. The renewable energy and energy efficiency targets for the local industry sector in the Western Cape is one example. For these decision-makers, technology change is a particularly critical component of the targets that respond to the climate-change debate. Subsequently, a desired feature of an integrated modelling framework is to dynamically represent the impacts of various policy measures on model outputs e.g. rates of change in technology adoption, under various scenarios.

Thereby the models allow better understanding of the rather non-intuitive positive and negative feedback loops between the economic, social and environmental dimensions of sustainable development.

Modelling the sustainability interactions and implications of technological interventions and sociological and ecological responses, is Dr Alan Brent, here next to a solar panel

The CSIR's research groups for sustainable energy futures; environmental and resource economics; sustainability science; ecosystems processes and dynamics; and waste management have responded to the research challenges by focusing on four energy-economic modelling approaches:

- Partial-equilibrium approach, i.e. cost-benefit analysis and cost-effectiveness analysis
- General-equilibrium approach
- Probabilistic/causal approach
- Systems-dynamics approach, i.e. fuzzy-logic/neural network, vector autoregressive and Threshold 21 (T21) models.



In terms of the latter the CSIR has joined forces with the Mauritius Research Council (MRC) and the Millennium Institute (MI) to develop the T21 model further. The development will support life cycle analyses of alternative energy value chains in the context of larger energy planning scenarios at provincial level. The model will allow the CSIR to investigate the best ways in which to promote the diffusion of alternative energy technologies. It will further advise government on public policy matters, by providing a robust scientific basis for decision-making. In particular, it will allow the testing of various assumptions and help build consensus in decision-making. Finally, the research will also assist to build capacity in the field of modelling in South Africa as these skills are desperately needed.

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Water-use project aims to bear fruit

by Mark Gush

THEY CAN BE FOUND along the country roads of South Africa – those neat rows of trees laden with fruit that make up orchards of apples, oranges, and other fruit for which our country is famous. Looking closely at the stems of the trees, a network of irrigation pipes that deliver life-giving water is visible.

The provision of water in the correct amounts, at the correct times is crucial to the fruit tree industry as 90% of production is dependent upon irrigation. The question is how do farmers know how much water a fruit tree needs and at what time, so that fruit quality and yield are optimised while water use is minimised?

A current CSIR project on the water use of fruit tree orchards aims to address such questions. Funded by the Water Research Commission and the Department of Agriculture, the research project is led by the CSIR's ecophysiology research group, in collaboration with plant production and soil science researchers at the University of Pretoria. Earlier studies on the water use of fruit trees in South Africa, conducted in the Eastern Cape and using weighing lysimeters, captured enough initial data to draft rough guidelines on the water requirements of some fruit tree species. These were published as the Green Book after the author, Dr George Green. However, the number of species actually monitored in that project was limited and broad assumptions regarding the extrapolation of results to other species were necessary.

Recent advances in the monitoring of sap flow (i.e. transpiration or actual water use) in individual trees, using the heat pulse velocity technique, together with an exciting new method of measuring total evaporation over an entire orchard, known as scintillometry, have made it possible to broaden and improve the accuracy of water-use measurements.

In this project researchers will use a combination of these two techniques to measure the water use of the most important fruit tree species in the winter and summer rainfall regions of South Africa. The impacts of this research in the stakeholder community will predominantly be in terms of improvements in water management and water-use efficiency. Economic benefits will include reduced irrigation costs (less water and electricity), with corresponding increases in profits for farmers, without reductions in fruit production and quality. Environmental benefits will include reduced leaching of nutrients into groundwater systems and increased stream flow and/or groundwater levels due to lower abstractions for irrigation.

As pressure on South Africa's limited water resources intensifies, and organisations such as catchment management agencies are established to oversee the equitable and efficient use of water, there is a growing need for accurate

Installation of the heat pulse velocity system in trees involves meticulous drilling for the accurate insertion of thermocouples and heater probes to measure sap flow (water use). The system is usually combined with an automatic weather station, soil moisture sensors and tree physiology measurements (e.g. leaf litter traps and photosynthesis measurements)

information on the water use of different land uses. Irrigated agriculture, including the fruit tree industry, is a major water user in a number of water management areas. Savings in water use within this sector consequently have the potential to have a significantly positive impact. The provision of improved fruit tree water-use information will not only contribute to the scientific body of knowledge in this field, but also facilitate water resources management.

Measurement of primary data in the natural sciences is notoriously difficult. Equipment is often expensive and must be protected from theft or damage by insects, animals and the elements. Field sites are often remote and costly to access. Phenomenal amounts of data are generated, which need to be assimilated, managed and analysed. Instruments sometimes fail and there is a high risk of data-loss. Finally, and most importantly in this context, it is impossible to measure everything.

One may decide to focus on the most important fruit tree species to measure, based on economic importance, extent of plantings and water-use savings potential. However, an infinite number of conditions (climate, soils, cultivars, root-stocks, management practices) exist under which those species may grow, all of which could never be accounted for in measurements alone.

Modelling is necessary to expand the measurable to the broader scale of scenario testing, usually through the processes of calibration, verification and extrapolation. Critical to this process is confidence that the model being utilised is the correct one for the application, hence the importance of model selection. The choice of model then informs what parameters need to be measured in the field to parameterise the model accurately. It is at this stage that the phenomenon of 'GIGO' applies. 'Garbage in garbage out' simply implies that the quality of data utilised to parameterise the model, and against which the model is calibrated and/or verified, affects the quality of the outputs directly.

The message? To model well you need to measure well.

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Understanding the National Poverty Alleviation System

by Mapule Modise

POVERTY REMAINS one of the major challenges facing South Africa today. New estimates of poverty show that affected households have sunk deeper into poverty and the gap between rich and poor has widened.

CSIR researchers have modelled South Africa's National Poverty Alleviation System (NPAS) and formulated insights that are set to improve the design of the system.

Poverty alleviation in South Africa is delivered through a variety of independent mechanisms. Numerous entities engage in the task of poverty alleviation, each with their specific objectives and focus areas. The current fragmented and uncoordinated nature of the existing delivery system requires a suitable approach.

The aim of the NPAS project was to apply systems methodologies towards a better understanding of the NPAS, to establish a suitable framework for analysis, and to describe and analyse the system such that stakeholders and decision-makers can engage towards a more effective poverty alleviation system.

The project's initial point of departure was to describe and analyse the South African NPAS using systems engineering (SE). Researchers needed to employ and test approaches used by scientists and engineers to gain a better understanding of this socio-economic system. The main characteristics of the NPAS were summarised as:

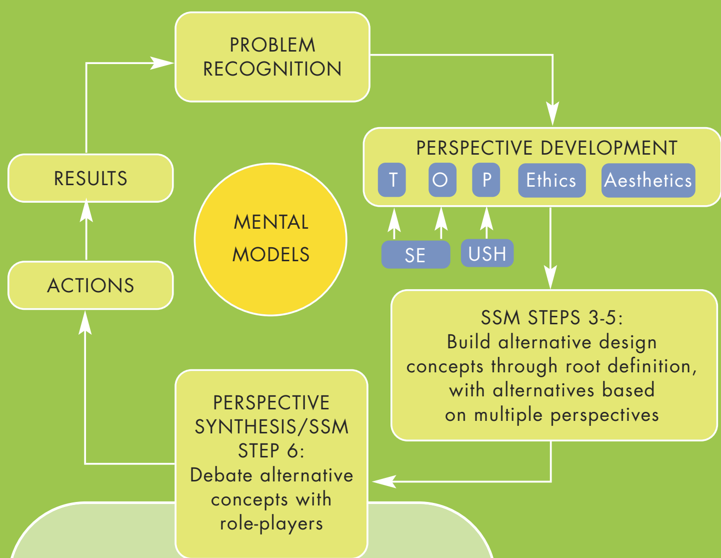
- The existing NPAS has evolved organically and is not centrally controlled by any party. It consists of multiple stakeholders with different and sometimes conflicting goals and views
- Information and communication breakdowns and difficulties exist between the users and implementers/designers of the system
- It has poorly defined and varying system boundaries, based on stakeholders' perceptions
- It is highly responsive and adaptable
- Interventions have long-term consequences
- It cannot be measured objectively
- There are ethical implications and it is often not feasible to experiment and build alternative systems.

A complex and non-reducible system mentioned above required a combination of both hard and soft systems approaches. As a result, a systems framework was derived, based on Courtney's (2001) new paradigm for decision support with SE, soft systems methodologies (SSM) and unified systems hypothesis (USH). The four phases systems framework mapped to the SSM learning cycle are:

Phase 1: Describe the intervention
Critical evaluation of the intervention in terms of poverty reduction; it describes the scope of the system of interest and identifies stakeholders and describes objectives, roles and responsibilities.

Phase 2: Modelling
SE was used as the main tool to develop the technical perspective on the system, while at the same time developing views from the O, P and E perspectives.

A SYSTEMS FRAMEWORK FOR STUDYING NPAS



- Courtney's framework consists of a decision-support cycle built around the multiple perspectives inquiry system. In the diagram, the T, O, P, E and A refer to the technical, organisational, personal, ethical and aesthetical perspectives on the system under investigation. 'Perspectives' refer to more than viewpoints - it is all the relevant information on which to base a decision, grouped under T, O, P, E and A
- SE contributed to the T and O perspectives. Something like the N2 chart would be classified as a technical perspective, and more subjective information supplied by an organisation would contribute to an O perspective
- Hitchins' USH contributed mainly to the O and P views, aspects such as simultaneous multiple containment of entities as well as lifecycles
- The perspective generation exercise was descriptive. The SSM is the design parts of the cycle, although it might also be used to evaluate existing designs
- Steps 3-6 of Checkland's (1981) SSM is proposed for systems design. Here, alternative systems concepts are proposed that are based on alternative perspectives rather than alternative technologies.

The framework is meant to assist with a descriptive rather than a normative process.

In addition, critical systems heuristics (CSH) was used to investigate aspects such as power relationships through the use of the 12 critical boundary questions.

Phase 3: Stakeholders' evaluation
Different perspectives on the system were collected and the modelling results were tested with the stakeholders.

Phase 4: Refinement
The problem definition was refined based on the outputs of phases 2 and 3. This last phase entailed a problem description based on a refined problem with enough clarity to suggest (untested) solution. The final output of the enquiry system provided a comprehensive view of the problem to a decision-maker.

