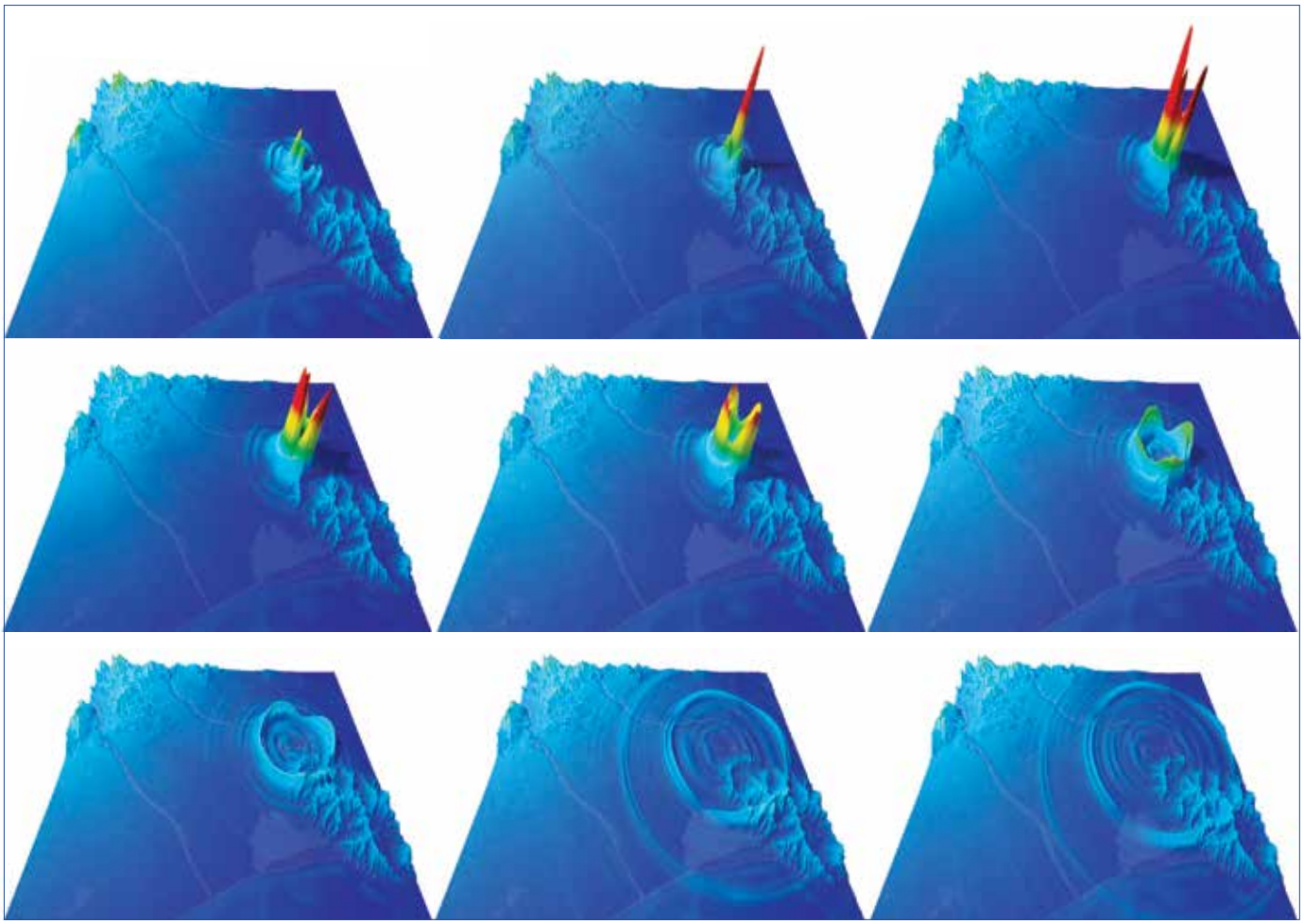
THE UNIVERSITY OF AUCKLAND
Te Whare Wānanga o Tāmaki Makaurau
NEW ZEALAND

CENTRE FOR ERESEARCH ANNUAL REPORT 2015

Contents

Centre for eResearch Annual Report 2015

A selective of images (below) of ground motion simulations of the 4 September 2010 Darfield Christchurch earthquakes. Simulation produced by B.Bradley, University of Canterbury. Staff at the Centre helped to create 3D visualisations of the simulation results.



Welcome message

Another year, another 25 million core hours. This year has seen some intense computational activity within the Centre for eResearch, with near 100 researchers now having passed the mark of consuming over 100,000 core hours each. Our High Performance Computing (HPC) service is provided via a partnership with the New Zealand eScience Infrastructure (NeSI: https://www.nesi.org.nz), and we are grateful to their HPC and user-support teams which have helped us achieve some great outcomes this year.

Our activities have broadened in 2015, we started new projects to offer university-wide services for research Virtual Machines, and the use of an advanced visualisation facility. We also launched a data publishing tool (figshare: https://auckland.figshare.com/) and began work a range of tools to support various research data needs. Within a modern university, such services are now an indispensible part of the research infrastructure. Finally, we started two important educational activities in 2015: (i) a regular slot in the PhD induction program to connect with our newest researchers, and a HackyHour weekly casual meet up to encourage shared approaches to problem-solving and support for researchers (https://uoa-eresearch.github.io/HackyHour/).

In this report, you will find details of our major outcomes and successes of 2015, details of our new activities and a brief overview of our plans for 2016. All of the showcased material, the feedback and the lists of research outcomes relies on responses from the University's researchers to our requests for information. I'd like to take this opportunity to thank all those researchers who put their trust in us, and those who shared their outcomes and achievements back with us to help us create this report.

Professor Mark Gahegan
Director, Centre for eResearch

Enabling computationally intensive research in 2015

One role of the Centre is to provide a gateway for researchers within the University to access the NeSI High Performance Computing facilities. Staff at the Centre engage with researchers to assess their needs, provide training, support and advice in order to help them achieve better research outcomes. The range of services and support offered by the Centre are listed below.

The report is structured as follows. The opening sections outline the broad range of work carried out in the Centre for eResearch (hereafter the Centre) during 2015. The second section details how the Centre is planning to meet the future needs of IT enabled research at the UoA. The final section of the report contains case studies taken from work undertaken using facilities and services available from the Centre or through the NeSI HPC facilities in 2015, followed by details of research outputs which have been produced using our resources over the last 12 months.

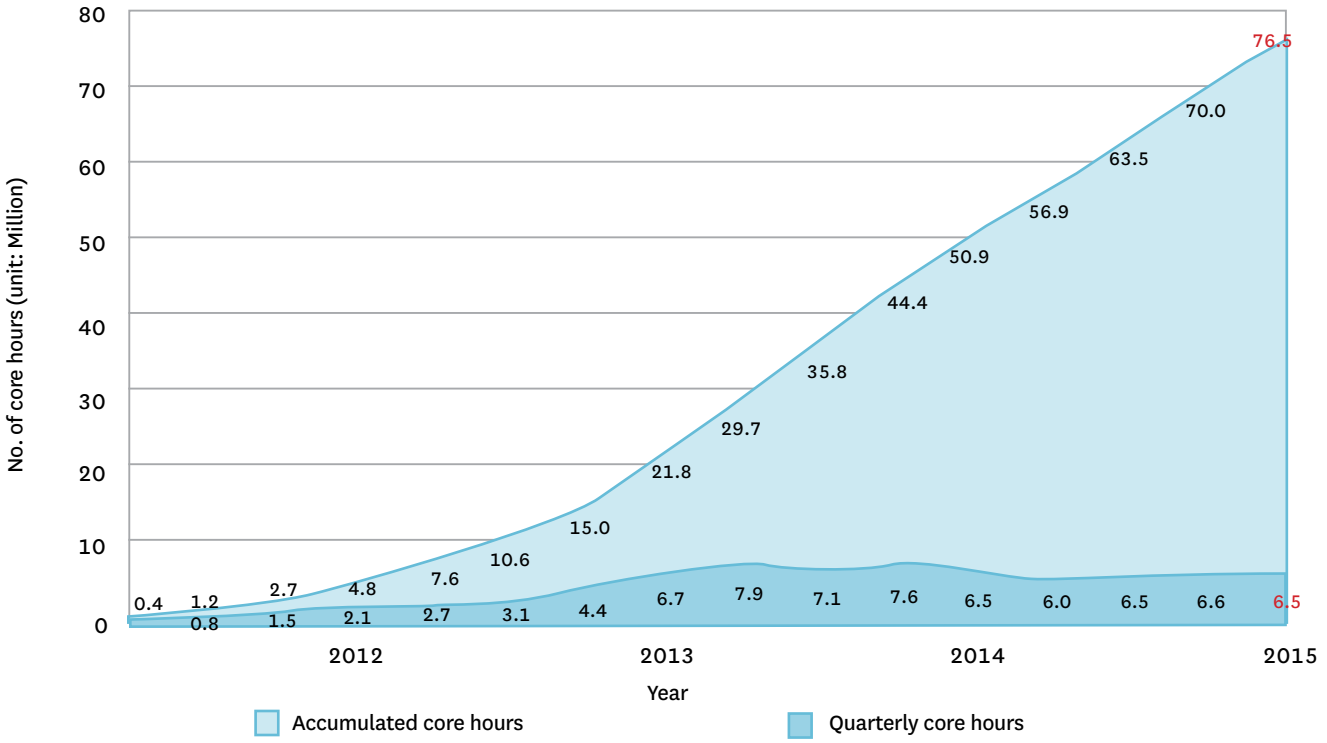
High Performance Computing (HPC) platform

The Centre has been involved with the provision of support for HPC services via the New Zealand eScience Infrastructure (NeSI) platform since 2011. The NeSI service provision contract with government was renegotiated over the past year in order to put in place a further four years funding. Under the new contract the Centre will continue to host the Auckland NeSI team and work closely with NeSI to invest hardware on behalf of the University into the national HPC platform. The extension of the NeSI initiative will allow researchers at the University of Auckland to access a range of HPC facilities.

The two graphs below provide details of the number of active researchers and live projects, and the number of core hours of compute used by researchers since 2012.

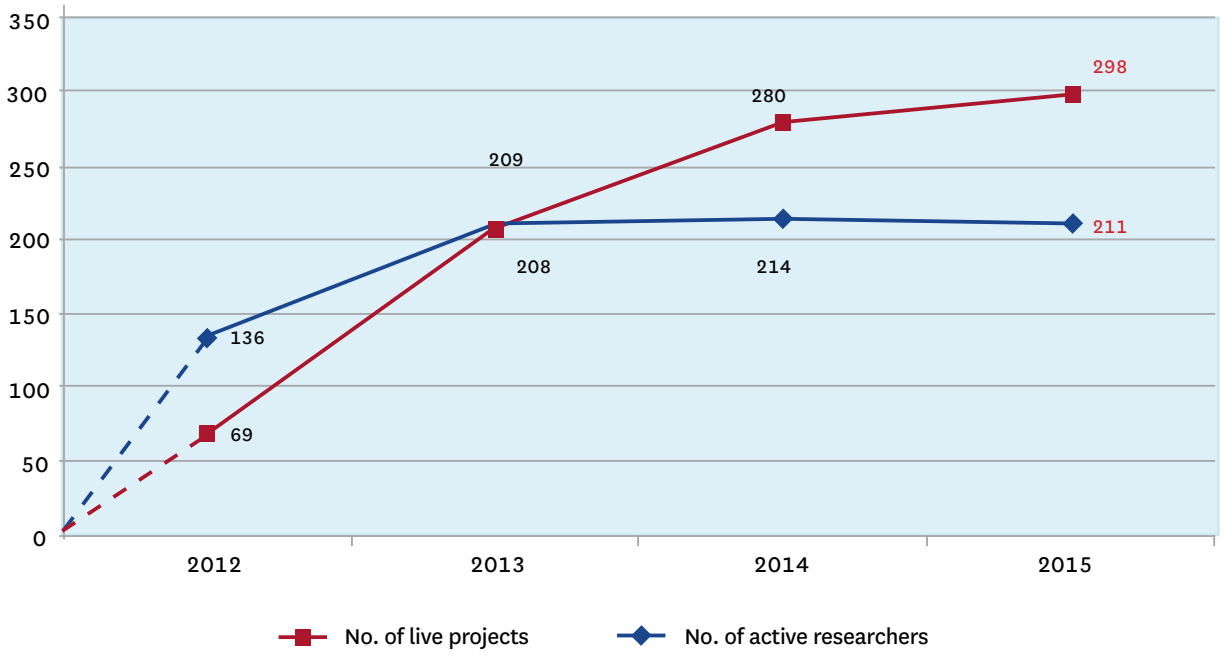
Number of compute core hours usage

Actual accumulated core hours recorded on 30 Nov is 74.7.
Forecast accumulated core hours to 31 Dec 2015 is 76.5.



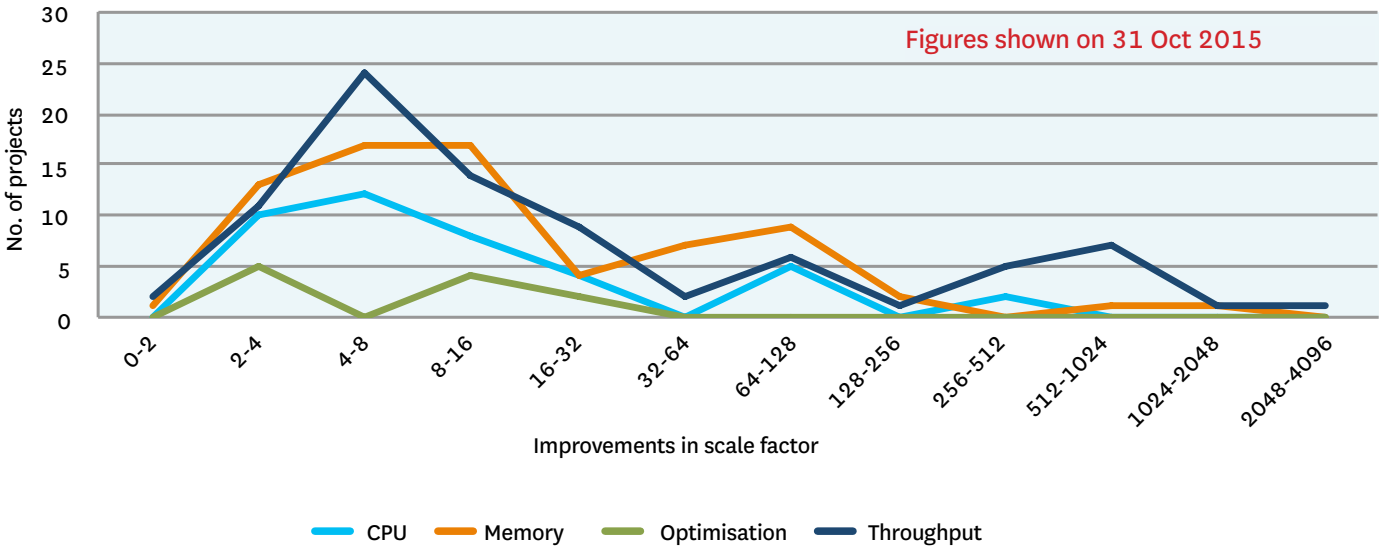
Number of active researchers and live projects

Figures shown on 30 Nov 15



Using the HPC facilities helps researchers to scale up their work – by analysing more data, performing more experiments, tackling bigger problems and so forth. The facilities help overcome common limiting factors such as the availability of memory and the number of processors available. The graph below shows the number of UoA research projects that the HPC support and the definition of the scaling factors.

Research project scale up in 2015



CPU:	Using multiple CPU cores concurrently running software applications across one or more computers.
Memory:	Enable researchers to work on large data set and detailed models on either a signle node or leverage memory across multiple cluster nodes.
Optimisation:	Optimise research programming codes and workflows to reduce the amount of time required to generate results, including program efficiency and extension to enable parallel processing.
Throughput:	Multiple similar simulations are performed test important key parameters in an underlying model which greatly improve research productivity.

Research Virtual Machines (VMs)

In collaboration with IT Services at the University of Auckland, the Centre provides support for the hosting of research-oriented virtual machines. Centre staff assist researchers to choose appropriate hardware, install and test software, document solutions and provide application support. ITS hosts the hardware in a managed VM Farm and provide the networking. Over the year, staff at the Centre worked closely with ITS to improve the delivery time frames for the establishment of virtual machines.