The developed systems framework was tested on CBPWP1 and the analysis allowed the CSIR project team to identify some limitations enshrined in the design of the programme. The insight drawn can be used to improve the system. The learning from this case study is relevant to the analysis of other infrastructure interventions designed with objectives of poverty alleviation.

The NPAS project team comprises Isabel Meyer, Mario Marais, Mwansa Saidi, Marita Turpin, Geci Karuri and Leanne Scott.

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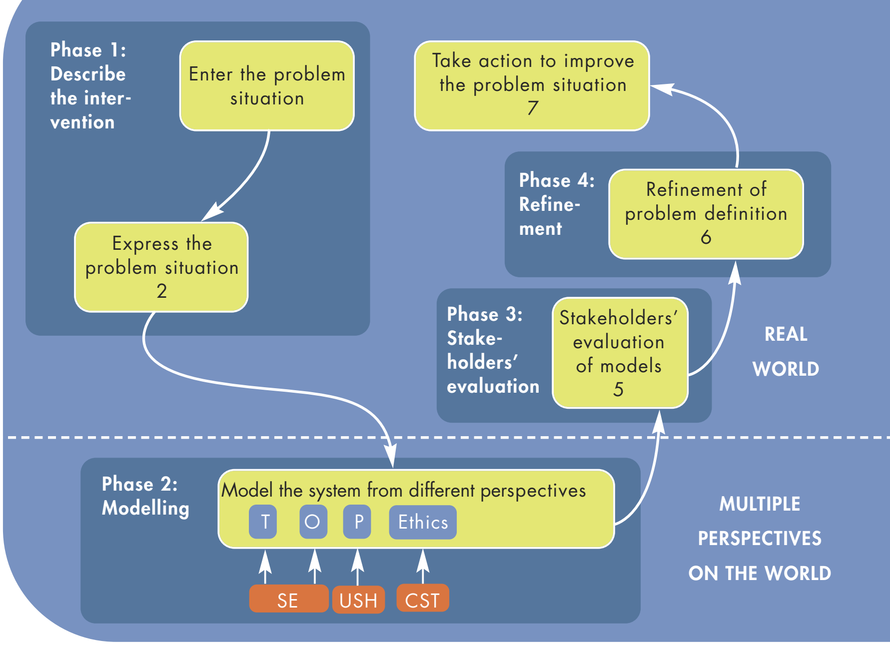
THE MODIFIED SYSTEMS ANALYSIS FRAMEWORK



Urban growth modelling for enhanced service delivery

by Dr Sharon Biermann

URBAN AND REGIONAL planners are continuously seeking ways of enhancing the quality of life of inhabitants through improved spatial planning. The physical form of cities and settlements is the consequence of a myriad of interacting, dependent and independent decisions and actions of private individuals, entrepreneurs and public role-players, responding to external and internal stimuli. Any change to the system, both intended and unintended, can take many years to manifest, often with unforeseen consequences.

Urban and regional planning models are instruments that enable scientists and designers to explore, predict and plan these environments, prior to acting in some irrevocable way. The ability to experiment on simulations of the real world rather than the real world itself is crucial in testing alternative development concepts and hypotheses for more sustainable urban and regional futures.

Through its spatial analysis and urban and regional modelling and simulation research, the CSIR supports key service delivery line departments at national, provincial and local spheres. The aim is for departments to achieve infrastructure investment and development spending that are aligned, focused and directed, in terms of location and form, and thus ensure sustainable and maximum impact through service delivery of the right kind and amount, in the right place and at the right time. In addition, the CSIR's modelling endeavours are being brought to bear on the critical aspect of restructuring current spatial forms for the eradication of inequalities and inefficiencies and the achievement of sustainable human settlements.

Dr Sharon Biermann manages the CSIR's planning support systems group

The CSIR has been instrumental in influencing integrated development planning processes and subsidised housing locality choices, amongst others. This is achieved through developing a range of model types used in urban and regional planning – from models of planning processes through to ones as abstractions of the system being planned, i.e. the city or neighbourhood. When it comes to issues of sustainable urban form, urban sprawl and compact cities, low-income housing location, transportation and energy efficiency in South African cities, the CSIR has led the way in the development of empirically-based tools and models to measure, compare and evaluate alternative development trajectories.

From the more traditional land-use transportation modelling approaches, the CSIR's urban growth modelling research is evolving with international trends to incorporate new ideas in economics, network science and complexity theory. Spatial interaction modelling remains a strong competence within the CSIR, with accessibility modelling having significant impact in cities like Ethekwini, where locality decisions about new social facility investment are not made without reference to modelling outputs.

In a current research project, funded by the Department of Science and Technology, the CSIR is making significant enhancements to well-established, more deterministically-oriented land-use transportation modelling approaches. To address deficiencies in current spatial planning practice, products and processes, the purpose of the project is to develop context-specific – yet scale interrelated – evidence-based, decision-enhancing spatial planning tools to ensure that decisions regarding resource allocation (focusing on housing and transport infrastructure) are underpinned by a strong empirical base. These are supported by:

- Rigorous and robust analysis of spatial and temporal development dynamics – trends, patterns, potential, need, linkages and flows
- Scenario-based, multi-scaled growth modelling to facilitate strategic choices, prioritisation and trade-offs, multi-scale with the capability to ask 'what-if' questions about the urban systems being planned.

In parallel, the CSIR is exploring the modelling of change in cities from the bottom up, resulting in emergent patterns formed by the myriad of land development decisions, rather than modelling cross-sections of urban structure from the top down. In addition to static models, which are useful in simulating how the aggregate of decisions that have created a city, leads to the structure currently observed, the CSIR pursues more dynamic approaches that involve attempts at simulating the evolution of decision-making processes through time.

Most recently, the CSIR investigated agent-based city models where individual behaviour of objects or events locating and moving in space is simulated. The possibility of adapting and extending UrbanSim (a software-based simulation model for integrated planning and analysis of urban development) for the unique conditions of a developing country context, where the formal economy co-exists with the informal, offers exciting collaboration opportunities with the developers at the University of Washington.

While keeping pace with international research trends in urban modelling is stimulating, emerging approaches do not necessarily represent alternatives to past models but are rather complementary, with the advantage of providing less abstract representation of the system and its behaviour. The fact that modellers, professionals and policymakers cannot only see how agents as actual individuals move within the city, but can jointly reason about agent behaviour, offers a unique opportunity for improving the communication between all stakeholders.

The CSIR follows a collaborative innovation and adaptation approach in the processes of developing, testing and refining its models, especially in contexts where complex and/or multiple problems need to be solved for networks of multiple actors. This approach enables the co-creation and validation of mental models describing the specific context, key concepts, back-end methods and tools and collaborative processes of extracting, collating and validating tacit and non-tacit content and information in support of the modelling endeavour.

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Platforms in modelling and simulation

Albert Gazendam

SCIENCE AND TECHNOLOGY are inseparable. In the context of modelling and simulation as a tool that researchers employ to uncover hidden truths in their subject matter, platforms are enablers that allow us to push the limits of precision, complexity and ultimately, scientific productivity. These platforms take the shape of physical or virtual representations of subsets of reality, allowing us to focus intellectual resources on that which is of most interest while cutting out the negligible.

Information and communications technologies play a key role in technology platforms utilised for modelling and simulation. The extent to which electronic signals, digital circuitry and binary logic have changed the world of modelling and simulation is immeasurable. Scientific computing and high performance computing in particular are making significant impact by speeding up the computational elements of the research cycle and inspiring researchers to start dreaming of a future with less simplifications and more fundamental insight.

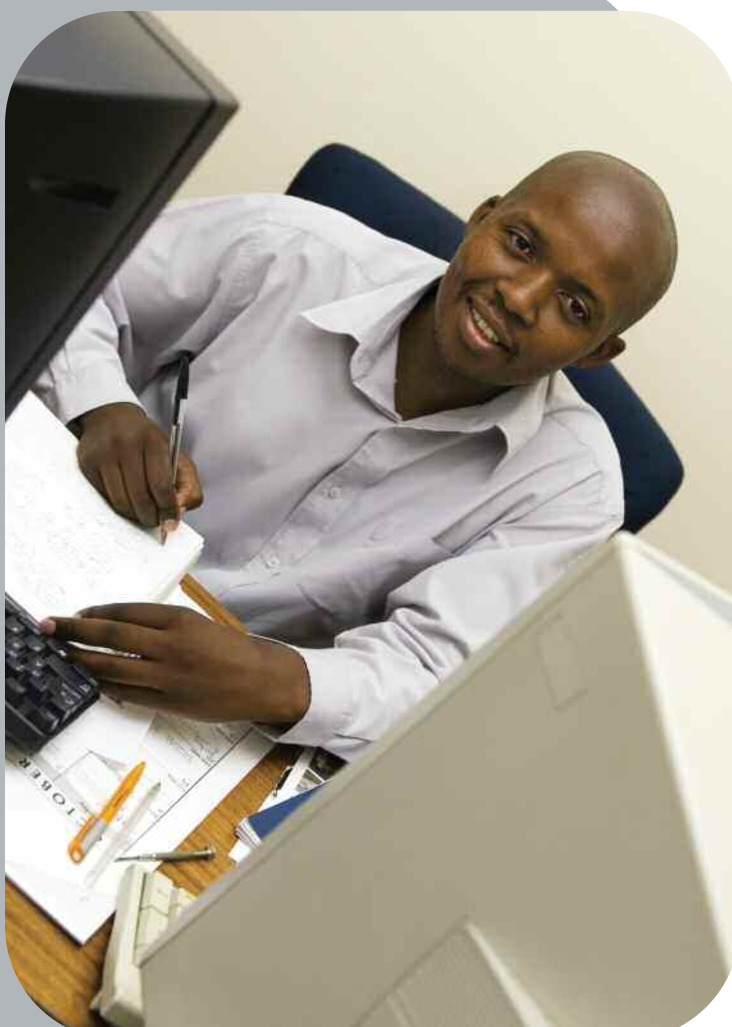
– Albert Gazendam

ALBERT GAZENDAM works at the Meraka Institute. His research interests include high performance computing and new applications of virtualisation, as used in the enablement of cloud computing and new understanding of computing subsystems.

Borehole radar system

improves planning in gold and platinum mines

by Teboho Nyareli

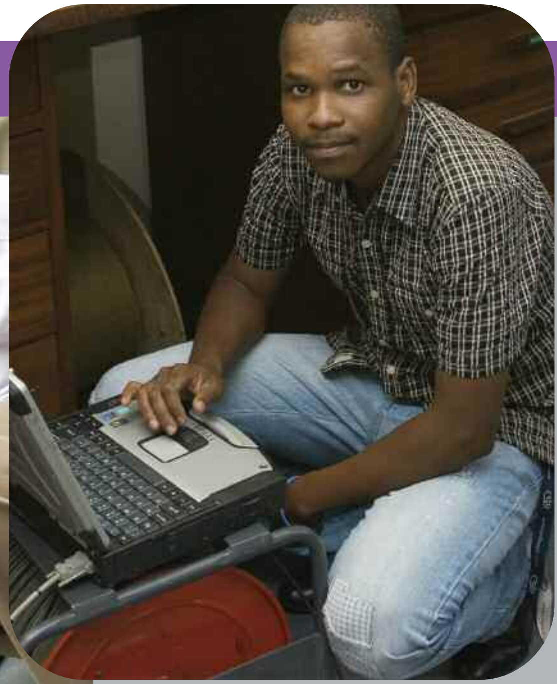


A BOREHOLE RADAR SURVEY conducted prior to the start of the mining process improves mine planning and ensures that less waste is mined. Borehole radar systems are the tools used to conduct these surveys. The technique has been used successfully to delineate reefs and other geological features in South African gold and platinum mines.

One such system is the Aardwolf BR40, designed and developed in recent years by the CSIR. The Aardwolf borehole radar system can determine the distance between the reef and the borehole, but cannot locate the position of the reef relative to the borehole. The reef may be above or below the borehole (Figure 1). Developing a borehole radar system with directional capabilities can solve this problem. Directionality can be achieved by implementing directional antennas and direction finding techniques on the borehole radar system.

Directional antennas and direction finding techniques have been used for many different applications. An example is direction-finding antennas on a police helicopter. This system relies on antenna elements being at least a quarter of a wavelength apart. In the case of a borehole radar system, the borehole diameter is usually 48 mm, which constrains the antenna elements to less than 48 mm apart. This is much less than a quarter of a wavelength of an antenna operating at a maximum frequency of 500 MHz. The receive antenna elements are therefore affected by mutual coupling.

The challenge is to model the feasibility of implementing an array of dipole antennas in a receiver probe that is less than 48 mm in diameter and to understand the effect of mutual coupling. The antenna should be modelled such that the signal that propagates from the transmit antenna to the receive antenna is preserved as much as possible. A ground



Teboho Nyareli and Josias Nonyana bench-testing the directional borehole radar system

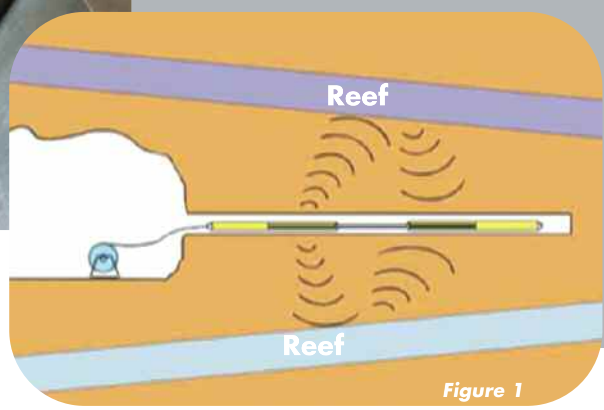


Figure 1 Geometry of a borehole radar survey

penetrating radar (GPR) modelling tool called GprMax3D is used to determine if the implementation is feasible. GprMax3D is an electromagnetic wave simulator for GPR modelling based on the finite-difference time-domain (FDTD) numerical method.

The borehole radar system determines the distance to the reef by measuring the time of flight of an electromagnetic wave travelling from a transmit antenna to a receive antenna. To determine the direction of the wave, the difference in time of arrival at a number of antennas in an array is measured. GprMax3D is used to simulate the transmission of electromagnetic waves between transmit and receive antennas of a borehole radar system.

Transmit and receive antennas are usually in line in a borehole, with the receiver measuring reflections from targets that are illuminated by the transmitter. To simplify the modelling, transmit and receive antennas are physically separated (Figure 2) and the direct signal from transmitter to receiver is considered.

Due to the computational power needed, the models were run on a high performance computing cluster, (C4) at the CSIR in Pretoria. A resistively loaded antenna (damped antenna) has broadband characteristics. Modelling proves that a damped dipole antenna is less efficient than an undamped dipole one, but because of its broadband characteristics, the pulse shape of the signal is preserved. This is shown in Figure 3 for signals received when using undamped and damped dipole antennas, respectively, in the model.

The mutual coupling effect was also investigated at the array of four receive antennas (shown in Figure 2). The modelling results show that as the distance between the receive antenna is decreased from 80 mm to 20 mm, the effect of mutual coupling on the signal increases. GprMax3D also calculates the time difference between signals received at four receive antennas. When a model is set-up as shown in Figure 4, the time difference between antenna 1 and 3 can be determined for the direct and reflected signal.

Figure 5 shows that the direct signal is received at about 14 ns and the reflected signal at about 22 ns. Modelling results obtained using GprMax3D prove the fact that, if time of arrival of a signal at an array of receive antennas is known, the direction of the signal can be determined.

A GprMax3D model can also generate an output file called snapshot. A snapshot represents an electromagnetic wave within the area of model at any given

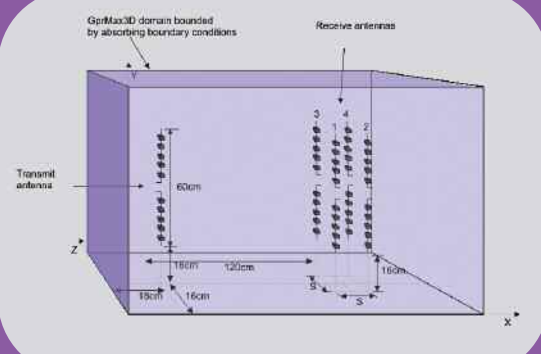


Figure 2
GprMax3D model domain that includes antennas of a borehole radar system

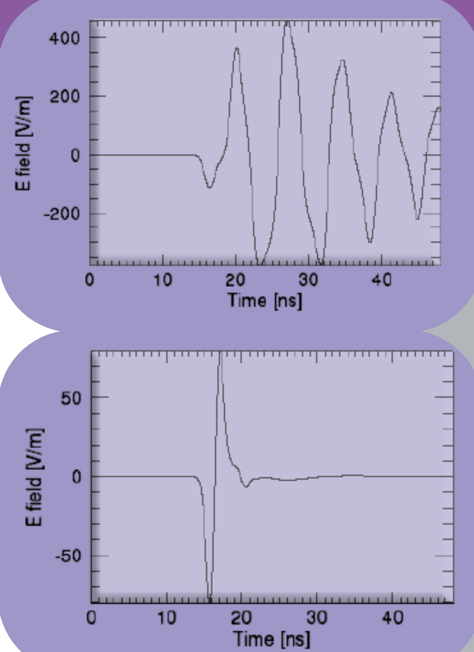


Figure 3
Signals received by an undamped and damped dipole antenna, respectively

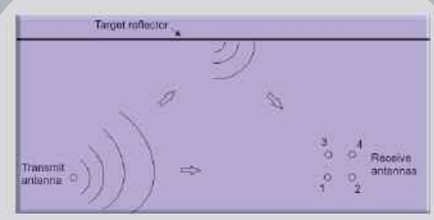


Figure 4
Path of signal when a target is included in model

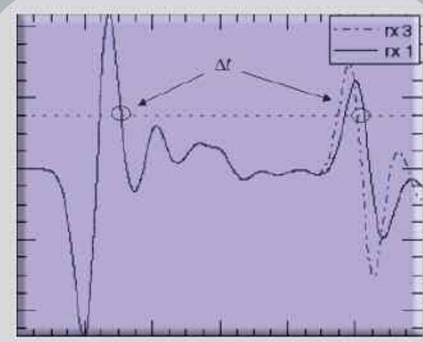


Figure 5
Signals captured from receive antenna 1 (rx 1) and receive antenna 3 (rx 3)

Figure 6
Snapshots of electromagnetic waves propagating from the transmit antenna to the receive antennas

time. Figure 6 shows snapshots of an electromagnetic wave front as it propagates from the transmit antenna towards the receive antenna. It is evident that the direct wave arrives before the reflected wave at the receive antennas.

The modelling results are important, because they show that the proposed method of deriving directionality is physically feasible, and they allow design parameters to be determined empirically without having to build numerous physical antennas. Testing of the antennas designed using the GPRMax3D models has validated the numerical work, and led to faster development times.

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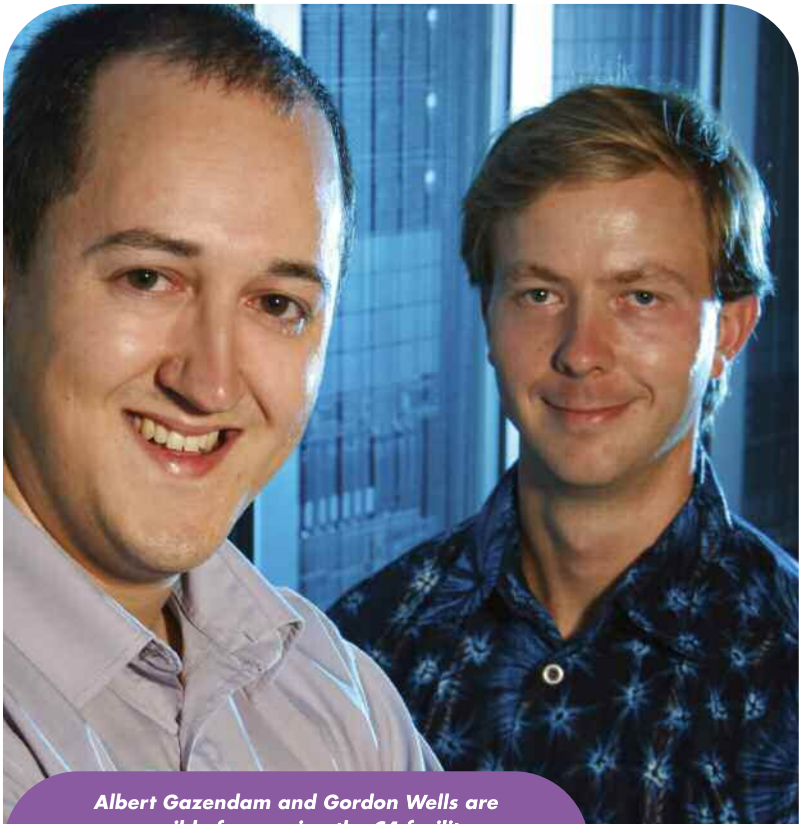
C4: Enabling modelling and simulation through scientific computing