In 2015 staff at the Centre set up 12 computational virtual machines for the Faculty of Science, Faculty of Engineering, Faculty of Medical and Health Sciences and the Faculty of Business and Economics. While most of them serve a scientific purpose and enable researchers to run simulations for which their desktop environment is not suitable, the Centre has also supported Learning and Teaching by setting up VMs for the Data Science Practice course run by the Department of Statistics in semester 2. Case study 6 is based on the Research VM support.

Large scale visualisation

The Centre provides researcher access to a large visualisation data facility. Visualisation can be very helpful in many fields of research, from archaeology to zoology, from modelling the early universe to exploring the structure of a geological fault. Visualisation is powerful tool that helps researchers to understand, effectively capture and act on complex problems especially when dealing with huge volume of information.

The visualisation wall at the Centre was upgraded in 2015 to include six 4K resolution displays powered by a computer with three high end graphics cards. These synchronised displays allow researchers to investigate high resolution visual data using Windows compatible software. The large amount of memory on this machine (128 GB) provides researchers with the capacity to render large data sets that are unsuitable for standard desktop or research lab computers. This facility is showcased on the front cover and in case studies 3 and 5.

Research data management

Research data management infrastructure is seen as an essential part of research support within the University. As well as open and accessible research data and publications, increasingly funding bodies require research data management plans for the research projects they fund. The Centre for eResearch is working with the Library and ITS to develop the tools, strategies and an overall research data management framework to support researchers.

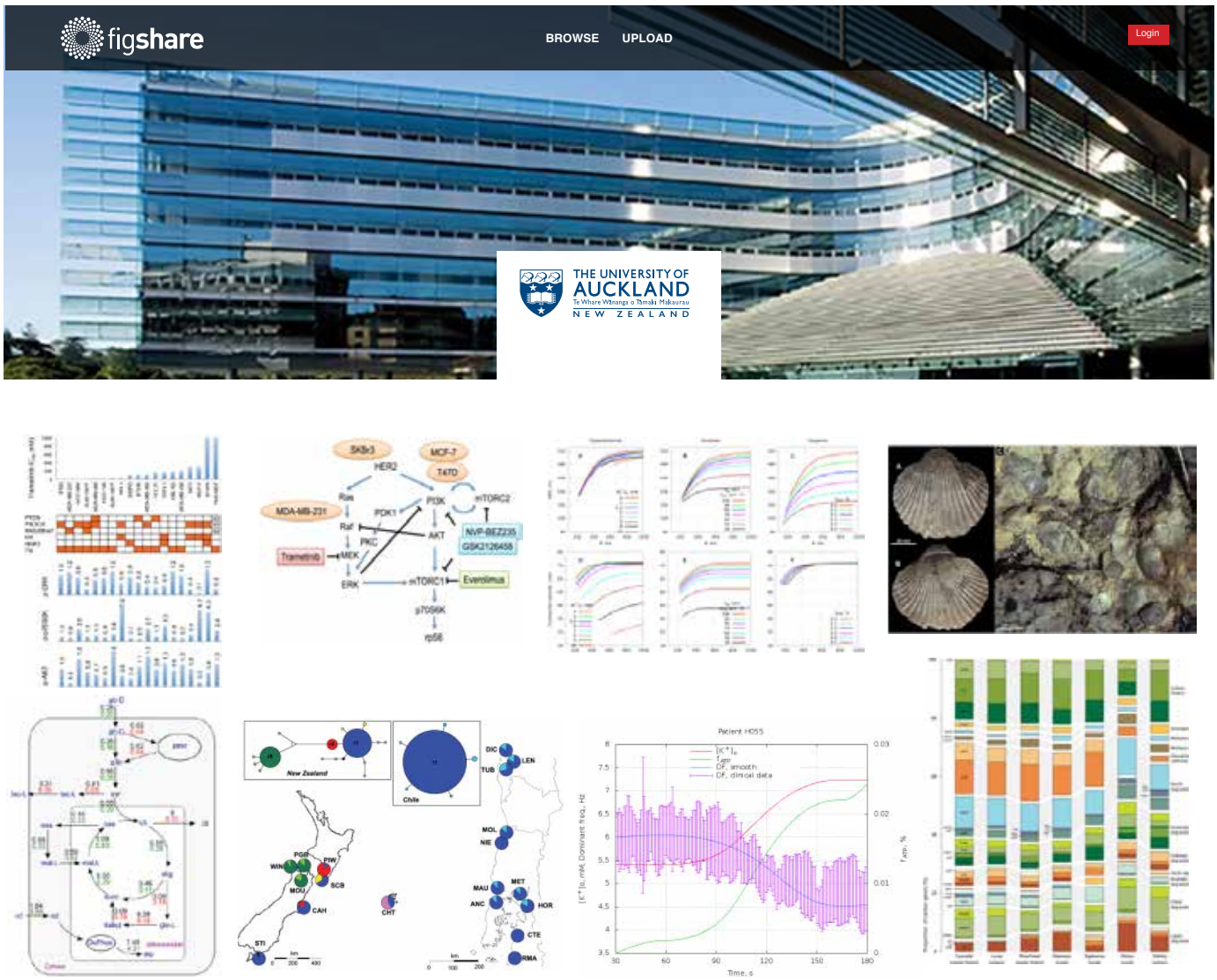
As part of the development of research data services at the University over the past year the Centre has partnered with the Library and the COMPASS research centre to find a suitable infrastructure for the storage, delivery,

discovery and continued reuse of the datasets. This project was funded by a Vice Chancellors Strategic Development Fund grant. This project is an opportunity to explore repository solutions and develop best practice exemplars in data management while also realising the practical goal of archiving at-risk datasets.

Over the past year the project team have been examining the use of Figshare as a suitable tool for this purpose. The Figshare service was launched in January 2015 and allows researchers to store, share and publish research data. It helps the research data to be accessible by storing Metadata alongside datasets. Additionally, every uploaded item receives a Digital Object identifier (DOI), which allows the data to be cited. If there are any ethical or copyright concerns about publishing a certain dataset, it is possible to publish the metadata associated with the dataset to help discoverability while sharing the data itself via a private channel through manual approval.

The current Figshare pilot project (See figure below) has over 1,000 university datasets research artefacts published with appropriate metadata for discovery.

In its final stage, the institutional version of Figshare will allow sharing of non-published datasets within a research group and with external collaborators. The work on this service is ongoing and we are collaborating with Figshare to improve user experience and overall usefulness. This service will facilitate the discovery, access and reuse of research data and helps research collaboration to enhance research impact and help researchers to comply with funding rules.



Enabling computationally intensive research

Informal weekly HackyHour drop-in session

Education and training

Over the past year training has been provided to staff and students across the University to enable them to use the facilities available through the Centre. The courses range from those for inexperienced compute users to more sophisticated software modelling assistance and were offered throughout the year. In 2015 the following courses were run at regular intervals throughout the year:

- Introduction to High Performance Computing on the NeSI Pan cluster.
- High Performance Computing with MATLAB and GPUs

In addition a number of new training initiatives were put into place in 2015. Staff implemented a HackyHour session in 2015. These are informal weekly 'drop-in' sessions for researchers to meet and collaborate with their peers on computational problems in their research. The Centre provides a staff member with support from PhD candidates at the Centre whose role it is to help with issues in coding, workflow design and data management. As the initiative becomes more popular, it is expected that there will be a regular pool of researchers experienced in eResearch which can offer additional support. For more information see http://uoa-eresearch.github.io/HackyHour. Centre staff also offer a course titled 'Big Data and High Performance Computing' as part of the Doctoral Skills Programme offered to Ph.D. students through the School of Graduate Studies. The course provides an overview of services available to researchers as well as best practices for working with high performance computing and research data. While there are similar efforts to introduce researchers to these concepts in some research groups, this is currently the only course of its kind being offered to all Ph.D. students at the University.

The figure below details all the training courses that the Centre has provided throughout 2014 and 2015.

In-experience HPC users

Introductory training

- What is high performance computing?
- Concept of parallel programming.
- Shared memory and distribution.
- Hardware and software resources .
- High Performance Computing with MATLAB and GPUs.
- Access, job submission and data back-ups.
- Best practice and security measure.

Job scheduler

SLURM workshop

- SLURM installation, extension and support.
- Resource management.
- Daemons.
- SLURM commands (job/step allocation, system information, accounting, scheduling and administration.
- C-groups and scheduling plugins.
- Examples and submitting jobs.

In-depth expert support

Project consultation

- Expert consultation for in-depth support needed, can be arranged through appointment with our consultants.

During 2015 a number of staff at the Centre became certified as Software Carpentry instructors (see https://software-carpentry.org/ for more information). This allows the Centre to formally offer training under the Software Carpentry brand which has been immensely popular with researchers as an introduction to digital research skills.

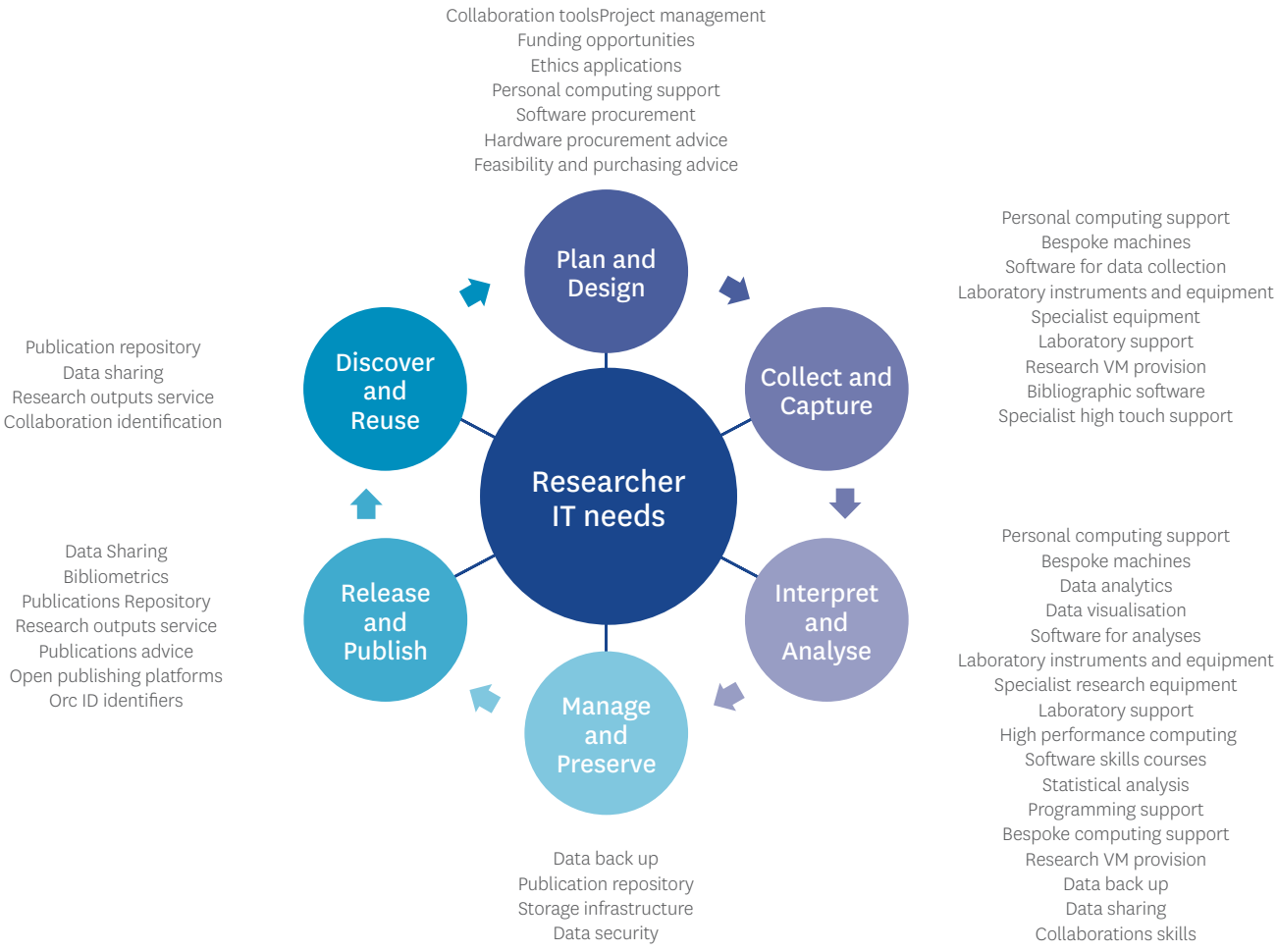
Looking to the future

The very nature of research is constantly testing and pushing the boundaries of knowledge, as it seeks to tackle more complex multidisciplinary problems. This means that IT support for research must be constantly pushing the boundaries of networking, data, computational, and collaboration support. It is becoming clear that a growing number of researcher's IT-related needs are not being met from standard desktop offerings at the University. While some of these needs are covered by the NeSI High Performance Computing (HPC) platforms, a growing number are not. HPC is very useful for those who can create or utilise its applications, but there is a long tail of researchers whose needs fall somewhere between HPC and desktop computing. Added into this mix are the critical needs for a raft of data support services, the drive towards data sharing and methods (open science), and better data management. All of these issues combine to create a need to rethink how IT support is delivered to researchers at the University.

To help understand how IT support for research is delivered at the University, staff at the Centre produced a report developed with information obtained through a series of interviews with various IT service providers within the University, from interactions with a range of university academics and support staff, and from global trends in how research is conducted. The diagram below shows the results of this investigation mapped onto a model of the research lifecycle.

To develop services to meet this changing and expanding demand the Centre has obtained funding for three projects. These projects will extend the Research VM and visualisation services available at the University and explore research data management services and implementation strategies. In addition, the Centre is working with academics elsewhere in the University to further develop IT training for researchers. The Centre is also awaiting confirmation of funding which will enable it to establish a single web portal coalescing all the services offered by ITS, Centre for eResearch, NeSI, Faculty IS and Libraries and Learning Services, and provide a staffed researcher IT advisory service. Each of these is discussed below.

Mapping Researcher IT needs at different stages of the research life cycle



Looking to the future

Research Virtual Machines (VMs)

Researchers often have computing needs that do not fit neatly into the NeSI High Performance Computing facility or the ITS general purpose VM clusters where 30-50 Virtual Machines (VMs) co-exist and share the resources of each individual physical server in the cluster. For example, research VMs may require 100s of gigabytes of memory dedicated to a single VM instance, or require Microsoft Windows Operating System (hence be unsuited to the NeSI HPC offering), or real-time interactivity with the software, or massive amounts of storage, or the installation and setup of a complicated set of application programs. Currently, researchers request access to Research VM resources through the Centre's support team.

There are, however, gaps in the current Research VM services where available bespoke solutions require significant compute, memory or data resources which exceed the existing capacity. To address these gaps the Centre has obtained funding for a project whose purpose is to deliver a computational service for researchers who need to move beyond the computational confines of their desktop.

The project outcomes will include:

- The design and implementation of a dedicated VM cluster to support specialised, research-focussed virtual machines, which provide virtualised support for (computationally aspirational) research application; and
- the creation of a set of service offerings and support structures for this service.

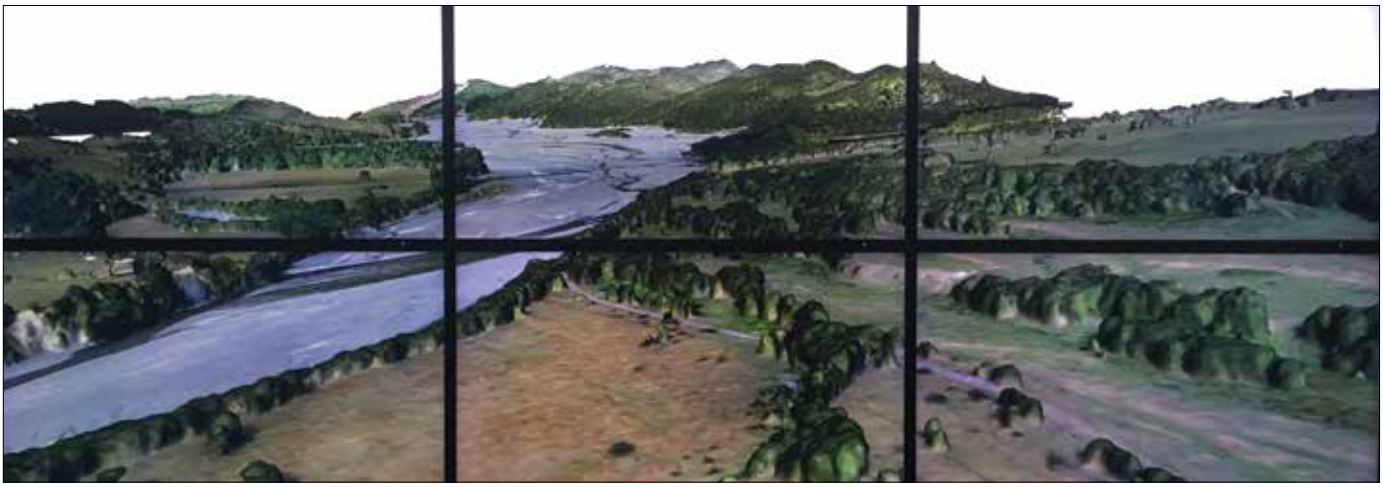
In the coming year the Centre is aiming to improve our service offerings by adding more hardware, hiring a full-time employee to support researchers on the virtual machines and to advertise the service more widely. This project will run until the end of 2016.