by Albert Gazendam

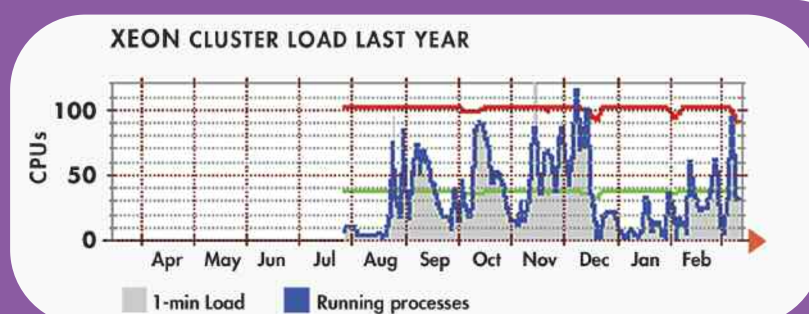
HIGH PERFORMANCE computing (HPC), often referred to as supercomputing, is a technology area in the broader domain of information and communications technologies (ICTs). At the most basic level, the purpose of HPC is to enable computer software with demanding computational requirements to be executed in acceptable time frames. The pieces of software are typically aimed at solving research problems in the scientific and engineering world, but there are also many examples of commercial and industrial applications that utilise HPC. The matters of computational requirements and acceptable time frames often go hand-in-hand, which is simply demonstrated by the intuition that an increase in the number of processing cycles per second will yield results in less time than before. In HPC, the aim is thus to enable the solution of computational problems that are so large and complex that they could not be addressed feasibly by conventional techniques.



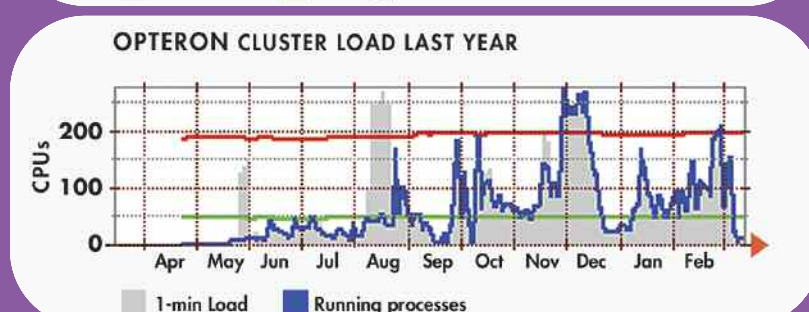
Albert Gazendam and Gordon Wells are responsible for running the C4 facility

In mid-2006, the CSIR invested in the establishment of a new HPC platform to be used as a research tool into the technologies of HPC itself, as well as an enabler of computational science in the organisation and beyond. The platform, known as the CSIR Cluster Computing Centre (C4), has subsequently grown through various additions and enhancements made possible by several CSIR research groups and projects, especially its Meraka Institute. C4 is among the most substantial HPC resources in South Africa, and offers computing capacity to the wider scientific community in addition to its core users in the CSIR. There are currently more than 70 registered scientific users, many of whom depend directly on C4 for the advancement of various research efforts. Usage of C4 is at no cost to scientific users; clear registration instructions are available at http://lists.meraka.csir.co.za/mailman/listinfo/c4-users.

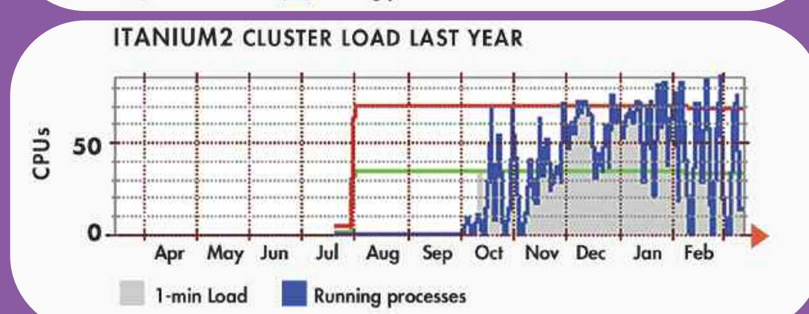
A graph showing the utilisation statistics of the xeon cluster in C4 since the most recent significant software rebuild in July 2007. The blue line's value relative to the red line relates utilisation percentage, with the period during early December 2007 clearly showing an overloaded condition. Utilisation is only now picking up again following the year-end vacation



A graph showing the utilisation statistics of the opteron cluster in C4 since the most recent significant software rebuild in April 2007. The blue line's value relative to the red line relates utilisation percentage, with the period during early December 2007 clearly showing an overloaded condition. A dip over the year end vacation is also clearly visible



A graph showing the utilisation statistics of the itanium2 cluster in C4 since the most recent significant software rebuild in July 2007. The blue line's value relative to the red line relates utilisation percentage. This system achieves some of the best utilisation percentages in the South African research community



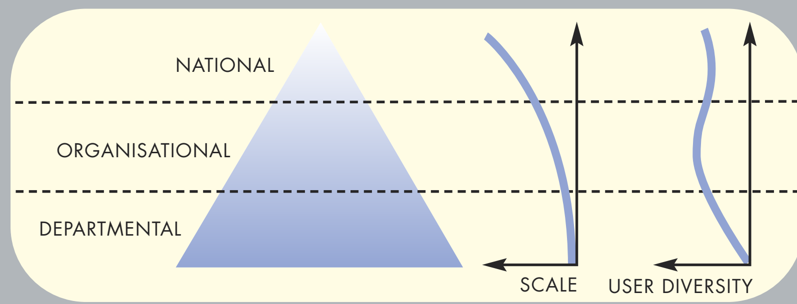
Dr Shadrack Moephuli (left), CEO of the Agricultural Research Council (ARC) with Dr Sibusiso Sibisi, CSIR President and CEO at the C4. Research collaboration between the ARC, the University of Pretoria and the CSIR on an ultra high-resolution climate simulation study has been boosted significantly through the use of the C4.

Examples of where C4 is being used in research projects range from the modelling of DNA substitution in HIV, to experiments in artificial intelligence, the simulation of stresses and strains below road surfaces, and the development of improved radar processing techniques, to the refinement of data compression algorithms. The flexible and open nature of C4 makes it possible for researchers to explore the benefits of HPC in new ways. In essence, C4 is an HPC laboratory where perceptions are meant to be challenged and rules are meant to be flexible. This approach can be interpreted as an 'infrastructure commons', in line with the liberating philosophy that lies at the heart of open source software (OSS).

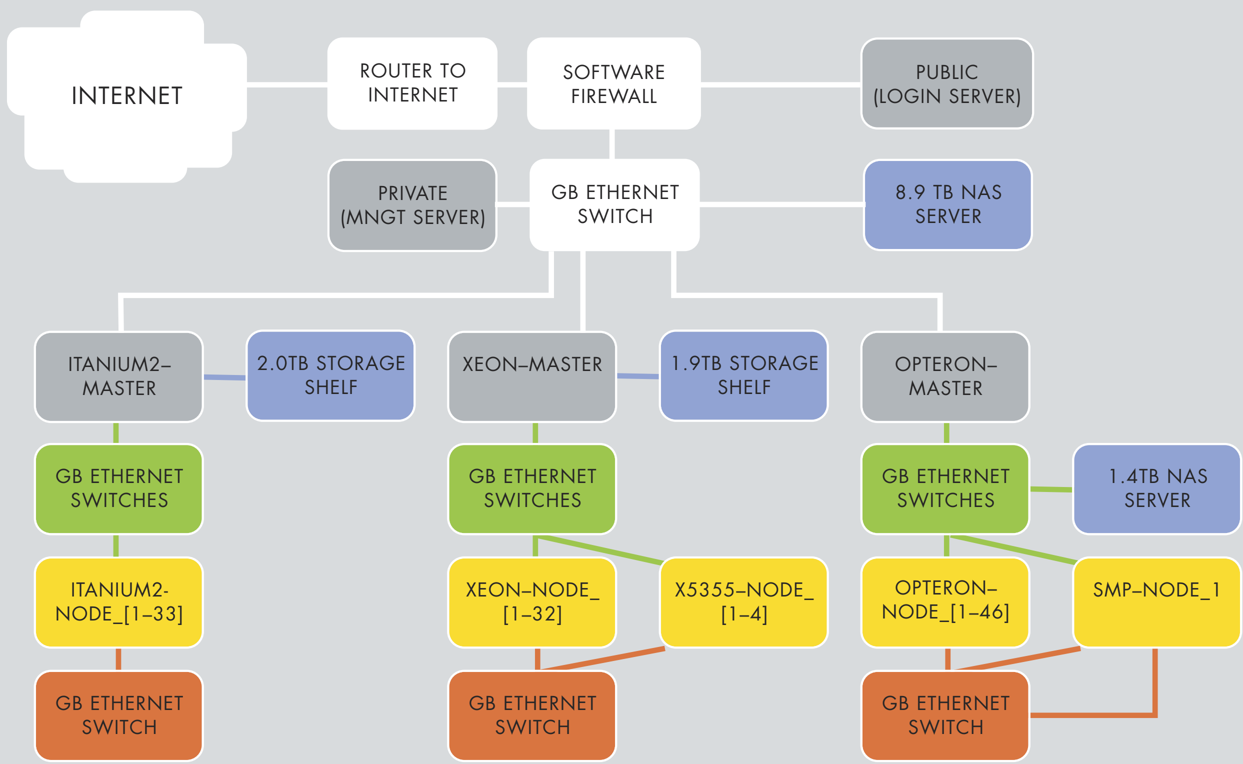
The technical characteristics that contribute to the openness and flexible nature of C4 are attributable to the fact that it consists of a number of computing clusters all built up from standard, albeit very high-end, hardware components that are available off-the-shelf from multiple suppliers. There are thus very low risks of vendor and technology lock-in with regard to expansion and support matters, while it is still possible to exploit the benefits of economies of scale. These hardware components are configured in what is known as a Beowulf architecture, which allows for the creation of a modern supercomputer based on open hardware standards and OSS. Each of the three clusters currently incorporated in C4 runs Linux-based operating systems and is equipped with a multitude of scientific OSS libraries and tools, the number of which are continuously growing.

Computing technology ages very rapidly. The most basic measure of an HPC system's mettle is the number of floating point arithmetic operations that it can perform in a second.
When considering the international top 500 list of supercomputers (www.top500.org), it is worth noting that the 500th most powerful HPC system in the world today scores around 4 Tflops (this ranking will require about double that number in a year's time), while C4's aggregate score is only slightly more than 1 Tflops.
At utilisation numbers that are rapidly growing beyond month-to-month average levels of 60%, it is critical that scientists continue to look beyond the horizon of what today's technology can provide.

The world of HPC is changing rapidly, and is now entering a new age of growth following that which started in the mid 1990s with the advent of the Beowulf cluster. This new age centres around the proliferation of multi-core processing, virtualisation technology



This pyramid illustrates the hierachy of HPC facilities, with C4 being a good example of an organisational class facility that is typified by moderate scale and high scale levels of user diversity



- 1 headnode providing 4 x single core Itanium®2 1.6GHz and 16GB of RAM
- 33 nodes providing 2 x single core Itanium®2 1.6 GHz and 4GB of RAM

- 1 headnode providing 4 x single core Intel® Xeon® 3.6 GHz (model Irwindale) and 16GB of RAM (xeon)
- 31 nodes providing 2 x single core Intel®2 Xeon® 3.6 GHz (model Irwindale) and 4GB of RAM (xeon-node_1– xeon-node_32)
- 1 headnode providing 4 x single core Intel® Xeon® 3.6 GHz (model Irwindale) and 4GB of RAM (xeon-node_27)
- 4 nodes providing 2 x quad core Intel®2 Xeon® 2.6 GHz (model Cloverton) and 2GB of RAM (x5355-node_1 - x5355-node_4)

- 1 headnode providing 2 x dual core AMD® Opteron® 2.6 GHz (model 285) and 4GB of RAM (opteron)
- 46 nodes providing 2 x dual core AMD® Opteron® 2.6 GHz (model 285) and 4GB of RAM (opteron-node_1 - opteron-node_46)
- 1node providing 4 x dual core AMD® Opteron® 2.6 GHz (model 885) and 64GB of RAM (smp-node_1)

This diagram shows the various components of C4 and their relative positions in the high-level network architecture

and increasing levels of abstraction that attempt to hide resource and infrastructure complexities from a new breed of software user that hungers for limitless processing, storage and networking resources. Not only does this open up vast opportunities in all domains of science and industry, but also a growing number of engineering challenges in managing the trade-offs between abstraction and efficiency.

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Modelling and simulation the supercomputer way

by Dr Happy Sithole

Dr Happy Sithole, acting director: CHPC

MANDATED BY the Department of Science and Technology, the Centre for High Performance Computing (CHPC) aims to enhance the computational research output of the South African scientific computing community. High profile projects in material science, astrophysics, oceanography, climatologies, bioinformatics, fluid dynamics, finite element modelling, astronomy, high energy physics and quantum computing modelling are currently utlising the CHPC computational infrastructure.

Funded under the cyberinfrastructure initiative, the CHPC supports users across all spheres of the tertiary education institution system, with various requirements for computational resources. The type of applications range from nanometre to light-year scale, applicable from scientific to engineering domains.

Traversing across these modelling scales, several demands exist on computational resources, due mainly to the mathematical formulations behind a specific modelling method and partially due to the type and size of a system being modelled. For example, some of the codes require efficient input/output (I/O) during parallel processing whereas others demand sufficient memory allocation. High performance computing (HPC) architecture suitable for multiple processors, which share the same memory and high-speed connection for efficient I/O between subsystems, are symmetric multi-processing (SMP) and massive parallel processors (MPPs). It is specifically these various demands in computational platforms that present the CHPC with opportunities to carefully scrutinise the available technologies in developing its infrastructure.

THE CENTRE FOR HIGH PERFORMANCE COMPUTING (CHPC) started operations in June 2007 with the major objective to amass and manage computational infrastructure, and avail it to the South African research community. The first HPC system has been put at the Rosebank campus of the CSIR. The IBM (e1350) Linux-based cluster, consisting of 640 processing cores distributed across 160 nodes, has 2,5 Tflops capacity, and plans are under way to increase the capacity by the end of 2008.

The imperative demand for a critical mass of skilled HPC practitioners forms the central activity of the centre. For this purpose, a training programme on skills relevant to HPC, such as parallel programming and scientific applications, is being facilitated.

Detail in modelling

An important factor to take into account when modelling is the detail of the model. A basic principle of modelling is to try to reduce the detail in the model in the context of accurately portraying the essential aspects of interest to the system.

Even if it were possible to build a detailed model, excessive detail would slow down the run time and be irrelevant to the results.

An indication of the efficiency of the simulation is expressed in terms of the speed-up or slow-down factor. The speed-up factor is the number of seconds that can be simulated of the real system for one second of the processor time. The slow-down factor is the number of seconds of the central processing unit's time needed to simulate one second of the real system. The detail in the model should represent only the detail of the data that are available to us, otherwise correlations might be necessary.

Techniques and challenges

A choice of methods can be used to gain insight into systems and to gain results from these through models. It may be possible to have an analytical solution to a model, but not always. This is due to the fact that the system does not reduce to a product form solution, nor is it close to one – a result of passive resources and priority schemes being used. Embedded heuristic algorithms also present a problem.

When it is not possible to get an analytical solution computer, simulation is an alternative. However, there should be some crude analytical checks on the results from the simulations against the real system. Sometimes the models are not static but vary with time, thus further complicating the analytical methods. Different modelling landscapes each has its own limitation.

For example, it is unnecessary to model a system based on molecular mechanics, if the aim is to understand the influence of electrons in a system, and thus limit such simulations only to *ab initio* approaches. These limitations also extend to the time frame required on the model and the size of the system. However, one should recognise the mutual dependence of one technique on the other. In most cases, accuracy and refinement of a model on larger landscapes might require input from a model at lower landscapes, and *vice a versa*.

The challenges of these varying approaches to modelling are unique from one technique to another. At electronic level, good approximations to exclude some electrons in calculations are being addressed through density functional theory (DFT) and at atomistic level, through the use of efficient inter-atomic potentials. The finite element analysis looks at various methods of mesh refinements, which will be less costly in computational resources. However, the common challenge in all these methods is to take advantage of the fast increasing computational power.

These are issues of scalability, where a decision is required on whether a problem is of an HPC nature. Most of the applications have been written whilst parallel programming was still in its infancy, hence the developments were not sensitive to such challenges. It is only through the developments in the MPPs that we see the effort to parallelise these codes.

CHPC scientists are currently using the HPC techniques in their research areas, including meteorology modelling, space physics and astrophysics, visualisation and virtual reality, and computational mechanics and electromagnetics.

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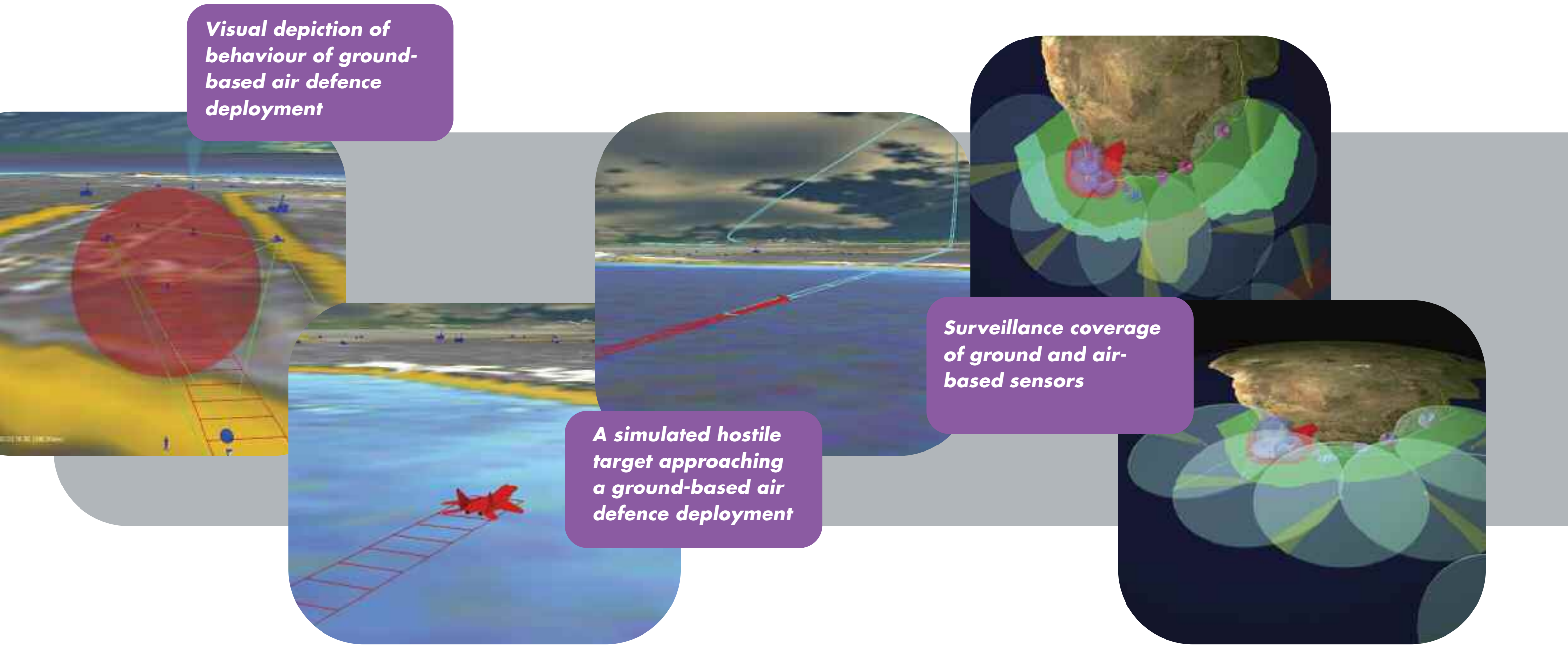


Visual depiction of behaviour of ground-based air defence deployment

A simulated hostile target approaching a ground-based air defence deployment

Surveillance coverage of ground and air-based sensors

Cyclops 2 pushes boundaries for simulation interaction and feedback

by Bernardt Duvenhage and JP Delport

THE CSIR HAS GAINED considerable experience in simulation visualisation within the recent past due to the prominence of its simulation work. One of the tools that has evolved considerably during this time is the Cyclops visualisation and visual analysis tool. The current version, Cyclops 2, has been under development since 2005.