Visualisation

As noted earlier in this report, the Centre has some requisite hardware infrastructure already in place to help the University to address the rising needs for visualisation where massive, interactive or immersive display technologies could be leveraged. Further hardware investment is planned for early 2016 which will build on the existing infrastructure to create a fully functional and supported set of visualisation platforms and services including:

- Volumetric scientific visualisation (3D, stereo, large format, immersive tiled-wall display and workstation solutions).
- Massive data visualised information, using multiple screens in a shared space.
- Advice on graphical display creation and composition.
- Visual analytics support and development work.

The facility will be made available to all researchers within the University, and bookable through the Centre.



3D reconstruction of Tapueaeroa River. Refer to case study 3.

Research data management

Researchers and academics in the University produce vast amounts of data every day, generated through different processes and for different purposes. These data may include text, word documents, spreadsheets, Lab notes, transcript, video tapes, photos, images, slides, specimens, data files, models, algorithms etc.

Such data and information are of value to the University and the wider research community. It is crucial to manage these data to increase the research efficiency, integrity, dissemination of knowledge and validation of results.

Although there is a data management policy at the University, there is currently no coherent set of research data management services available for researchers to use. Typically researchers are unclear about how to manage their data, and if research data management is done it usually is in an ad-hoc manner. In addition, there is no data register, so the University currently does not know which data it holds, where and how it is stored.

Recently the Centre has obtained funding to conduct preliminary work around data management to feed into a longer term plan for the implementation of a research data management strategy and the development

of services for the University of Auckland. The purpose of this project is to focus on sizing and scoping a research data management infrastructure for the University. Scoping will be carried out by investigating infrastructures in use by comparable institutions, as well as working directly with a number of research groups on actual use cases, recording their work-flow, and conducting an analysis of the demand for services not yet in place. This will include prototyping various solutions, in order to see how they would fit the use cases, and provide incentives to research groups to work with us.

The project will continue the work on the 'Figshare' pilot project (mentioned earlier in this report): decide on a technology to use for production (either Figshare or a competing product/service) and build out that service for adoption by a wider community in preparation of a full-scale production deployment, enabling the publication of research datasets for a wider group of the University researchers.

The experiences gathered in working with our researchers will be used to identify other, complimentary and possibly interconnected data services on order to develop research data capability at the University of Auckland.

The services developed are likely to include a Dropbox-like service for sharing & remote syncing of research data, and the provision of access to a scratch file system for research projects with high-volume data.

The project will also develop resources for researchers and students on how to manage research data and create data management plans, and develop training material for staff and students.

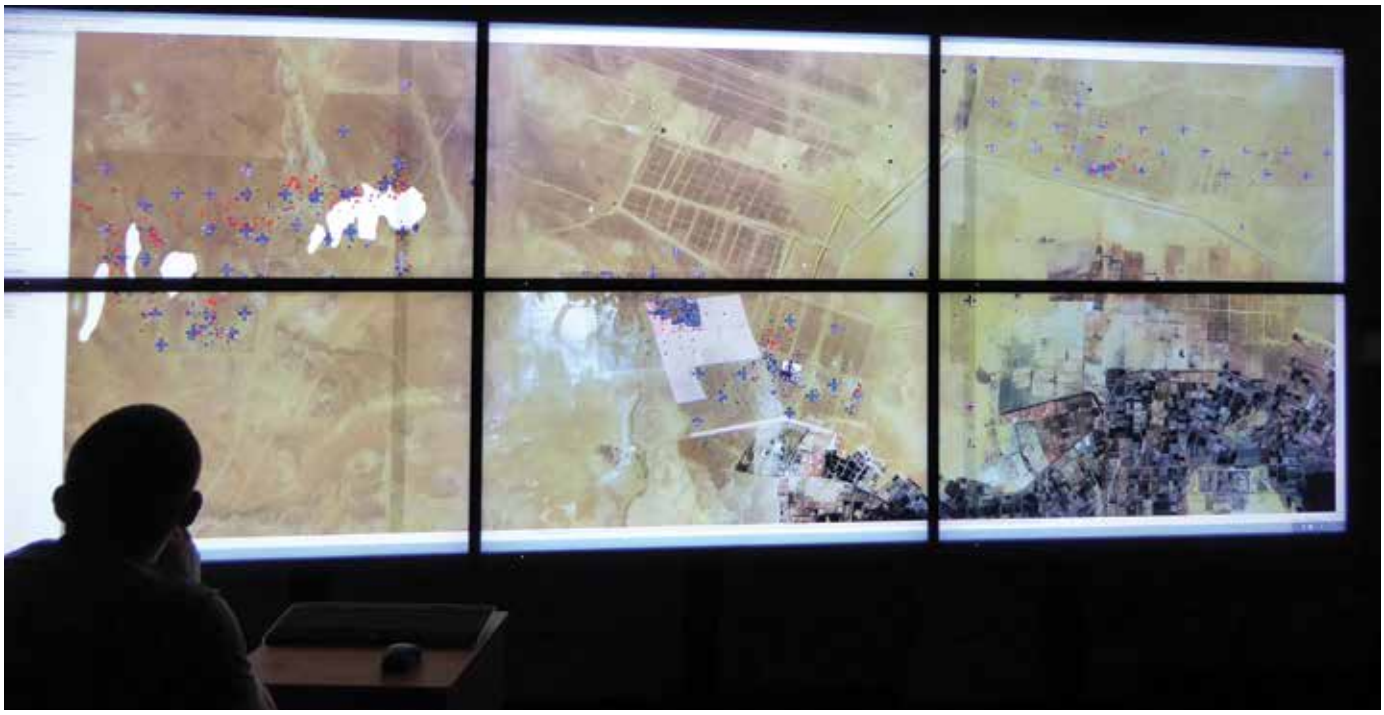
Lastly, the project will also deliver a research data management strategy for the University, to guide future developments in this area.

Education and training

Staff at the Centre, along with other interested staff elsewhere in the University are examining ways to enhance the IT skills of researchers to enable them to engage effectively in computationally intensive research. There are a number of groups within the University which provide training courses for staff and Doctoral researchers such as CLeaR for teaching and research development and POD for capability development. For the basic software programming skills required for research IT upskilling, however, there is no consistent and cohesive strategy to raise the level of digital capability. As a consequence many gaps still exist where core HPC skills are not being taught to students. For example, there are no introductory level programming courses for researchers nor a single place that the researchers can learn about available courses at the University. In collaboration with others, the Centre aims to provide scheduled training to researchers and doctoral students:

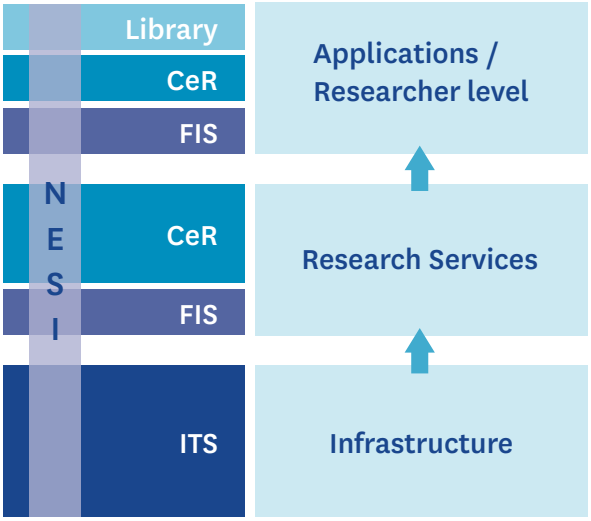
- Extended Software Carpentry courses.
- Specialised training in scientific computing, scripting.
- Doctoral Skills programme.
- Possibly designed course as required papers in scientific computing, eScience, high performance computing as part of the University degree structure (perhaps at the honours level).

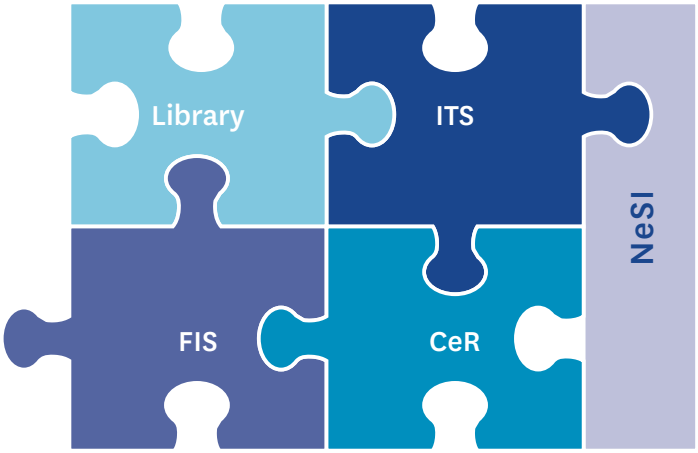
The provision of these extended training resources will ensure that the staff and students at the University of Auckland have the IT skills they need to undertake computationally-intensive cutting edge research.



Distribution of artefacts in the Fayum, Egypt. Refer to case study 8.

Looking to the future





Creating a service catalogue for the University

University of Auckland researchers and academics currently have no single place where they can find information about which IT support and services are available to them to enable them to undertake computationally intensive research. Given that most fields of research are experiencing significant growth in their computing and data support needs, due to the availability of increasingly larger and richer data sources, and the growth of computational analysis, simulation and modelling, easily accessible information about what tools, service and support are available to staff and students is a high priority.

To address this gap staff at the Centre are scoping, and have applied for funding for a project which would establish a single web presence coalescing all the services offered by ITS, Centre for e Research, NeSI, Faculty IS and Libraries and Learning Services, and a staffed researcher IT advisory service.

The project will deliver the following:

- A Researcher IT Services portal. This will organise and provide supporting resources for the research IT services as the front page of a web portal that then provides links to the services and support on offer. All service providers have a suitable landing page for the services they offer and this will link back to the portal described above so that researchers can find other services. A thorough review of related roles and responsibilities, service entitlements (what researchers can expect), will be conducted. Service maturity will be lifted where needed.
- A research advisory role. This role will act as an advice centre for researchers, help connect them with the services available to coordinate service provision from the various providers involved, and to offer customisation support where it is needed.

Provision of these services and support will assist in providing an infrastructure of the highest quality possible to support teaching, learning, and research at the University of Auckland.

CASE STUDIES

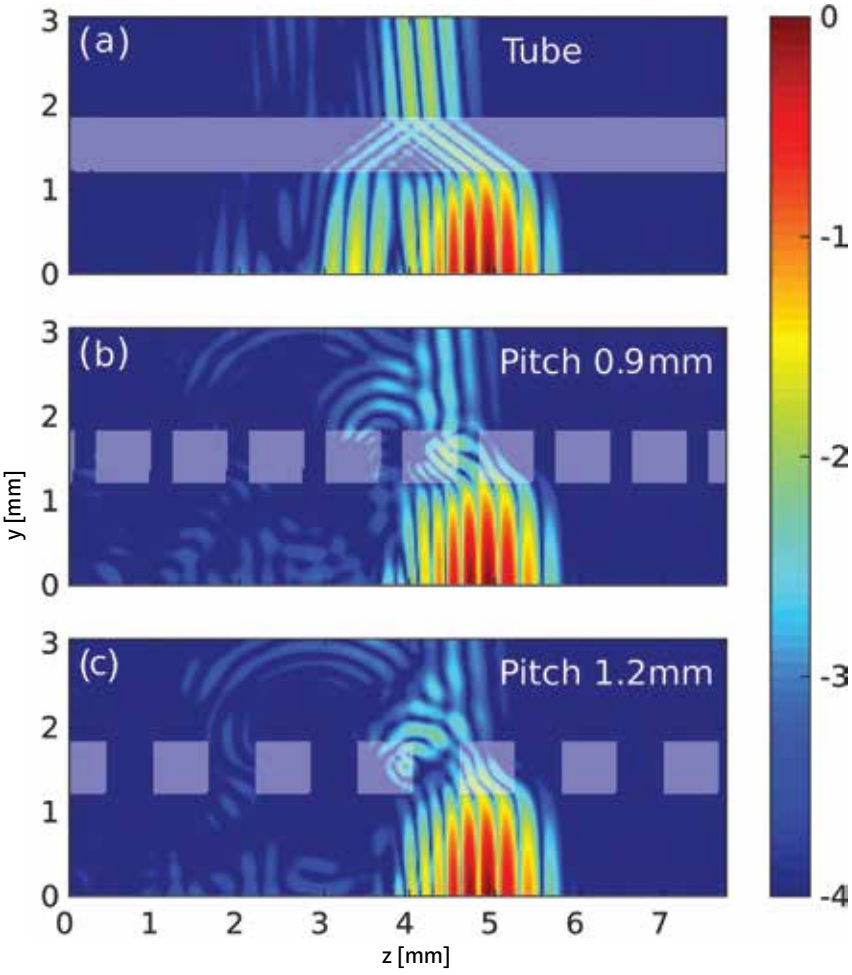
Development of novel waveguides in the terahertz (THz) region

Dominik Vogt, PhD candidate, Dr Jessienta Anthony, Research Fellow, Assoc Prof Rainer Leonhardt, Dodd-Walls Centre for Photonic and Quantum Technologies, Department of Physics

Terahertz science

Terahertz (THz) radiation, often referred to the frequency range from 0.1 to 10 THz, is the focus of an active and fast growing research community. This frequency range, located in the electromagnetic spectrum between the microwave band and infrared band, was known as the "THz-gap" until the late 1980's.

A lack of available coherent sources and detectors rendered this frequency range inaccessible. The breakthrough was achieved with the generation of THz-radiation by means of femtosecond laser pulses in the visible or near-infrared range. The generation is usually achieved by either photo-conductive antennas or nonlinear crystals: while a biased photo-conductive antenna emits THz-radiation due to a time dependent photo-current induced by a femtosecond laser pulse, a nonlinear crystal hit by a femtosecond pulse generates a THz-pulse by difference frequency generation. Further development of THz-detectors and THz-sources like the introduction of a quantum cascade laser suitable for Terahertz frequencies provided the access to a vast variety of THz applications. In the past two decades a Terahertz technology in various fields like information and communications technology, biology and medical sciences, non-destructive evaluation and homeland security were established. Moreover, Terahertz radiation is suitable to study fundamental processes present in this frequency range like e.g. phonon excitation as well as inter-band transitions in condensed matter and rotational transitions of molecules in gases.



FDTD simulation of a THz pulse propagating in a) a dielectric tube waveguide and b)-c) a 3D-printed dielectric helical waveguide with different pitches.

Terahertz waveguides

However, to take advantage of these promising applications and to realise bench top THz devices, waveguides capable of guiding broadband THz radiation with low loss and low dispersion are essential. A first approach to utilise the well-known waveguides from microwave or near-infrared systems, namely circular/rectangular metallic waveguides and dielectric fibers, proved to be impractical. Novel waveguide designs were necessary to overcome the increasing ohmic losses at metal surfaces and the high dielectric absorption in the Terahertz frequency range. Although extensive research over the past ten years led to a number of new waveguide designs and materials, there is still a high demand on further improvements and investigations.