The design goals are growing along with the requirements of the user group. The user base of, and therefore requirements placed on the tool have steadily expanded and led to enhanced visualisation features. Cyclops 2 is currently used as a visual verification and validation aid by modellers, as a platform for generating experimental stimulus, for analysing simulation results and as a simulator in its own right used in playing out simulation runs to deduce or infer new knowledge.

The tool has, for example, been applied in:

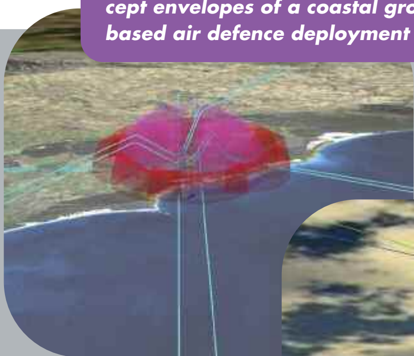
- Behavioural analysis of a system-of-systems level ground-based air defence system (GBADS) simulation
- Construction of human-machine-interface mock-ups of simulated equipment for the incorporation of human behaviour in experiments
- Analysis of high fidelity one-on-one infrared missile against aircraft engagements
- Study of the surface coverage of satellite and other airborne sensors for surveillance purposes.

The visualisation style is one of augmenting a synthetic 3D environment with representations of possibly time-stamped simulation results. The synthetic environment includes digital terrain elevation data, GIS data overlays and satellite or map imagery much like that of Google Earth.

The characteristics of the current version of Cyclops include:

- Generic network or log file interface for live or off-line simulation visualisation
- High performance history buffer that provides live pause and replay functionality of the simulation action
- Flexible hierarchical filter that removes unwanted visual clutter
- Visualisation component that produces the 3D representation of the simulation results.

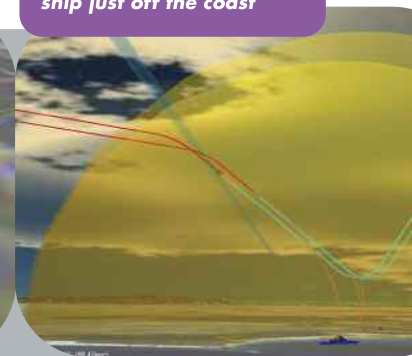
The interface to Cyclops uses an XML protocol that allows for the inclusion of user-defined attributes. The attributes are used by the visualisation component to create the 3D geometry and are also used for constructing the hierarchical filter tree.



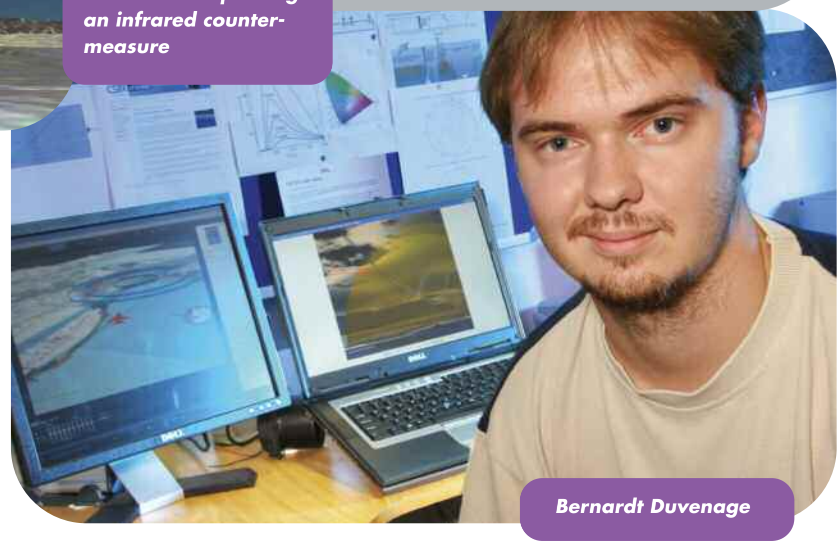
A 3D depiction of the virtual areas of responsibility and weapon intercept envelopes of a coastal ground-based air defence deployment

The view from an approaching missile towards a transport aircraft soon after an infrared countermeasure was dispensed

The view from a transport aircraft towards an incoming missile soon after dispensing an infrared countermeasure



Simulated hostile aircraft being tracked and engaged by a Corvette ship just off the coast



Bernardt Duvenage

The first three Cyclops 2 characteristics, as mentioned earlier, are consistent across a large range of visualisation domains without modification.

The visualisation component, on the other hand, is employed to construct, augment and visually represent the simulation results by mapping the abstract simulation entities and concepts to a 3D representation. The mapping to and inferring of the 3D representation therefore require domain-specific knowledge. For example, to represent a simulated anti-aircraft gun turret, it must be decided how the turret will be represented in 3D, how it will be fixed to the terrain and what shape has to be used to represent the gun's virtual envelope of target intercept. Such 3D representations then allow the behaviour of simulation entities, the internal processes of these as well as the temporal and spatial interactions with other entities to be visualised.

The domain-specific information is currently not actively transported over the XML interface. Research is, however, being done on making Cyclops more domain independent and configurable with the goal of providing maximum benefit to the modellers and simulation analysts.

The visualisation component provides an interface to 3D scene graph functionality and makes use of the well-supported open source open scene graph (OSG) library. The use of OSG allows access to cutting-edge visualisation techniques that exploit the performance and programmability of modern hardware graphics processing units (GPUs). The use of a scene graph also allows for efficient manipulation and rendering of a large number of 3D objects and extensive high resolution terrain databases.

The visualisation component exposes a number of geometric primitives that can be used for the 3D representation of the simulation results. The current set of primitives includes cones, ellipses, sphere segments, lines, polygonal areas and, specifically for the current military domain, primitives such as flight paths and trail ribbons, particle system explosions and screen-aligned or entity-aligned 2D icons. Texture-mapped 3D objects constructed using packages such as 3D Studio Max or Blender can also be inserted as geometric primitives. The set of primitives is continually extended as the need arises.

Cyclops 2 is pushing the boundaries for simulation interaction and feedback. It has been shown that such a tool facilitates situational awareness for the domain expert and non-expert user alike. This has resulted in an effective communication tool to present simulation results to clients and the general public, while intuitively conveying the credibility of the simulation.

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Simulating a wireless solution for remote areas

by David Johnson

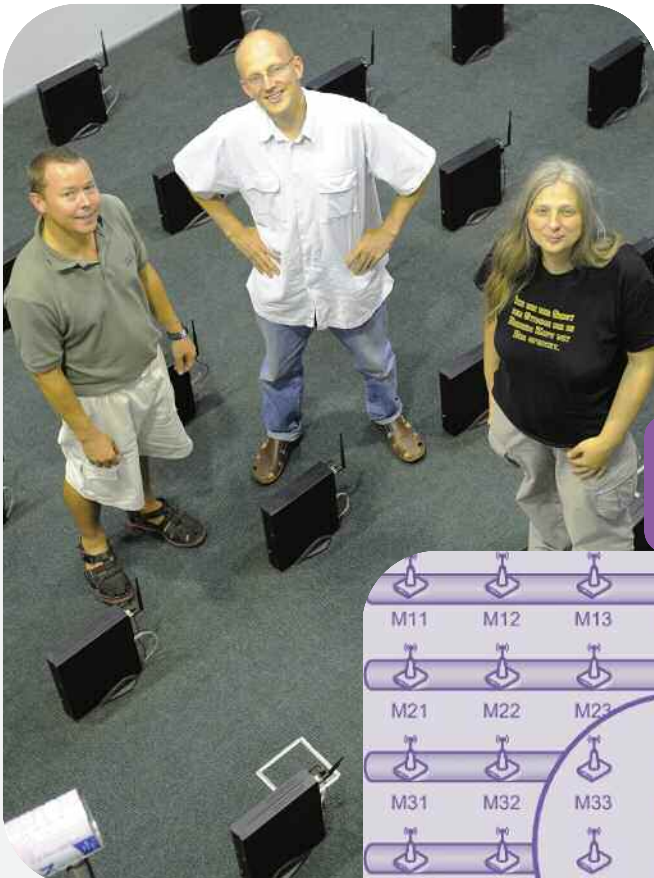
THE MAJORITY OF PEOPLE living in rural areas of developing and underdeveloped nations have not yet been able to take advantage of the internet revolution. This increasing gap between the technology-enabled sections of human society and the underdeveloped rural population has created a 'global digital divide'. Most of the research focus to date has been around improving connectivity in urban areas while rural areas often have very little or no connectivity options.

Wireless mesh networks have the potential to provide much needed broadband connectivity to these under-serviced areas but studying the behaviour of such networks is a complex modelling problem. To overcome these challenges, the Meraka Institute of the CSIR built an indoor scaled grid-based wireless test bed.

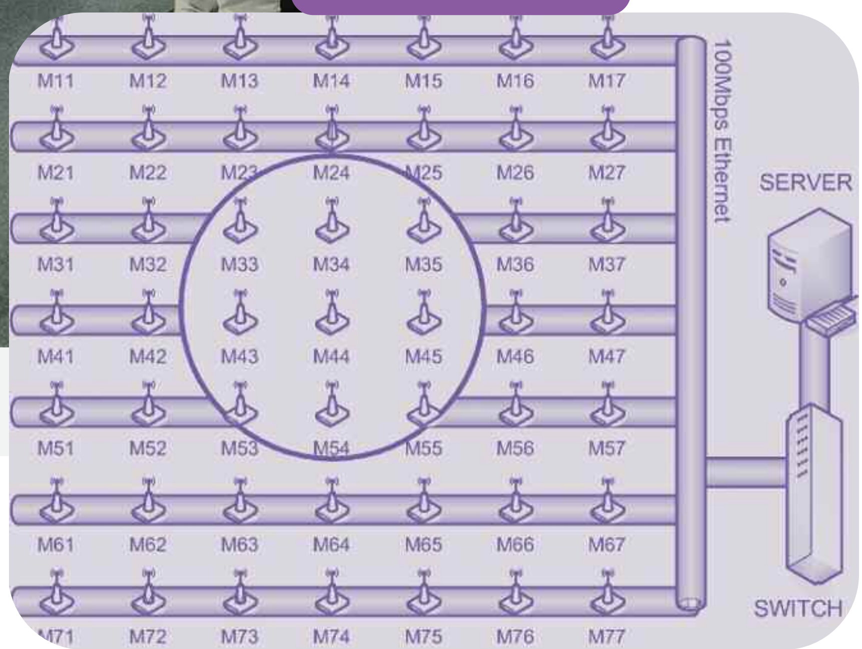
Wireless mesh networks function very differently to conventional communications networks such as a global system for mobile communication (GSM), in which all client devices communicate with a central base station. In mesh networks a signal travels from its source to its destination by making use of wireless routers to relay the signal from one device to the next using an optimal route. A wireless router is a dedicated communications device installed at the user's premises to ensure that data are received and delivered in a timely manner. In a mesh network there is no concept of a master device and all devices are equal in terms of function and form a self-configuring, self-healing network that is simple to deploy.

A network needs to be able to scale up from small, 10-device networks to large rural villages consisting of hundreds or thousands of devices and still ensure timely delivery of real-time data such as voice communications, while simultaneously delivering bursty web traffic to users. This is a complex problem as routing protocols need to find optimal routes through a non-uniform collection of wireless routers with a range of connectivity characteristics. There are numerous other challenges such as adapting to different types of traffic flows as well as overcoming problems such as interference in a shared channel multi-hop environment.

Modelling a system like this is typically done using computer-based simulation tools. However, recent analysis of research papers, in which well-known computer-based simulation tools are used, has shown a lack of consistency between results run on different simulation packages. It is thus difficult to know



John Hay and David Johnson with visiting researcher Elektra Aichele in the mesh laboratory



which results to trust, were they to be implemented on a physical wireless network.

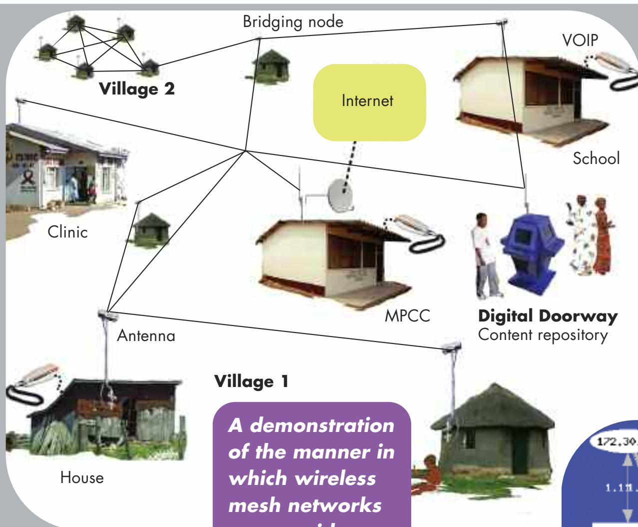
The Meraka wireless test bed consists of a wireless 7x7 grid of 39 wirelessly-equiped nodes, built in a 6x12 m room. Each node consists of an 800 MHz PC equipped with an 802,11 based radio connected via Ethernet to a central server. The nodes are uniformly spaced 800 mm apart to fit into the room dimensions and the operating system is loaded from the central server using a net-boot environment.

One of the key challenges in the grid was attenuating the signal enough to simulate large distances between nodes. The inverse square law of radio propagation, where the electric field strength is attenuated by 6,02 dB for each doubling of the distance in any free-space loss scenario, makes it possible to build an indoor scaled version of a far larger network using attenuators.

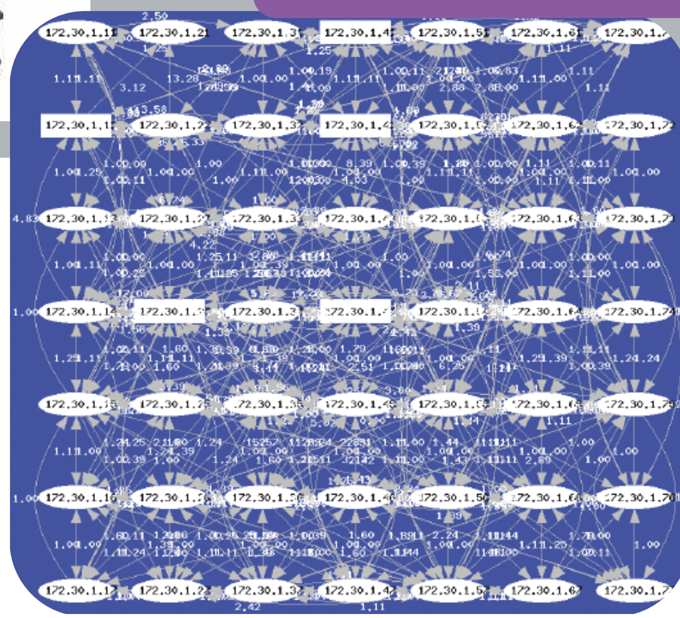
To achieve this, each radio was equipped with a 30 dB attenuator to introduce a path loss of 60 dB between the sending and receiving node.

The software framework for running experiments in the lab consists of a number of useful scripted tools, such as executing a single command on all the nodes at once or logging various results on each node back to the central server. All nodes are also connected to a relay-bank that allows a remote user to power-down and power-up all seven rows in the grid. This is especially useful if an experiment causes nodes to freeze up and a hard-reboot is necessary. The environment allows a researcher to quickly upload a new operating system or protocol to the central server and deploy this on all 49 nodes within a matter of minutes.

An extensive electromagnetic model has been constructed for the grid and compared against actual signal strength measurements to help understand the effects of the physical environment on the grid's performance. Some useful insights were gained from this exercise, such as the antennas re-amplifying the signal when placed in a closely spaced straight line and the attenuation of the signal due to metal PC boxes. Some improvements to the electromagnetic environment, such as placing antennas on higher pedestals, will be explored. To date, a number of comparative tests between various routing protocols have been run on the test bed.



A demonstration of the manner in which wireless mesh networks can provide connectivity in a rural village



Routing topology formed in the wireless grid when running a mesh routing protocol on each node in the grid. Each oval represents a computer and rectangles represent computers that handle the most traffic. The lines connecting each shape represent wireless links, the numbers next to these lines represent the quality of the link. (The higher the number, the poorer the link: 1 is a perfect link). Data will try to traverse this grid such that the sum of the individual links is as low as possible

These tests have helped expose the strengths and weaknesses of these protocols under various network conditions. For example, one of the problems analysed was the ability of a routing protocol to scale to large networks. The network size was iteratively grown in a spiral fashion from four nodes up to 49 nodes while monitoring parameters such as routing traffic overhead, percentage of successfully delivered packets and delay. These results have already shown new insights previously unavailable in the research community that relied only on computer simulation tools.

The most recent work carried out is a detailed analysis of a protocol developed by a wireless mesh community in Berlin, called BATMAN (Better Approach To Mobile Adhoc Networking). The originator of this protocol, Corinna Aichele (aka Elektra), spent two months at the Meraka Institute using the test bed to quantify BATMAN's advantages over existing mesh routing protocols. It is expected that this lab will be used remotely by researchers from all over South Africa and the rest of the world to help build a realistic view of how mesh networking protocols perform in a range of network conditions on real wireless hardware.

Typical graphs that can be generated by the wireless grid: This graph compares the number of outbound routing overhead packets per node per second as the number of nodes increases for four different routing protocols. Routing overhead needs to be minimised as it uses up valuable capacity in the network that needs to be used to send data over the network

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Microfluidics – disruptive technology for the future

by Mesuli Mbanjwa and Kevin Land

CSIR researcher, Mesuli Mbanjwa, using the confocal microscope

A FULL-SCALE LABORATORY, the size of a credit card? Impossible. It is, however, exactly towards this end that the micro-manufacturing research group of the CSIR is heading.

The advancement of micro-manufacturing technology has fuelled the development of microsystems for a wide range of electronic, biomedical and energy applications. The CSIR has taken the lead in South Africa in establishing the first micro-manufacturing laboratory to focus on the manufacture of micro-scale components.

Interest in microfluidics started 20 years ago. One of the first commercially successful applications was in the inkjet-printer. The mechanism behind these printers is based on microfluidics and the manufacture of very small tubes to carry the ink for printing.

Modelling and simulation are considered essential and indispensable tools for microfluidics research.

Microfluidics is the science and engineering of fluids in very small volumes, typically in microscopic and nanoscopic ranges. Fluids on these scales can be handled better while being more precisely controlled than in conventional fluidic systems. Microfluidics is a multidisciplinary area that combines different elements of physics, engineering, biology, chemistry and biotechnology with a wide range of applications spanning from manufacturing industries to diagnostic and therapeutic medical applications.

A diagnostic 'lab-on-chip' microfluidic device may, for example, be the size of a credit card, able to perform analysis on a micro-scale that is normally done in a full-scale laboratory.

Such a device, depending on its function, would have different functional components including channels, valves, mixers, separators and pumps manufactured on a micro-scale.

Micro-manufacturing research at the CSIR focuses on building a competence in the design and manufacturing of microfluidic devices. Current work involves design and modelling of single, modular microfluidic elements that include mixers, separators, pumps and flow channels. Related manufacturing issues, such as machining, materials, and sealing are also considered. Future plans are to model complex microfluidic systems that may consist of a number of these complete elements. This could include technologies and techniques not yet implemented, such as fluorescent and other detection methods, micro-optics, integration of electronics into chips, and various other control methods.

The research group currently has two applications areas that are funded by the Department of Science and Technology's Advanced Manufacturing Technology Strategy (AMTS) implementation unit, which is hosted by the CSIR.

The applications are microfluidic devices for biological applications and the development of direct alcohol micro-fuel cells, respectively. The micro-fuel cell modelling is aligned with the design of flow fields for fuel cells to be used in portable applications.

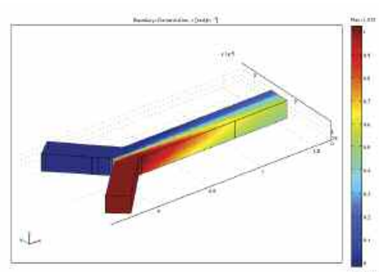
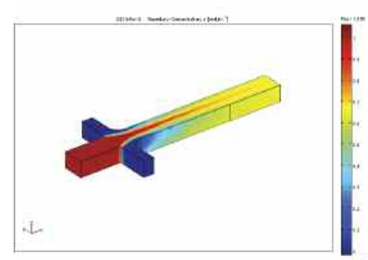
The designs are evaluated using computational fluid dynamics (CFD) modelling in order to eliminate a trial-and-error approach to manufacturing. This serves to save considerable time in the process chain as manufacturing is often cost-intensive and time-consuming.

Modelling and simulation also allows for innovation as future designs can be developed and evaluated without being limited by existing experimental testing systems.