The intention of our work is to contribute to the development of novel single-mode waveguides with low loss and low dispersion. The picture shows the electric field energy density of a THz pulse propagating through three different waveguides: a dielectric tube, and two different dielectric helices. The THz pulse is propagating in positive z-direction, and the grey areas are the dielectric material. The centre axis of the waveguide is just below the x-axis of each sub-figure. The novel waveguide designs are experimentally investigated with a THz time-domain spectroscopy setup based on photo-conductive antennas. Moreover, a comprehensive numerical study based on the finite-difference time domain (FDTD) method is performed to support the measurements. The basic idea behind any FDTD method is to approximate the continuous space derivatives and time derivatives of the time dependent Maxwell's equation with discrete finite-differences. This is necessary as the boundary conditions are so complicated that there is no analytical solution. The time-domain method, compared to a frequency-domain method, provides the advantage that we can investigate the broadband frequency response of our waveguides with only a single simulation. All FDTD simulations performed in this work are done with the Unix-based open-source software "MIT Electromagnetic Equation Propagation" (MEEP). It is important to note that our simulations are performed in 3D as our waveguides do not have a uniform cross-section and we therefore cannot employ the 'usual' software packages used for more traditional waveguides.

The extensive numerical study of the waveguides is indispensable for the development of high performance THz waveguides. The simulations provide detailed insight into the guidance mechanism of the waveguides and facilitate the design process for the most efficient THz waveguides as different configurations can be compared easily.

By using the Pan High Performance Computing resource, it enabled our simulations to gain detailed insight into the guidance mechanism of the waveguides and facilitate the design process for the most efficient THz waveguides as different configurations can be compared easily.

3D FDTD simulations of THz waveguides on the NeSI Pan cluster

The New Zealand eScience Infrastructure (NeSI) Pan cluster provides us the only possibility to perform our simulations with the required resolution. Our 3D FDTD simulations involve extremely time consuming calculations and have such a high memory demand that implementation on a normal desktop computer is not feasible.

A typical three dimensional simulation for a 100mm long waveguide is running on up to a 100 cores and requires approximately 400GB of memory. A typical processing time for such a job is about 30 hours. Moreover, the cluster allows us to investigate multiple waveguide designs simultaneously which provides a great ease for our research. As can be seen in the picture, a slightly different pitch for the helix can result in quite different losses. We have also numerically investigated metal helices with and without a dielectric coating using the Pan cluster.

Results and future work

Recent work facilitated by the NeSI Pan cluster includes our investigation of broadband guidance of THz radiation in both metallic and 3D printed dielectric helical waveguides. Each type of waveguide has been presented at the annual International Conference on Infrared, Millimeter, and Terahertz Waves (IRMMW-THz) in Tucson (USA) and Hong Kong (CHN). The work is also published in the corresponding conference proceedings. Future work will concentrate on further studies of these waveguides and the development of sophisticated high performance waveguides for the THz frequency band and their application.

Computational investigation of catalysis mechanisms for polyurethane synthesis

Dr. Tilo Soehnel[1], Senior Lecturer, Neil Edmonds[2], Senior Lecturer, Ransi Devendra[3], PhD candidate. [1&3] School of Chemical Sciences, [2] Department of Mechanical Engineering

Introduction

Polyurethanes are polymers made with a series of urethane linkages formed as a result of reaction between a polyisocyanate and a polyol[1]. Catalysis is an important part of polyurethane technology as it promotes the reaction between an isocyanate and an alcohol group to give the urethane linkage. Depending on the ratio of isocyanate to alcohol the final polymer will have different end groups. The products with isocyanate end groups are called pre-polymers and they are intermediates used in some polyurethane application. Catalysts used in pre-polymer preparation also play a role in the performance of the pre-polymer system in final applications. However the present knowledge on polyurethane catalysis cannot explain all behaviours of polyurethane systems. In this investigation mechanisms of various catalysts were investigated.

A complete understanding of the reaction mechanism allows for better control of the reaction at each stage. Experimental methods for investigating reaction mechanisms have been investigated by many researches to elucidate each step of the reaction. However, these investigations are mainly based on analyses of products formed in a chemical reaction using varying concentrations of reactants without considering the intermediates that are formed. This procedure can miss some of the important data related to the reaction and provide false leads on the actual mechanism. Computational techniques based on quantum mechanical methods can give information related to interactions between reactants and intermediates formed in a chemical reaction. These also have the ability to investigate specific interactions between selected functional groups to give a better insight as to intermediates formed. The most useful outcome is the ability to visualize the interactions, this gives an opportunity to test possible reaction pathways involved in reactions.

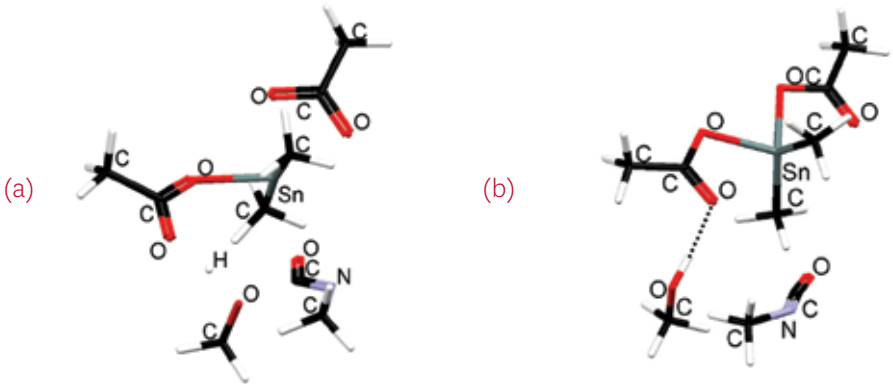


Figure 2: Three molecular interaction: (a) van der waals complex (b) transition state.

NeSI Pan cluster

In this project, the quantum chemistry software package Gaussian 09 available on the NeSI Pan cluster was used for computational modelling to investigate catalysis reaction pathways for urethane formation using electronic structure theory. In these investigations, DFT and *ab-initio* computational methods were used. Since it is possible to carry out several jobs at any given time, many different experiment models were simulated to relate catalysis of urethane formation. This feature gave the ability to achieve results in a fraction of the time compared to performing the investigation on a desktop computer.

Investigation into urethane catalysis

Organotin carboxylates are one of the common types of catalyst in synthesis of polyurethane used industrially. These catalysts are used in the synthesis of polyurethanes based on both aliphatic and aromatic isocyanates. It is reported in literature[2] that organotin carboxylate interact with alcohol to give an organotin alkoxide which becomes the dominant catalyst for urethane formation. It is also believed that the same mechanism is true for both aliphatic and aromatic isocyanates. However, computational and experimental model compounds studied showed that organotin carboxylates do not undergo alkoxide formation by interacting with alcohol. A result of the computer simulation is shown in Figure1; this simulation does not show a transition state that would indicate the formation of an organotin alkoxide intermediate. Modelling, however, shown that the urethane formation takes place through a triple molecular interaction between organotin carboxylate, alcohol and the isocyanate[3] as shown in Figure 2.

These investigations were performed in a non-polar medium and showed that urethane formation for aliphatic isocyanates is different to that for aromatic isocyanates. For aliphatic isocyanates, the carboxylic ligand found in organotin carboxylate catalyst contributes to catalysis and for aromatic isocyanates it does not contribute to catalysis. The computational findings were supported by experimental work. Based on this data it was possible to propose mechanisms for urethane formation for aliphatic and aromatic systems in a non-polar

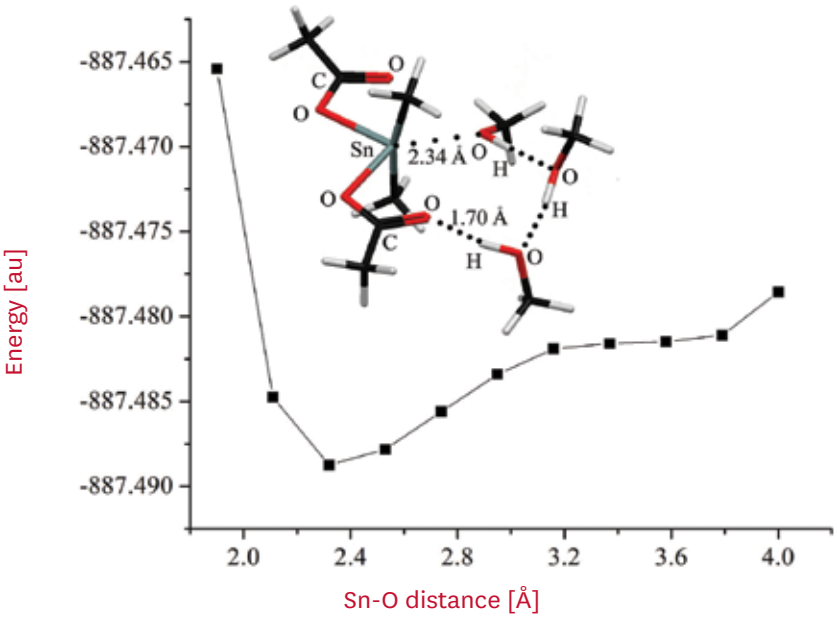


Figure 1: Computational modelling of the alcoholysis step of the reaction of Dimethyltin diacetate (DMTDA) with three methyl alcohol molecules.

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4. Devendra, R.; Edmonds, N. R.; Söhnel, T. *RSC Advances 2015, 5*, 48935.
5. Devendra, R.; Edmonds, N. R.; Söhnel, T. *Journal of Molecular Catalysis A: Chemical* 2014, *395*, 72.

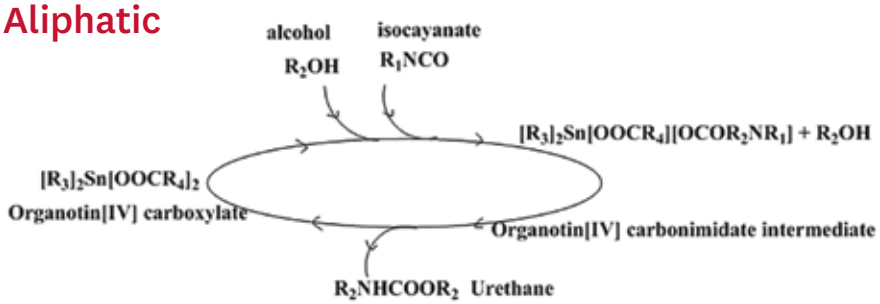
medium. Schemes 1 and 2 show the proposed mechanisms for organotin carboxylate catalysed urethane formation for aliphatic and aromatic isocyanates. The findings were implemented in aliphatic, a pre-polymer manufacturing industry, to give coating systems with improved their performance. The products were marketed worldwide under a world leading surface coating brand.

Computational methods were also used to study interactions in different solvent environments and relate them to experimental results[4] as well as understand specific interactions between organotin alkoxide and phenyl isocyanate that were reported in literature[5]. Investigations were also carried out for other metal catalysts such as titanium and zinc in urethane formation. The final aim of the investigation is to develop a tin free catalyst for aliphatic moisture cure polyurethane pre-polymer systems.

Student training

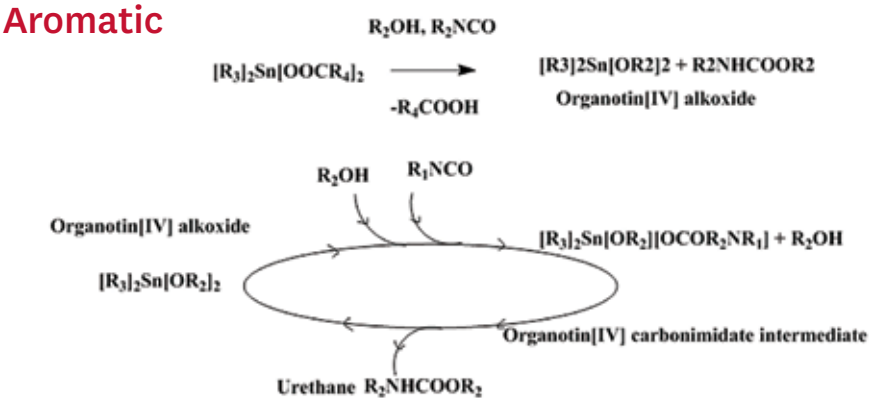
The project also has trained many undergraduates in the application of computational methods for understanding catalysis mechanisms for urethane formation. This will encourage students to select areas such as computational chemistry in their future studies.

Aliphatic



Scheme 1: Mechanism for urethane formation using aliphatic isocyanate with organotin carboxylate catalyst in a non-polar medium.

Aromatic



Scheme 2: Mechanism for urethane formation using aromatic isocyanate with organotin carboxylate catalyst in a non-polar medium.

Processing structure-from-motion photogrammetry on the cluster

Dr Jon Tunnicliffe, Lecturer, School of Environment

Introduction and research

The nature of earth surface processes analyses and simulation has changed dramatically in recent years, owing mainly to new capabilities in the acquisition and processing of high-resolution point cloud data. The availability of new photogrammetric "bundle adjustment" methods has had a notable impact on how we can represent and model the landscape. Using a highly overlapping sequence of photos from a ground-based or aerially-mounted camera, it is now possible to generate very accurate, high resolution topographic models. The photogrammetric technique is computationally quite demanding, and thus for relatively large study areas (thus many photos), generating point cloud models moves beyond the realm of desktop computing.

In the following work, we used a 24 MP camera mounted on an unmanned aerial vehicle (UAV) to acquire more than 5,000 photos of the braided Tapuaeroa River in East Cape New Zealand. The catchment is noted for its very high rates of sediment production through landsliding and mass wasting, resulting in highly dynamic river systems. Morphologic adjustments such as channel avulsions and bifurcation, and bar erosion occur quite frequently. The aim in developing a high resolution model of the river was twofold: (1) to provide a basis for numerical simulation of river hydrodynamics and these morphologic processes, and (2) to generate a baseline model against which we can quantitatively compare future change. The dataset will have a number of important applications in catchment management, landuse planning, habitat assessment, and improved understanding of river response to long-term sedimentary disturbance.

Figure 1 - An example of point cloud data on the Tapuaeroa River. The point density achieved was close to 25 pts/m2, along a 12.5 km transect of valley floor. Fine details of river morphology are resolved, such as abandoned channels and bar-top sheets of fine sediments. Even grain roughness can be resolved, in coarser sediments.

Figure 2 - Merged point cloud, representing five surveys, with over 160 million data points, generated using 2,700 photos.

What was done on the Pan cluster and how it helped

We used the NeSI Pan cluster to process our aerial photos using Agisoft Photoscan, a structure-from-motion software package that features fine-level task distribution, such that processing tasks can be passed out to hundreds of cores. The Centre for eResearch helped to develop this parallel workflow, reducing the working time for a large survey such as this from many weeks to a few days. We generated a point cloud for the full valley floor, with 30 ground-control points, and many tens of millions of topographic points. Gridding, manipulating and clipping portions of the resulting point cloud requires significant RAM resources, which, again, is not easily handled on a desktop computer. The Centre for eResearch's visualisation facility with its large tile-wall display provided an impressive view of the point cloud in a single display frame. Once the topographic surface was subdivided into tiles, it could again be handled by desktop machines.

What's next?

We will be flying over the Tapuaeroa River in early 2016, with the aim of developing a 'difference map'. By subtracting the 2015 model surface from this later surface, it is possible to develop a highly detailed, quantitative picture of morphologic change in the river system. We have developed a research group with students and researchers from the University of Auckland and Massey University's Institute of Agriculture & Environment (Ian Fuller) to leverage the full analytical potential of this technique, and expand our survey coverage. The work will be featured at the upcoming 11th International Symposium on Ecohydraulics (2016) in Melbourne. This project forms the basis of a series of papers that will be submitted to Earth Surface Processes and Landforms and Geomorphology.

Anya Leenman has been working toward completion of her MSc in Geography, with her thesis 'Interpreting the Changing Morphology of Tributary-junction Alluvial Fans in Response to Catchment Wide Disturbance' due to be completed by March, 2016. Anya has been able to reconstruct the decadal-scale dynamics of tributary fans in this valley, based on very high resolution models of the alluvial fans in tributaries that join the Tapuaeroa River.

Homodynamics in the microcirculation

Tet Chuan Lee, PhD candidate, Dr Richard John Clarke, Supervisor, Dr David Scott Long, Co-supervisor, Department of Engineering Science

Overview

The microcirculation is the network of smallest blood vessels that deliver nutrients to the body's organs and tissues. The walls of these blood vessels (and in fact the majority of blood vessels) are coated in a structure known as the Endothelial Glycocalyx Layer (EGL). It is a porous brush-like layer that consists of many different components. The EGL is believed to serve a number of important physiological functions including the protection of the vessel walls from potentially harmful levels of fluid shear stress from the blood and as a transducer of mechanical stress from the vessel lumen. It is also hypothesised that it may play an important role in regulating vessel permeability and in the body's inflammatory response. As such, it has received a great deal of research interest in recent years.