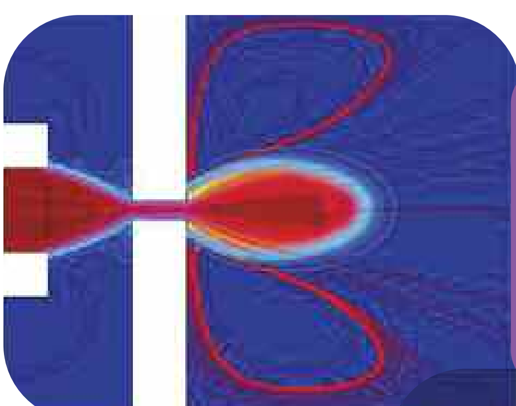
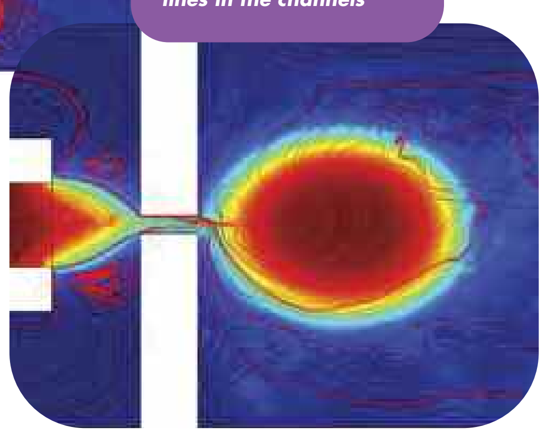
In microfluidics, CFD modelling and simulation employ three types of models, mechanistic, analytical, and semi-empirical.

Mechanistic models are theoretical mathematical models where the physical phenomena are described by differential and algebraic equations. Modern modelling software programs are used to solve these equations, often iteratively.

Analytical models also use mathematical equations that give approximate solutions, but not a comprehensive representation of physical phenomena. These models are very useful when dealing with simple systems where quick solutions are required. Semi-empirical models are used when phenomena are too complex to be represented by mathematical equations. Experimental data are obtained and experimental correlations are combined with known mathematical equations in the models.

Concentration profiles in static microfluidic mixers a) Y-type and b) hydraulic flow focusing modelled with COMSOL software

CFD model visualisation of a two-phase flow of a microdroplet of water dispersing from its phase into a continuous oil phase in a 963 μm coaxial flow focusing device. The red lines represent velocity streamlines in the channels

Semi-empirical models are often limited to specific operating conditions in which they can be accurately applied. In many cases, experimental relationships do not adequately explain physical phenomena since correlations are made between input and output parameters. Certain experimental data are used to validate theoretical models, although some models are validated mathematically.

CFD modelling and simulation in microfluidics differ slightly from macro-models because the general physical phenomena of fluids at a small scale differ from that of fluids at a larger scale. This is due to domination of surface effects over volume effects because of scaling laws. It, therefore, becomes necessary to combine modelling of these diverse physical phenomena with conventional CFD models. Called multi-physics modelling, these models require additional mathematical equations for inclusion in conventional CFD models. COMSOL Multiphysics is one of the commercially available CFD software packages, and has been chosen by the micro-manufacturing group for its modelling needs.

Once designs have been evaluated they can be manufactured. The group currently has an Excimer laser work-station that can be used for machining of microchannels in various materials, such as metals, glass and polymers. In addition, the group utilises aspects of soft lithography for replication of micro-structures and is actively investigating the establishment of an advanced soft lithography manufacturing facility.

Machined components can be studied under a Zeiss laser scanning confocal microscope for dimensional accuracy and surface finish on the components. This equipment will also be used in the future to visualise fluid-flow through channels. In this way, the models can be analysed to ensure design accuracy. Often termed a disruptive technology, microfluidics requires science and research to take a whole new approach to handling liquid in a laboratory environment.

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Physical scale modelling helps predict in-mine geophysical responses

by Michael van Schoor and Dr Stoffel Fourie

PHYSICAL SCALE MODELLING offers an attractive alternative to conventional numerical modelling for predicting the response of a geophysical system. Recent experimentation with modern potting and casting materials, such as various types of resins, has rekindled the interest in scale modelling. In particular, the use of transparent resins enables one to construct models that can be used primarily for demonstration purposes, but which can also serve as scale modelling and calibration facilities.

The idea of dabbling in scale modelling was prompted by ongoing research by the CSIR's applied geosciences research group into the application of in-mine electrical resistance tomography (ERT) and induced polarisation (IP) tomography.

Why physical scale modelling?

Although computer simulations are relatively easy and economical to conduct, these do have some disadvantages. Some simplifying assumptions are inevitable and restrictions in terms of model construction, especially in the case of complex 3D problems, usually apply. Consequently, synthetic modelling results may not always represent an accurate simulation of real field parameters and measurements. Scale modelling offers more flexibility in this regard and synthetic material properties can be matched to known or expected geological material properties. In addition, scale models can serve as testing and calibration facilities for geophysical instrumentation, while they also offer excellent demonstration and instructional possibilities. It is also more cost-effective to work on scale models than to mobilise a team of people to experiment underground.

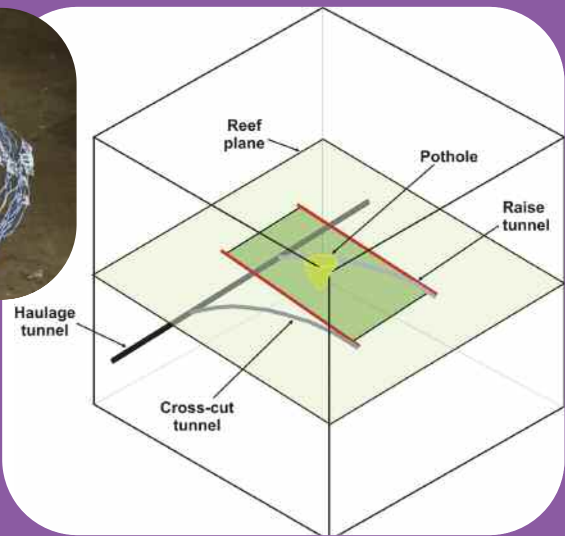
Scaling down a mine

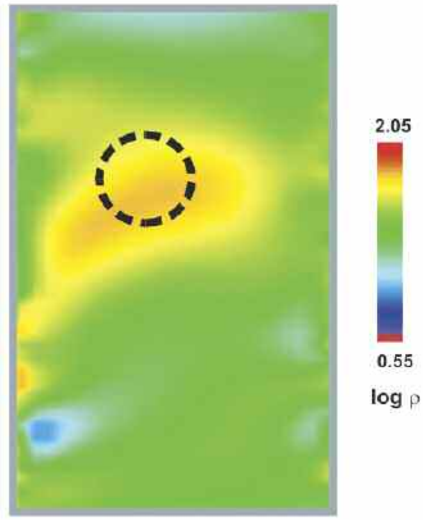
In recent years, the CSIR has conducted research into the application of tunnel-to-tunnel ERT and IP tomography in South African platinum mines. The typical Bushveld Complex platinum orebody is a thin, gently dipping, planar deposit or 'reef' that is relatively continuous on a regional scale. The average thickness of the two major platinum-bearing reefs, the Merensky Reef and the UG2, is approximately 1 m and mining typically occurs at depths of several hundred metres below surface. The reef is accessed through a system of vertical shafts and horizontal tunnels. Ore extraction starts from within the raise tunnels and the virgin blocks between adjacent raises are systematically mined out. Depending on factors such as the locality, mining method and the dip of the reef, the raise tunnel spacing may vary from some 35 m to 200 m.

The targets of interest in these studies are localised slump structures or 'potholes' that disrupt the lateral continuity of the Merensky or UG2 reefs.

Michael van Schoor and Dr Stoffel Fourie conducting geophysical measurements on a scale model designed to simulate a typical platinum mining problem

The 1:400 cement model is a scaled equivalent of the 3D mining layout and geophysical sensor configuration depicted in the schematics shown to the right





ERT output image revealing the presence of the known pothole target, manifesting as a high-resistivity anomaly (warm colours)

Since the imaging plane for tunnel-to-tunnel surveys coincides with the more conductive reef plane, the potholes effectively constitute targets that are electrically more resistive and less polarisable than the background (undisturbed, continuous reef).

In-mine ERT surveys comprise a combination of in-line dipole-dipole measurements (source and receiver dipoles located in the same tunnel) along the respective raise tunnels, and tunnel-to-tunnel measurements, in which the source and receiver dipoles are located in opposite tunnels. The electrodes are placed along the tunnel sidewalls of the survey block – a typical in-mine survey would involve between 30 and 50 equidistant electrode locations and several hundred dipole-dipole measurements. For the scale model experiments, a tunnel spacing of 36 m and a survey site aspect ratio of 2:1 are assumed. This equates to 21 electrodes per tunnel and a unit electrode spacing of 3 m.

A pothole target is placed between the two tunnels to disrupt the reef horizon as well as some of the immediate hanging and footwall layers. A 1:200 scale model based on the generic mining layout and geological problem described here has been designed. This model, which is currently under construction, is being made using an ultra-clear resin so that the model can serve primarily as a demonstration facility. The pure resin, once set, would have an extremely high electrical resistivity. This would also afford the opportunity to study a physical mechanism by which the thin reef acts as a preferential pathway for current flow, thereby enabling the tomographic imaging of the pothole targets.

As part of the research a smaller (1:400) version of the model was constructed from cement-based materials and a pilot ERT survey was conducted. Tomographic images were produced using a complex resistivity-based 2D imaging algorithm. The inversion result confirmed the hypothesis that a thin, relatively conductive reef acts as a preferential pathway for current flow: The ERT output image clearly shows the manifestation of the pothole target as a high-resistivity anomaly. The pothole effectively causes the current flow paths to be distorted and lengthened and the corresponding increase in measured resistance can be explained in terms of the proportionality between resistance and path length in an electrical circuit and Ohm's Law. These initial promising results were presented at the 2007 South African Geophysical Association's (SAGA) biennial conference.

The future

The 1:200 demonstration model will soon be completed and further small-scale ERT and IP tomography experiments will be conducted on both the 1:200 and the 1:400 models. In future, the same or similar models could be used to investigate other geophysical applications such as IP tomography or complex resistivity as well as other geological problem scenarios such as cavity or old workings detection, mapping of reef disruptions, and environmental applications such as the delineation of acid mine drainage and other pollution plumes.

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