One of the difficulties in conducting research on the EGL is that it is extremely sensitive to changes in its environment. Some of the components that make up the EGL exist in a dynamic equilibrium with blood flow and so in-vitro experiments may degrade the EGL. In-vivo measurements are also extremely challenging, in part due to the small sizes involved in the microcirculation. As such, this work seeks to develop computational models that will enable us to better understand the EGL and its roles in the microcirculation.

Previous models have generally assumed an idealised geometry such as a vessel with a circular cross-section or have worked in two dimensions. A physiologically realistic microvessel, however, is unlikely to be circular. Instead, it will have an undulating shape due to the presence of the endothelial cells that make up its surface. These endothelial cells will protrude into the vessel due to their cell nuclei. The EGL itself is also believed to have a non-uniform distribution along the vessel surface. In fact, it has been hypothesised that the EGL redistributes to the cell-cell junctions where the endothelial cell height is lowest in order to minimise the shear stress experienced at the surface of the vessel.

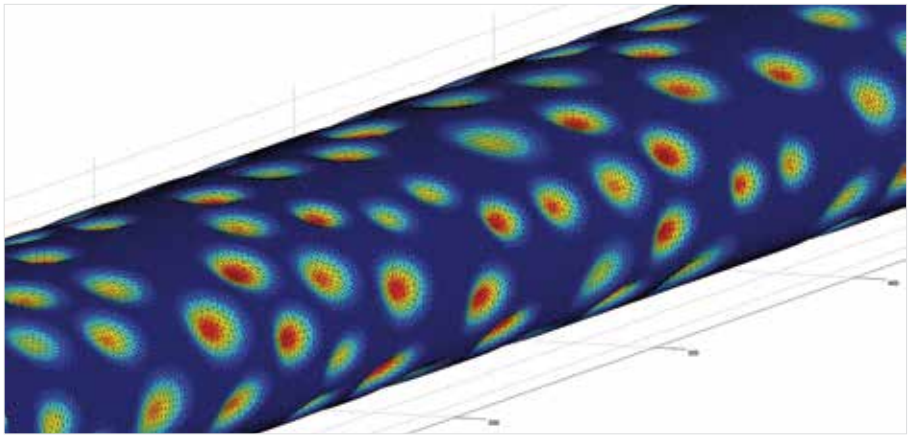


Figure 1 – A computational mesh of a microvessel used in these simulations. The undulating shape is due to the endothelial cells that make up its surface (colour rendering indicates height).

In order to investigate this, a computation model for an EGL lined microvessel was developed using the Boundary Element Method. In this model, the EGL was treated using volume-average Biphasic Mixture Theory equations. In Biphasic Mixture Theory, the EGL is made up of two components, the solid fraction, which is taken to be the glycocalyx and a fluid fraction which is the blood that flows through the porous EGL. The model was developed to allow the simulation of an arbitrary vessel shape and EGL distribution in three dimensions.

A more physiologically realistic vessel geometry was then constructed (Figure 1), informed by Confocal Microscopy Images of a post-capillary venule. The flow through the vessel was then simulated with different prescribed distributions of the EGL. This allowed us to compare vessels with an EGL that is uniformly distributed and one where it has been redistributed to the cell-cell junctions and found that the redistribution of the EGL does indeed appear to reduce the shear stress experienced by the vessel walls as seen in Figure 2.

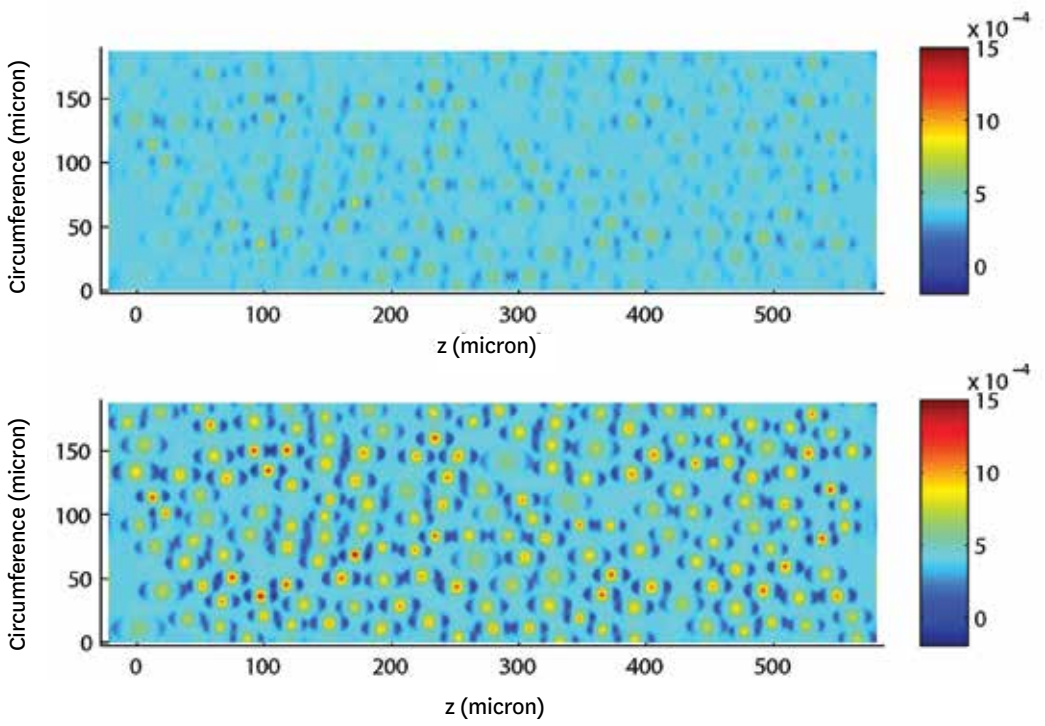


Figure 2 – Results from a simulation comparing a redistributed EGL (top) to one with a uniform distribution (bottom). As can be seen from the plots, the redistributed EGL experiences much less fluid shear stress than the one with a uniformly distributed EGL.

Computational resources

In order to perform simulations on the physiologically realistic vessel that has been created, a mesh fine enough to resolve the endothelial cells that make up its shape is required. As the Boundary Element Method (BEM) which was used to create the computational model produces densely filled matrices, the memory requirements to undertake these simulations was substantial. The Pan cluster provides access to the computational resources that are necessary to be able to undertake simulations of a microvessel with a geometry of this complexity.

The BEM leads itself to parallelisation as each entry in matrix it produces is independent of the other entries. As such, these simulations are particularly suited to being performed on a computational cluster such as the Pan cluster. By distributing the matrix onto multiple nodes and then constructing each part of the matrix locally, the construction of the matrix is greatly sped up. This matrix is then solved using PETSc which allows the interative solution of distributed linear systems using MPI communication.

Without the computational resources provided by the Pan cluster, it would not be possible undertake these simulations due to the memory constraints of a desktop computer. Furthermore, the time taken to perform these simulations would be much greater, potentially up to hundreds of times longer. Finally, the Pan cluster allowed a greater number of simulations to be undertaken which allowed more comparisons to be made between the different distributions of the EGL.

Geographic and temporal information retrieval on massive document collections

Dr Benjamin Adams, Research Fellow, Department of Computer Science

Overview

The project aims to discover the relationships between the topics, places, and events that can be found in a very large document corpus. By understanding these knowledge relationships we build new kinds of exploratory ad hoc search systems that use the contexts of geography and time to help people search and discover otherwise hidden information using interactive map and timeline based search interfaces.

Frankenplace

Frankenplace is an interactive thematic map search engine that uses geographic context as a means to discover, organise, and interactively visualise the documents related to a search query. The current version of Frankenplace indexes over 5 million articles from the English version of Wikipedia and online social media blog entries.

Cartographers have known for centuries the power of organising thematic information by geographic context and visualizing it on a map. A thematic map allows you to understand the spatial dynamics of a topic within a structure that has strong reference points in human experience - myriad places and regions around the world. At the same time a thematic map can show us important relationships between these places because they are similar or differ with respect to some property of interest.

Frankenplace is also an ad hoc search engine designed to help users find relevant documents that match a query. By visualizing the interaction between the thematic and geographic content of documents, users can use the map interface to quickly explore through hundreds or thousands documents that match their query while bringing their background knowledge about geography to bear on their interpretation of the results. Likewise, unexpected patterns that arise on the map provide opportunities to learn new things about how a topic of interest relates to places.

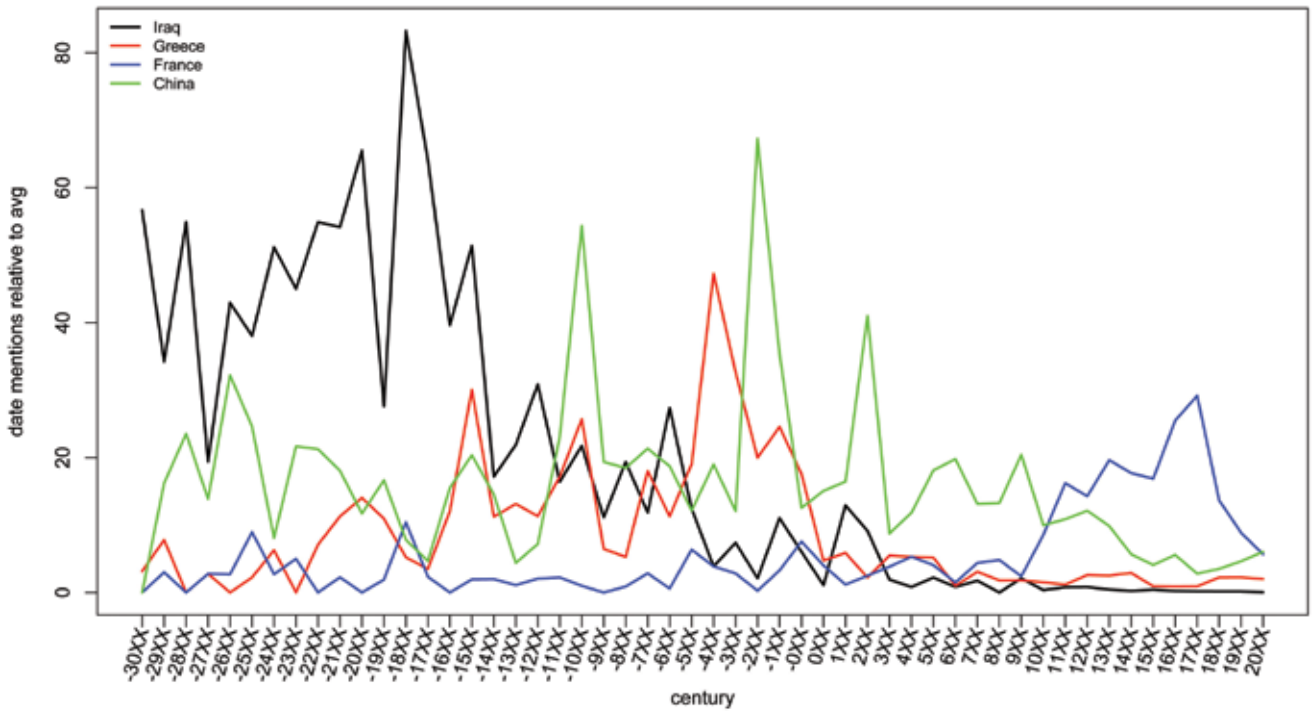


Figure 1. This chart shows the relative number of references to dates by century for China, France, Iraq, and Greece. These results come from over 68 million references mined out of the English Wikipedia.

Figure 2. The Frankenplace tool running on 64K screens in the Centre for eResearch visualisation facility.

How are times and places related?

There is demonstrated need for knowledge systems that can organize large document collections through space and time (e.g., for the digital humanities). However, little is actually known about the statistics of how places and times are written about in these document collections. We are currently using the Pan cluster to mine these relationships. Our goal is that these insights will lead to more useful schemas to spatially and temporally organize and present search results in interactive information retrieval systems.

How High Performance Computing has helped

The NeSI High Performance Computing (HPC) facilities have been a critical resource in our research. It has allowed us to build the indices for Frankenplace orders of magnitude faster than we would have been able to otherwise. We were able to pre-process millions of documents in parallel to clean the text to remove irrelevant HTML and other noise and run natural language processing code to tag place names and dates. In order to build the indices we also needed to perform millions of spatial intersection operations to match text paragraphs in these documents to cells on a discrete global grid. Here again the ability to run these operations in parallel has been a tremendous help in allowing us to test, improve, and re-run our algorithms. In future work, we plan to use the advanced GPU facilities on the cluster to create better geographic and temporal taggers using deep neural networks.

The role of visualisation facility

In addition to the HPC infrastructure that NeSI provides, the Centre for eResearch also offered the advanced visualisation facility with an entirely new avenue of research, exploring the impact of large collaborative and interactive visualisation for map-based search. The ability to see search results for the entire world at high granularity has led to new opportunities to evaluate the role of human computer interaction in our research.

Quality of care and outcomes in children with cleft lip and/or palate

Louise Ayrey, Project Manager, PhD candidate, Department of Paediatrics - Child and Youth Health

Objectives

This study has two main objectives in relation to cleft lip and palate (CLP). Firstly it will investigate the health care delivery pathways from the time of diagnosis to the primary surgery for children with a cleft lip and/or palate and their families. This will ensure that CLP patients are receiving health delivery to the standard expected and required. Secondly it will provide the first consistently collected outcome data in relation to cleft lip and palate in New Zealand, including surgical outcomes, speech, dental care and importantly quality of life. This study will be compared to data from the UK to determine how cleft lip and palate patients in New Zealand fare compared to their contemporaries worldwide. This will allow any deficiencies to be identified and processes put in place to ensure improved outcomes in the future Cleft lip and/or palate (CLP) is a most common birth defect affecting approximately 1 in 700 newborn infants. In New Zealand we have found a higher incidence (1 in 566 live births). Of note was a higher rate of cleft palate alone in Maori (the highest reported in the world), followed by Pacific and others.

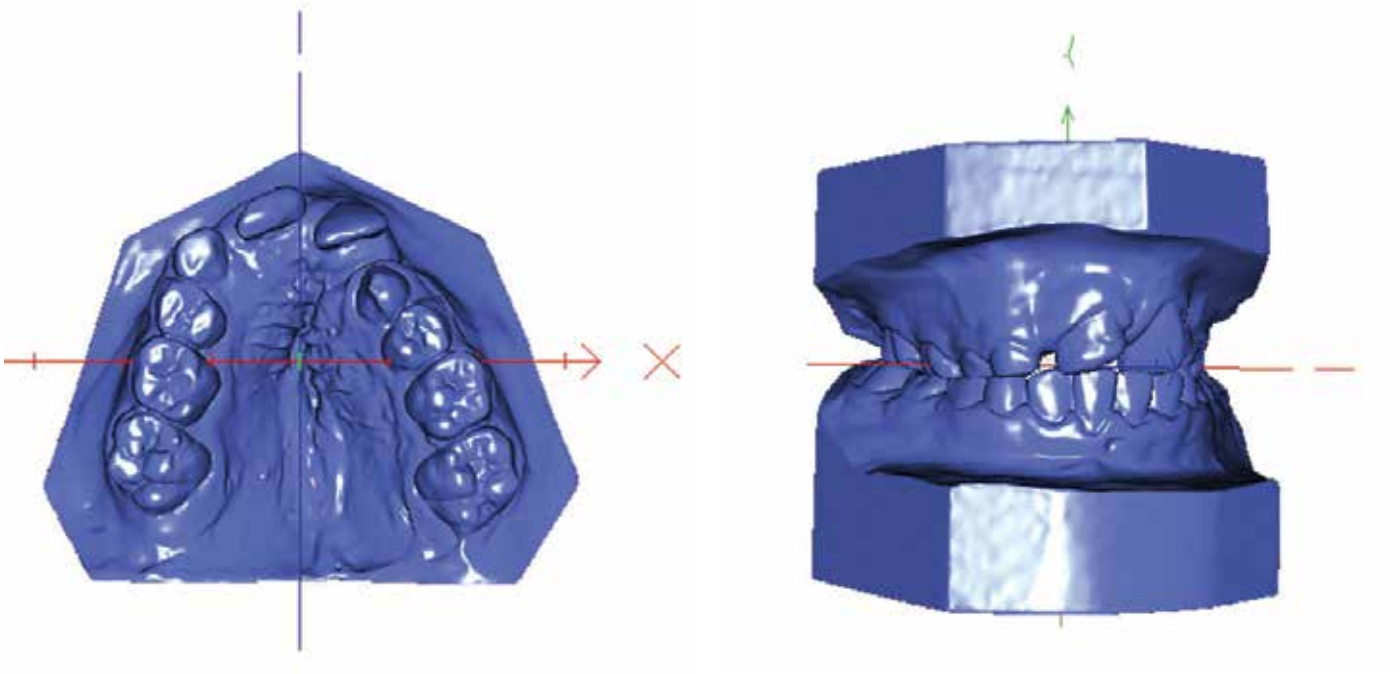
The treatment for those born with CLP is long term (usually till at least one's early 20's) and multidisciplinary (involving multiple surgeries, speech language therapy, and orthodontic treatment) as well as having an impact on quality of life of both the child and the family. There is little data relating to health delivery of cleft services in New Zealand and the outcomes associated with the delivery of these services.

This project has three main aims

- To determine the care paths and family satisfaction of pathways from diagnosis to primary surgery and ensure cleft services are being provided at the highest level.
- To assess a range of clinical and personal outcomes in CLP patients at 5 and 8-10 years of age.
- To assess how outcomes for New Zealand CLP patients compare to those of CLP patients in Australia and the United Kingdom.

How are we doing this?

To ensure we meet the project's aims the cooperation and collaboration of a number of health professionals is required. We are utilising staff within the cleft multidisciplinary teams to ensure the timely and accurate collection and reporting of speech, orthodontic, photographic, growth and quality of life data. Dental health data is also being collected from 20 DHB's.



Using the university's research VM to upload and keeping data safe with Seafile

With numerous people uploading data from several hospitals across a number of locations in a timely manner, it was imperative a secure, safe portal was established from the outset. The Centre for eResearch support team has provided an encrypted secure mechanism for file sharing and storage services using open source Seafile software installed in the university's research virtual machines (RVM). This enables the upload of patient data with secure password protection for each user and the added protection of passwords within each sub-section of the study. Principal investigators can quickly assess how much of each data set is coming in, when it was uploaded and from whom. Assigning study ID and renaming files shortly after they arrive into the database enhances the speed at which we can ensure the study subjects remain unidentified for assessment purposes. The subsequent downloading of the de-identified data from Seafile to be used by the investigators for scoring and analysis is also fast and efficient.

Where to in the future?

This project aligns with the goals set out for the Health Delivery stream. It will be able to deliver robust information about pathways and outcomes that will enable changes to policy and practice to ensure consistency and best outcomes for CLP patients in New Zealand within 5 years. This research will impact on the delivery of cleft services in New Zealand and help to optimise appropriate standardised care pathways after antenatal diagnosis of a pregnancy with a cleft (through the Maternal=Fetal Medicine network). Early life data will enable health services to plan suitable health care for cleft children (via the newborn network). The outcomes will enable establishment of baseline data for New Zealand as well as providing detailed data on factors affecting outcomes in cleft children throughout childhood. It will also provide evidence of how New Zealand units are faring relative to our Australian counterparts as well as established best practice units in the United Kingdom.

Optimisation of blades on large wind turbines with individual pitch control and trailing edge flaps

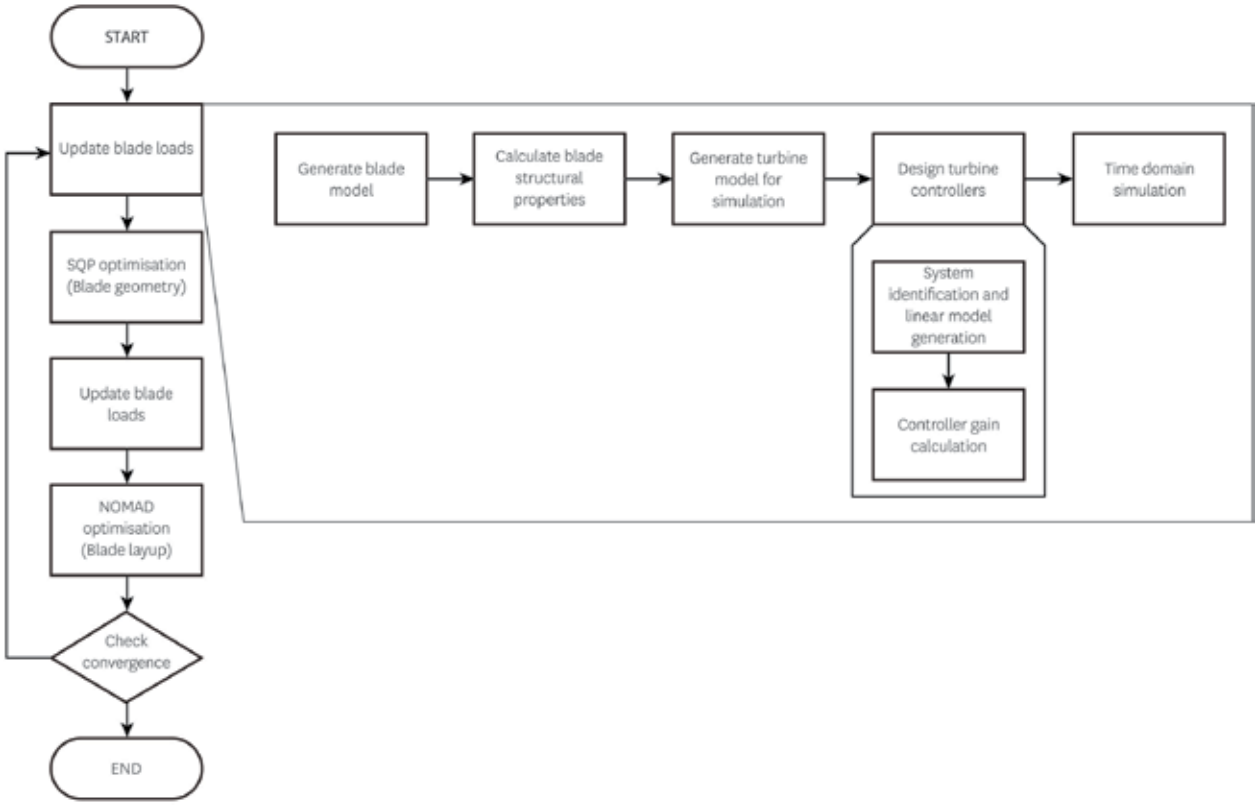
Zhenrong Jeremy Chen, PhD candidate, Dr Karl Stol, Senior Lecturer, Prof Brian Mace, Head of Department, Department of Mechanical Engineering

Overview

Advanced load control methods for wind turbines such as individual blade pitch (whereby each blade on a wind turbine is pitched at a different angle) and trailing edge flaps (near the blade tips) have been shown in previous research to be capable of reducing fatigue loads on the turbine, with load reductions at the blade root being the most significant. This project aims to explore whether wind turbine blade designs are able to take advantage of the benefits offered by these load control methods to reduce the overall cost of energy ($/kWh) from the turbine over its lifespan.

A process implemented in MATLAB which integrates blade design, structural analysis, turbine modelling, controller development and turbine simulation (time and frequency domain) is used with the SQP (Sequential Quadratic Programming) and NOMAD (Nonlinear Optimization by Mesh Adaptive Direct Search) optimisation algorithms to find a particular blade geometry and layup which minimises the cost of energy, which accounts for the capital and operational costs of the turbine, and its energy production, over its lifetime. A list of the tools used in this process, illustrated in Figure 1, is included in Table 1.

Figure 1 Overview of optimisation process.



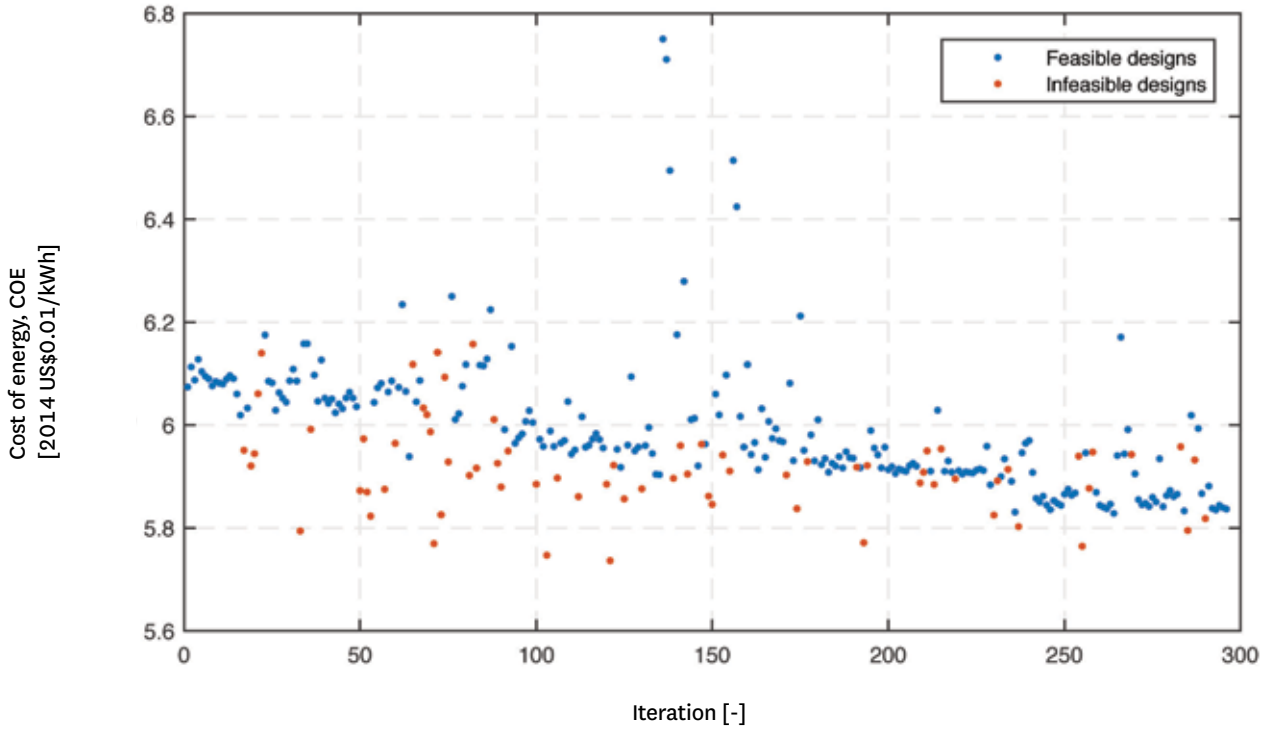


Figure 2 Sample results from NOMAD optimisation of blade layup.

Use of the university's research virtual machines

The optimisation process developed makes use of virtual machines at several stages to parallelise task execution. Within the SQP optimisation, sensitivity analysis of each of the blade geometry design parameters is performed in parallel. Time domain simulations of wind turbines for system identification experiments at different wind speeds are also performed in parallel, along with additional simulations to determine the loads experienced by the turbine over its lifetime in a variety of wind fields and operational states as specified by international standards. From the results of these extensive simulations (typically around 80 separate simulations), constraints for the optimisation algorithms which correspond to limits on ultimate loads, fatigue loads and blade deflection are also calculated in parallel. The use of the computing resources from the NeSI Pan cluster greatly reduces the time required for each of these tasks, reducing time required for development of the optimisation process and allowing for results to be obtained within a realistic timeframe.

Table 1 Tools used in blade optimisation

Tool	Purpose
NuMAD (Sandia National Laboratories)	Blade design
PreComp (National Renewable Energy Laboratory)	Blade structural analysis
HAWCStab2 (Technical University of Denmark)	Frequency domain turbine analysis
HAWC2 (Technical University of Denmark)	Time domain turbine simulation
NOMAD (integrated in OPTI Toolbox, Auckland University of Technology, University of Auckland)	Blade layup optimisation
MATLAB	Top level control of design and optimisation process, data processing

Current Progress

The blade design and optimisation process is currently being used to optimise the blades on a baseline 5MW turbine with a standard collective pitch controller (no advanced load control). The result of this optimisation will be used as a starting point for optimisation of blades on a turbine with individual pitch control, with the use of localised actuators in the form of trailing edge flaps introduced at a later stage. Future work may also involve the optimisation of larger turbines (10-20MW) to assess the scale of benefits provided to large wind turbines which integrate advanced load control. Initial results have shown that there is room for the cost of energy of the baseline turbine to be reduced, and we aim to demonstrate how the benefits of advanced load control can extend past load reductions on existing blade designs.

ARCI, archaeology eResearch collaboration initiative

Joshua Emmitt1, Graduate Teaching Assistant, Dr Rebecca Phillipps1, Research Fellow, Sina Masoud-Ansari2, eResearch Support, Prof Simon Holdaway1, Prof Mark Gahegan2, 1Anthropology, School of Social Sciences, 2Centre for eResearch

Background

Archaeologists are interested in human environment interrelationships over long spans of time and often engage in comparative analyses of these relationships. Data are compiled from a range of sources. The Archaeology eResearch Collaboration Initiative (ARCI) is a research group specialising in the management and analysis of data intensive archaeology. Currently the project is working with data from field projects in Egypt, New Zealand, Saudi Arabia, and Australia. These projects generate large amounts of data that need to be shared regularly between researchers around the globe.

Data collection

Data acquired in the field consists of high resolution sampling of archaeological phenomena, recorded as a collection of geographic information with corresponding attribute information. It is not unusual for tens of thousands of observations to be collected during a field season. In addition, survey data can include photographs of archaeological features, including high resolution GigaPan imagery, and LIDAR point data. This data often includes complex file structures or large file sizes, the reading of which by specialist software such as ESRI's ArcGIS are not easily shared in a structured way amongst researchers, both domestic and international. The Centre for eResearch provided access to the NeSI Data Fabric and customised servers which facilitated data sharing and collaboration, greatly increasing the productivity of the projects involved.

Methods for collection and recording archaeological data can vary between projects to accommodate different research interests, however, there are usually similarities between projects in that recorded artefacts and features need to show both geographic and archaeological context. The question is on what scale this information is recorded by different researchers, and how data can be meaningfully related. To facilitate this, each data point is given

Figure 1: Excavation on the Ahuahu Great Mercury Island Project, New Zealand. Artefacts are measured in space with a total station before being registered into a database in-field with a tablet.

Figure 2: In-field data collection using notebooks in the Fayum, Egypt.

a unique identifier (UNID), and each project is given a unique project code (PC). UNIDs are unique within a project, and the PC is never repeated. Together the UNID and PC form a dual-identifier system (PCUNID) which is unique across all projects. This enables the comparison of data between projects.

With the help of the Centre for eResearch, the ARCI team developed the pre-existing data representation schema that could be used to represent geographic and archaeological data across a wide range of physical environments. This improved schema can support both excavation and survey based data collection techniques, as well as incorporate data collected using different instruments and methods. It also enables the recording of metadata about the way the data was recorded. The schema was built into a PostgreSQL relational database and used PostGIS to link spatial attributes based on the PCUNID. This allowed both geographic and descriptive data to be stored in the same database and created a centralised, authoritative source for project data that could be accessed concurrently through various desktop and web-based applications. Using a database also had the benefit of providing fine-grained access control, so that access could be given to students who only needed to edit part of the dataset. This further aided the research workflow as it minimised problems in sharing and integrating changes made by different team members.

Workflows and tools

Projects which use the ARCI schema may not have started their data collection with it, meaning that data management and cleaning is required. The Centre for eResearch provided software development support and a number of different programs have been written to aid in the managing and cleaning of data. Some examples of this include tools that synchronise a collection of photos with their UNIDs in a photo database and software that creates attribute fields for geospatial data files based on their location in the filesystem. Some of the most important tools have been those that merge the attributes from a number of spatial data files into a standardised schema. In one project, this resulted in the merging of 1,200 shapefiles with different attributes to three, each with a common set of attributes which reflect the ARCI schema.

Data collected in the field is piece-provenanced meaning that the 3D position of each artefact is recorded (Figure 1). Attribute data is also collected on each artefact which could occur in-field (Figure 2) or in the lab. While the recording of information is systematic, errors can occur, and data collected is checked before integration into the main database. With this in mind a series of programs and database workflows were created to help clean the data before integration. These workflows identify duplicate, conflicting, or incomplete records. For example, one of the workflows compares the PCUNIDs between the descriptive and geospatial datasets to identify records that lack corresponding entries.

What's next

The ARCI project plans to roll out several of its interfaces over the next year. This includes a website which will make available several of the workflows developed by the project for other researchers to use. The website will also serve as a front end for our online database which will be at first accessible to researchers involved in the individual projects, with the future goal of facilitating the open-access of archaeological data, something that is increasingly required by funding agencies.

With increased public outreach as well as numerous articles which are being published in academic journals, it is hoped that more researchers will show interest in incorporating their datasets into our schema and database model. For more information please email the ARCI team at arci@auckland.ac.nz

High-resolution cryo-electron microscopy of protein complexes and machines

Dr Ambroise Desfosses, Research Fellow, Hari Venugopal, Teaching and Research Technician, Assoc Prof Alok K. Mitra, Department of Biological Sciences

Overview

In all walks of life, functioning of a living system is driven by proteins, the "workhorses" that direct the replication and survival of the constituting biological cell. Be it in a single cell or multi-cellular organism, the essential physiological processes require the interplay of thousands of protein molecules, each assuming an unique, folded 3-D structure, and each executing its biological function efficiently and with great specificity. In recent years, as part of Structural Biology, cryo-electron microscopy has developed into a powerful discipline. This method allows one to reveal high-resolution details of protein structure and protein-protein interaction in macromolecuar complexes to provide insight into many cellular functions that are important in human health and disease.

As part of our program to study the 3-D structures of complex protein assemblies, we use advanced image processing algorithms to generate 3-D structures from images recorded in our state-of-the-art 200kV transmission electron microscope equipped with an extremely coherent field emission gun as the electron source (TF20). These algorithms are used to analyze 2-D projection images of the 3-D complex, whereupon the knowledge of the orientation of the 3-D object that gave rise to individual 2-D image is deduced iteratively from an initial, approximate, reference model of the 3-D structure. This knowledge is then utilised to arrive at the 3-D structure from the many thousands of aligned images. This, so-called single-particle-analysis (SPA) for solving the 3-D structure is computationally demanding especially for large images containing near atomic resolution details.

Utility of the NeSI Pan cluster

We benefited from the ability to install parallelized versions of modern SPA softwares namely, Bsoft, EMAN2, SPIDER, Relion and most recently SPRING on the NeSI Pan High Performance Computing cluster, which provided exceptional computational power to fully utilise the power of these tools. Obtaining high-resolution information on a structure of interest depends mostly on the amount of 2D images combined in a single 3D structure, the fine sampling of each image, and a precise orientation determination. With a pixel corresponding to only 1 Angstrom (= 10^{-10} m) at the specimen level, each of the several ten thousands particle image gets as big as 500*500 pixels. Those images need to be compared to ten thousands of projections of a reference volume to determine the optimal translation and rotation to match the reference image. Therefore, in total, billions of cross-correlation have to be computed, and this for each iteration of the refinement. On a typical 4 CPUs machine, a full refinement would take up to a year ! Thanks to the large number of CPU's available on the NeSI Pan cluster, we can bring down those calculation to less than a week, allowing us also to test and optimise a number of crucial parameters for the 3-dimensional structure determination.

Below, we provide details focusing on the progress in our cryo-EM derived 3-D structural analysis of two macromolecular complexes at the highest resolution.

Insight into the function of a toxin-delivering protein nano machine

Many strains of bacteria have developed sophisticated protein assemblages that they use to gain a survival niche by either killing other sensitive bacteria through perforation of their membranes or by transferring toxins into eukaryotic hosts. Anti-feeding prophage (Afp) is a toxin-delivering micro-injection apparition released by gram-negative bacteria S. entomophila that is pathogenic to New Zealand agriculture pest grass grub (C. zealandica). Due to the fact that unlike for many other related systems Afp has a eukaryotic host, this has raised the possibility that apart from the benefit of using it as a chemical-free biological pesticide, Afp may be tailored for targeted delivery in anti-tumour immunotherapy. In order to facilitate such exercises, it is mandatory to reveal its detailed 3-D structure, which is composed of no less than 18 different proteins. Afp elaborates two different configurations - the resting extended state and the functional contracted state that is believed to enable extrusion of the toxin into the host (Fig. 1). We have in 2013 produced a modest (~15Å) resolution structure of the extended form by SPA coupled with specialised analysis of the helical symmetry of the sheath (1). Currently, using images from our TF20 microscope we are utilizing the Pan cluster to process simultaneously close to 10,000 images to arrive at a sub nanometre resolution 3-D structure for Afp as also for a structural mutant, the tube-baseplate complex (TBC) for an in-depth visualisation of the inner tube and the baseplate. This work is in collaboration with Dr. Mark Hurst of AgResearch Lincoln.

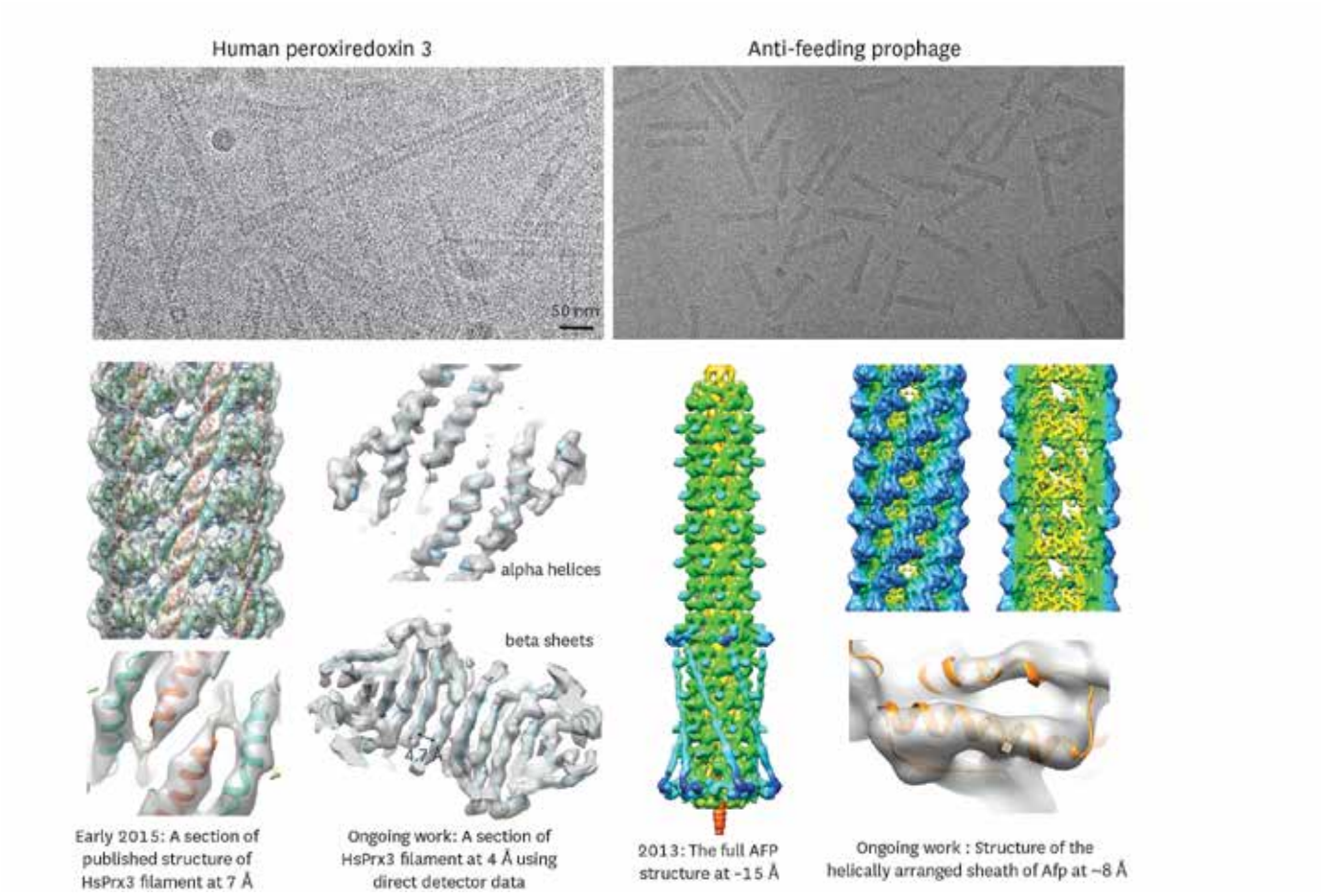


Figure 1: Top, Cryo-EM Micrographs of Human Peroxiredoxin 3 (left) and Anti-feeding prophage (right). From hundreds of such micrographs, the particles are segmented into tens of thoousands of images for which the relative orientations need to be determined. Bottom, example reconstructions obtained for both projects using the NeSI Pan cluster. Three-dimensional structures of those large protein complexes constitute a critical step towards the understanding of their biological function.

Insight into the 3-D architecture of a putative molecular chaperone

This study involved revealing the organization of high-molecular weight filamentous assembly of human peroxiredoxin3 (HsprX3). Peroxiredoxins (Prxs) are a ubiquitous class of thiol (Cys)-dependent peroxidases that play an important role in the protection and response of cells to oxidative stress and therefore is clinically very important. The catalytic unit of typical 2-Cys prx is a homodimer, which can self-associate to form complex assemblies that are hypothesized to have signaling and chaperone activity. Mitochondrial Prx3 forms dodecameric toroids, which can further stack to form filaments, the so-called high-molecular-weight (HMW) form that has putative chaperone activity. We imaged such structures formed at low pH using our TF20. We established the helical nature of these filaments and image processing using this deduced helical symmetry resulted in a ~7Å reconstruction (2), the highest resolution cryo-EM structure (Fig. 1) obtained using in-house data in whole of Australasia. We are currently pushing the resolution of this structure by processing data acquired on an electron microscope equipped with a direct detector. This structure establishes the molecular insight into the formation of the helical stacks of PrX3 dodecamers, and provides an explanation of the chaperone activity based on the elaboration of significant hydrophobic patches in the lumen of the filament. This work is in collaboration with Dr. Juliet Gerrard at SBS.

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Statistical modelling of carryover effects after cessation of treatments

S. Gwynn Sturdevant, PhD candidate, Department of Statistics

Hypertension, high cholesterol, and diabetes are responsible for significant mortality, morbidity, and cost in both developed and developing countries. Rather than intervening after these high-risk conditions develop, it would be preferable to intervene to prevent incidence hypertension, high cholesterol, and diabetes. Our research discussed trial design and analysis for evaluating interventions that prevent them, in particular, the problem of estimating the duration of response to treatment. Put simply, how long does the effect continue after the active intervention ceases?

Randomised controlled trials are generally considered the gold standard when testing for the efficacy of an administered treatment. Recently, a new genre of trial has emerged to test for a carryover effect. For analysis, these trials used naive comparisons of cumulative incidence at the end of the post- treatment follow up period. Diagnosis of hypertension, diabetes, and high cholesterol occurs when a noisy measurement crosses a threshold so incidence is difficult to localise. The purpose of our research is to explore sound methodologies to test a carryover hypothesis in these circumstances.

One such trial, Trial of Preventing Hypertension (TROPHY), can be used as a concrete example. In figure 1 we see 3 graphs. The top graph contains the long-term average systolic blood pressure (BP) of two simulated people: one has treatment given the first two years (red), the other is in the control group (blue). Long-term average BP varies throughout the day, over the year, and there is other non-negligible measurement error. The middle graph includes measurement error, the actual data obtained from a study. The bottom graph counts the number of measurements above the threshold; the measurement labelled 3 is when diagnosis occurs and subsequent data would be rendered useless due to trial protocol. Accurate trial design must consider these issues: a noisy measurement crossing a threshold and missing data after diagnosis.

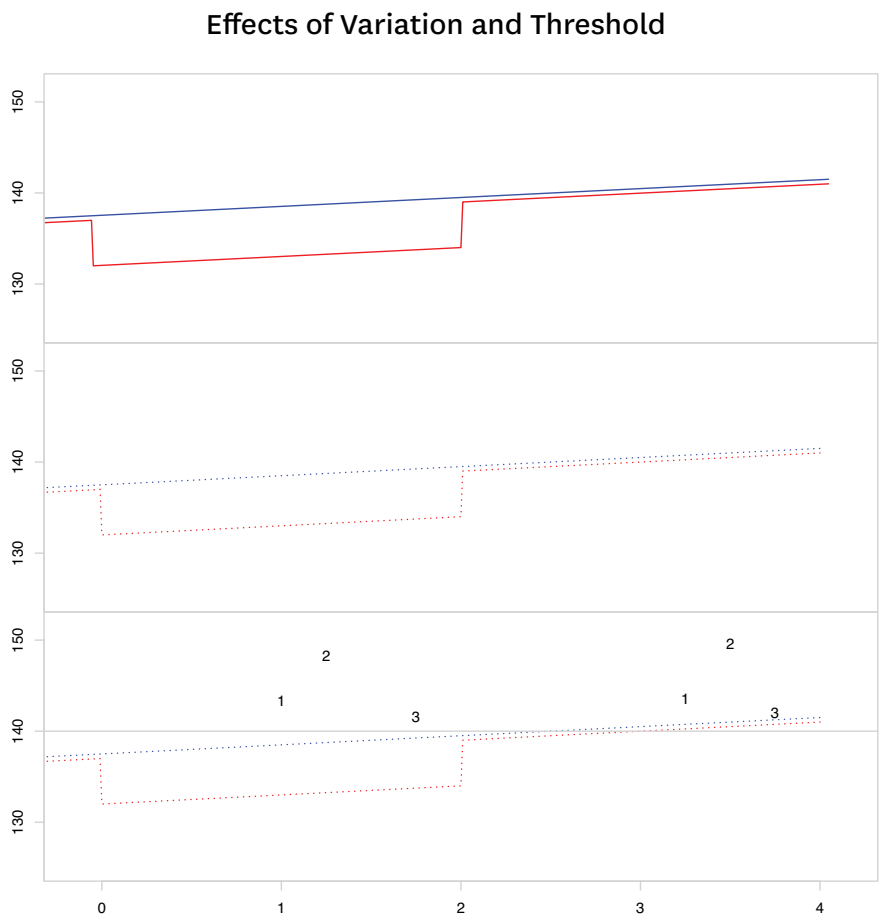

Figure 1: Long-term average BP on the top, measurement error included in the middle, and counting measurements above the threshold on the bottom.

Models with differing lengths of carryover can be seen in figure 2. Mathematically, BP is lowered for the initial 2 years then a carryover is included which varies from 0 to 2 years. At the end of treatment BP returns either quickly to a normal trend, or more gradually, depending upon if carryover does exist and its predefined length.

The error in TROPHY can be explained using figure 1. Due to random variation, the control arm of the trial is more likely to have measurements above the threshold than the treatment group for the initial 2 years. As TRO- PHY diagnosed hypertension when 3 measurements were above the threshold this

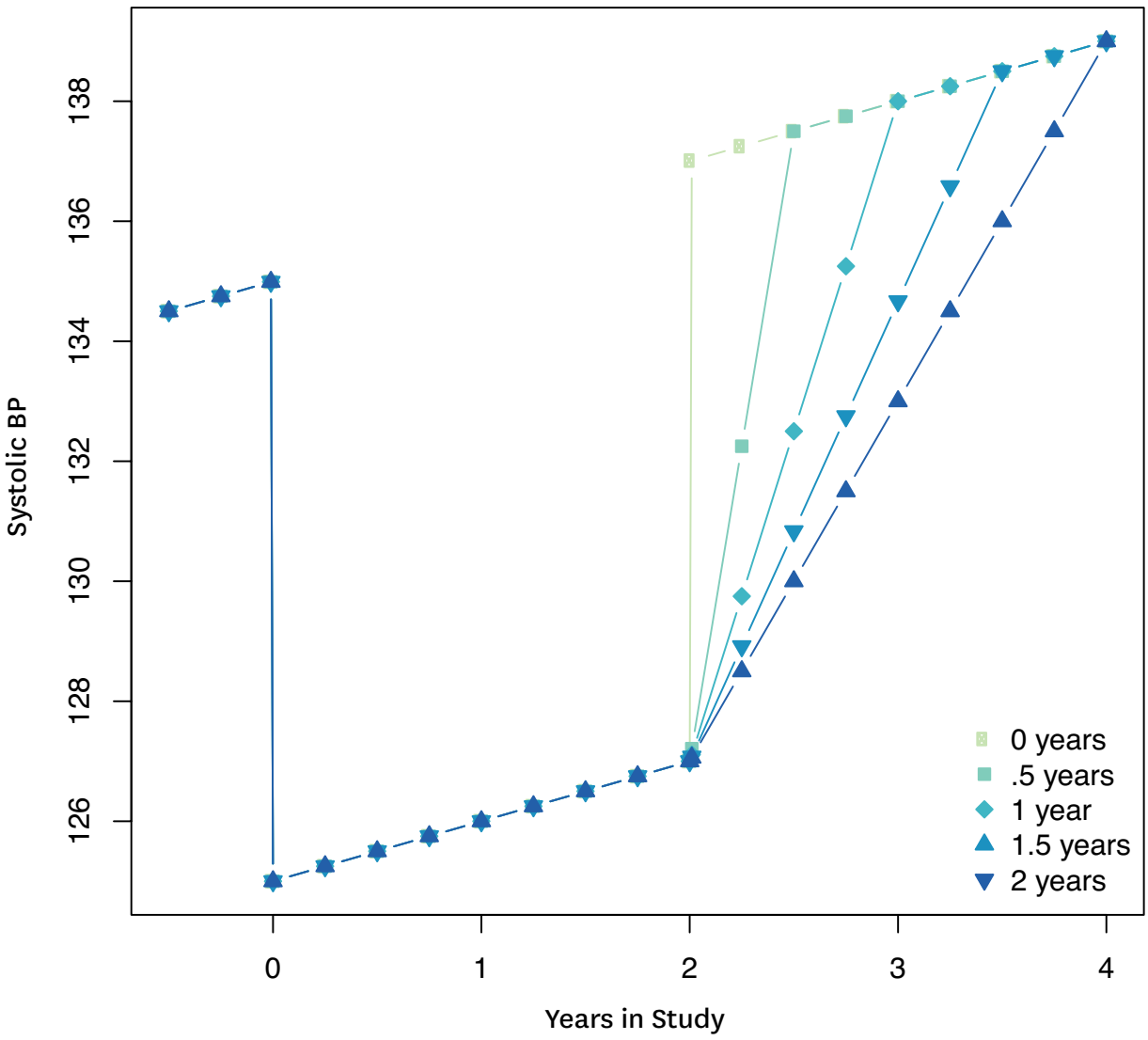

Figure 2: Systolic BP simulation with and without carryover. There are 5 different lengths of carryover: 0, 0.5, 1, 1.5, and 2 years.

resulted in a systemic bias in the design. This bias prior to the onset of the carryover period resulted in more diagnoses in the control arm of the study with or without carryover.

We explored four different approaches: parallel-group trial, crossover trial, linear mixed models, and survival analysis. We conducted systematic simulation studies over varying combinations of parameters to assess both parallel and crossover trials and compared incidence of systolic hypertension to determine power and Type I error rates. The linear mixed model was also assessed via simulation with coverage of relative risks used to measure efficacy. We assessed the survival analysis model by comparing results found from maximising our adjusted likelihood with true hazards found from the data.

The simulations would not have been possible without the support of the Centre for eResearch, in particular the NeSI Pan cluster. Our research utilised over 1,600,000 CPU hours — on one computer over 182 years — assessing new trial design is computationally intensive. Our design had to be tested on over 7000 differing combinations of parameters and each combination was tested 100 times to determine the biases of the mean estimates.

For the applications of interest researchers will need to apply a linear mixed model and parametric bootstrap to find relative risks. If 1 is in the confidence interval of the bootstrap our simulations suggest that it is 99% likely that the data came from a simulation that contained no carryover in the model.

Research outcomes

Staff at the Centre gathered information on recent research outcomes through a survey of researchers. The survey asked respondents to report on research outcomes produced using any or all of the following services: the NeSI High Performance Computing facility, the university's research VMs, the Centre's visualisation facility or the Centre's consulting services.

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1. **Edwards M, Meyer R, Christense N,** "Bayesian Semiparametric Power Spectral Density Estimation with Applications in Gravitational Wave Data Analysis". Physical Review D, under revision, May 2015.
2. **R Leonhardt**, Project title: "Simulations of Terahertz Waveguides". In preparation. Expect to submit to the Optics Express in Sept 2015.
3. **A J Dopheide.** "A Reference Set of DNA-barcoded Macro-invertebrates from A Forested Island". In preparation to submit to PloSon in late 2015 or early 2016.
4. **A J Dopheide.** "Methodological Considerations for Meta-barcoding of Terrestrial Biodiversity". In preparation to submit to Molecular Ecology Resources, in late 2015 or early 2016.
5. **A J Dopheide,** "Meta-barcoding of Island Biodiversity from Soil DNA". In preparation to submit to Molecular Ecology in late 2015 or early 2016.
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Oral presentations

1. **D Vogt; R Leonhardt,** "3D-printed Dielectric Helical THz Waveguides". 3133037. IRMMW-THZ Conference, Hong Kong, Aug 2015.
2. **E Bretscher,** "Fast and Economical Small Displacement Monohull Vessels". FiNZ, UoC, Christchurch, Jan 2015,
3. **HJ Carmichael, VSC Canela,**" Sub-Poissonian Light of High Photon Number: Stochastic Simulation and Control of a Quantum Light Source". NZIAS-MPIPKS Return Tandem Workshop Rotorua, New Zealand, Feb 2015.
4. **HJ Carmichael,** "Open Quantum Systems, Measurement and Feedback, Lecture 3: Intervention & Feedback". 71st Scottish Summer School in Physics, University of Strathclyde, Glasgow, UK, 21 Jul-2 Aug 2015.
5. **VSC. Canela, HJ Carmichael,** "Manipulation of the Photon Number Dynamics in a Micromaser". 23rd International Laser Physics Workshop, Sofia, Bulgaria, Jul 2014.
6. **MC Edwards, R Meyer, N Christensen,** "Signal Extraction and Power Spectral Density Estimation: A Bayesian Semi-parametric Approach". 30th International Workshop on Statistical Modelling, Linz, Austria, Jul 2015.
7. **T Pichugina, RS Grand, T Sugawara, W Schierding, K Masuda, J Uewaki, JR Allison, M Ueno, RA Martienssen, JM OSullivan,** "Understanding the Workings of the Schizosaccharomyces Pombe Epigenome in Three-dimensions". 8th International Pombe Meeting, Kobe Japan, Jun 2015.
8. **Eldridge JJ,** "Do Stars Always Explode in Supernovae or Do Some Just Go with a Whimper?" . CosPA, Auckland, NZ 2014.
9. **A Keane, B Krauskopf, C Postlethwaite,** "Bifurcation Analysis of a Model for the El Ni ño Southern Oscillation" . SIAM Conference on Dynamical Systems, Snowbird, Utah, USA, May 2015.
10. **Wang S, Rusak Z, Gong R, Liu F,** "On the Stability of a Solid-body Rotation Flow in a Finite-length Circular Pipe". Wang S invited Lecturer in Peking Uni China, Dec. 2014.
11. **Lin X,** " Using Core-collapse Supernova to Gain Insight to Stellar Population Model". CosPA, Auckland, New Zealand, 2014,
12. **P Medrano-Gracia, J Ormiston, M Webster, S Beier, C Ellis, C Wang, A Young, B Cowan,** "Construction of a Coronary Artery Atlas from CT Angiography". Medical Image Computing and Computer Assisted Intervention, Sept 2014.
13. **P Medrano-Gracia, J Ormiston, M Webster, S Beier, C Ellis, C Wang, A Young, B Cowan,** "Construction of a Coronary Artery Atlas from CT Angiography". Australia New Zealand Endovascular

Therapies (ANZET) Conference of Interventional Cardiologists, Mel, Au, Aug 2014.

14. **Medrano-Gracia, J Ormiston, M Webster, S Beier, C Ellis, C Wang, A Young, B Cowan,** "A Statistical Model of the Main Bifurcation of the Left Coronary Artery using Coherent Point Drift", Medical Image Computing and Computer Assisted Intervention, Oct 2015.
15. **S Beier, J Ormiston, M Webster, JE Cater, P Medrano-Gracia, A Young, B Cowan,** "Hemodynamic Assessment with Large Scale PC-MRI and CFD - a Study of Idealised, Stented and Patient Left Main Geometries", Medical Image Computing and Computer Assisted Intervention, Oct. 2015.
16. **M Xu, J Cheng, Damon WK Wong, A Taruya, A Tanaka, J Liu, S Beier, J Ormiston, M Webster, JE Cater, S Norris, P Medrano-Gracia, A Young, B Cowan,** "Automatic Image Classification in Intravascular Optical Coherence Tomography Images". MICCAI-CVII-STENT, Oct 2015.
17. **J Sneyd. MacLaurin Lecturer,** "The Dynamics of Calcium: Oscillations, Waves, Theories, and Experiments". Fall Southeastern Sectional Meeting at the University of North Carolina, Greensboro, Nov 2014.
18. **J Sneyd. MacLaurin Lecturer,** "Mathematics and Music: The Beauties of Pattern". 11 invited lectures in several universities in the USA during Oct and Nov 2014.
19. **J Rugis,** "Acinar Cell Modelling". eResearchNZ, Queenstown, New Zealand, Mar 2015.
20. **Sharp PW,** "Accurate N-body Simulations of the Solar System". Department of Computer Science, University of Toronto, Sept 2014.
21. **Sharp PW,**" Parallel in N-body Simulations of the Solar System", Uni of Ottawa, Aug 2014.
22. **Sharp PW,** "Accurate N-body Simulations of the Solar System on a GPU". Simon Fraser University, Apr 2015.
23. **Sharp PW,** "Long Accurate Simulations of the Planets and an Interacting Disk". University of Ottawa, May 2015.
24. **Sharp PW,** "A GPU-enabled Adams Integration for N-body Simulations of the Solar System". Bluenose Conference, Halifax, Canada, Jul 2015.
25. **HJ Carmichael,** "Dissipative Quantum Phase Transitions for Photon". Research Seminar, Los Alamos National Laboatory, Los Alamos, New Mexico, USA, Dec 2014.
26. **R Gutierrez-Jauregui, H J Carmichael,** "On Dissipative Quantum Phase Transitions beyond the Jaynes-Cummings Model". 24th Annual International Laser Physics Workshop, Shanghai, China, Aug 2015.
27. **Meyer R, Kirch C,** "Likelihood Approximations for a Bayesian Semiparametric Analysis of Stationary Time Series". Invited speaker, Business School, Uni of Sydney, Sept 2014.
28. **Sathar S,** "Tissue Model for Optimizing Gastric Pacing". 15th International Conference on Biomedical Engineering, Singapore, 2014.
29. **A Gavryushkina,** "The Total Evidence Approach with Sampled Ancestors: Direct ancestors of Morden Penguins". Allan Wilson Centre Annual Meeting, Palmerston North, New Zealand, 2014.
30. **A Santure,** "Using Genomics to Manage Adaptive Potential in Threatened Populations". Computational Genomics. Queenstown Research Week, Sept 2015.
31. **Douglass M, Davies B, and S Holdaway,** "Models and Measures: Approaches to Understanding Movement in Time-averaged Sequences". From a Landscape Perspective: A Celebration of J.W. K. Harris Career International Workshop, Healdsburg, CA, Apr 2015.
32. **Davies B,** "Simulating Late Holocene Landscape Use and the Distribution of Stone Artifacts in Arid Western New South Wales, Australia. Society for American Archaeology Annual Meeting, San Francisco, USA, Apr 2015.
33. **MC Stein, C Wild, A Scott,** "Approximating the Full Likelihood for Marginal2 x J Contingency Tables and Case-control Data. ". 60th ISI World Statistics Congress (WSC), Rio de Janeiro, Jul 2015.
34. **MC. Stein, C Wild, A Scott,** "Approximating the Full Likelihood for Marginal2 x J Contingency Tables and Case-control Data". Joint NZSA + ORSNZ Conference, Wellington, New Zealand. Nov 2014.
35. **MACSS Fernando, JM Curran, JA Bright, JS Buckleton, R Meyer,** "Bayesian Model Comparisons and Posterior Predictive Checks". Joint NZSA + ORSNZ Conference, Wellington, New Zealand, Nov 2014.
36. **Cooling MT, Soudlenkov G.** "Development of a Parallel, Distributed Fitting Platform for Systems Biology". eResearch NZ, Queenstown, NZ, Mar 2015.
37. **Cooling MT,** "Parallel Model Fitting", 9th International CellML Workshop, Auckland, Apr 2015.
38. **Depheide A, Thomas B,** "Meta-barcoding of Terrestrial Biodiversity from Soil DNA: Methodological Considerations and Application to an Island Ecosystem". Presented at Allan Wilson Centre Annual Meeting, Oct 2014.
39. **Holford, NHG,** "Evaluation of NONMEM 7.3.0 and Monolix 4.2.2 by Parametric Bootstrap". PAGANZ. Dunedin, 2014.
40. **Holford NY. Jiang DJM, TL, GG Milavetz,** "III-44 The Influence of Body Composition on Ethanol Pharmacokinetics Using a Rate Dependent Extraction Model." Page 24 Abstr 3405, Hersonissos, Crete, Greece, Jun 2015.
41. **H. Abbas, S. Alkhafaji, M.M. Farid,** "CFD Investigation of Pulsed Electric Fields Treatment" ICEF12,Québec, Canada, Jun 2015.

Conference proceedings

1. **Ukanwa KU, Clifton GC, Lim JBP, Sharma UK,** " Analysis of Concrete Filled Steel Tube Columns Using Plain and Steel Fiber Reinforced Concrete as infill". Steel Innovation Conference (SCNZ) Sept 2015.
2. **Adams B, McKenzie G, Gahegan M,** "Frankenplace: Interactive Thematic Mapping for Ad Hoc Exploratory Search". 24th International Conference on World Wide Web, pp. 12-22, 2015.
3. **Edwards M, Meyer R, Christensen N,** "Signal Extraction and Power Spectral Density Estimation: A Bayesian Semi-Parametric Approach". To appear, Proceedings of the IWSM 2015.
4. **Norris SE, & Richards PJ,** "Transient Flow Structures around a Cubic Building". Proceedings of the 19th Australasian FluidMechanics Conference, Melbourne, Australia, pp. 4 pages, Dec 2014.
5. **NJ Burbery, R Das, WG Ferguson,** "Establishing Effective Criteria to Link Atomic and Macro-scale Simulations of Dislocation Nucleation in FCC Metals". ICCM, Jul 2015.
6. **Fliegauf, Bryant, Frede, Slade, Woon, Lehnert, Winzer, Bulashevska, Scerri, Leung, Jordan, Keller, de Vries, Cao, Yang, Schffer, Warnatz, Browett, Douglass, Ameratunga, van der Meer, Grimbacher,** "Haploinsufficiency of the NF-kB1 Subunit p50 in Common Variable Immunodeficiency". 32nd Annual Meeting of the German Society for Pediatric Infection Biology, Freiburg, Apr 2015.
7. **Wasala S, Norris SE, Cater JE,** "Numerical Simulation and Aeroacoustic Noise Modelling of a Wind Turbine using a Blade Section in an Annulus". In Inter Noise, pp. 9 pages, Melbourne, Australia, Nov 2014.
8. **Storey R, Norris SE, Cater JE,** " Modelling Extreme Wind Events in a WindFarm using Large Eddy Simulation". 32nd ASME Wind Energy Symposium. National Harbor, Maryland, USA, 2014.
9. **Depheide A, Thomas B, Drummond AJ, Newcomb R,** "Meta-barcoding of Terrestrial Biodiversity from Soil DNA: Methodological Considerations and Application to an Island Ecosystem". New Zealand Ecology Society Conference, Nov 2014.
10. **Williamson N, Kirkpatrick MP, Armfield SW, Norris SE,** "Convectivelyunstable Turbulent Open Channel Flow with Stable Surface Stratification". Computational Techniques and Applications Conference (CTAC), Canberra, Australia, Dec 2014.
11. **Weber J, R Das, M Battley,** "Effect of Curvature on Structural Loading of Prismatic Bodies Subjected to Water Slamming". 8th Australasian Congress on Applied Mechanics, Melbourne, Australia, Nov 2014.
12. **Weber J, R Das, M Battley,** "Slamming Induced Loads on A Rigid Cylinder and Comparison with Rigid Wedges". 5th High Performance Yacht Design Conference, Auckland, New Zealand, Mar 2015.
13. **A Ashikov, C Clifton, B Belev,** "Behaviour and Design of EBFs for Seismic Actions - the NZ Experience". The XV International Scientific Conference Rzeszw Lviv Kosice, Sept 2015.
14. **Sathar S, Cheng LK, Trew ML,** "A Comparison of Solver Performance for Complex Gastric Electrophysiology Models". Conference Proceedings of IEEE Engineering Medicine Biology Society (In Press), 2015.
15. **Sathar S, Trew ML, Cheng LK,** "Tissue Specific Simulations of Interstitial Cells of Cajal Networks Using Unstructured Meshes". Conference Proceedings of IEEE Engineering Medicine Biology Society (In Press), Milan, Italy, Aug 2015.
16. **Verleye B, Swery EE, Kelly P,** "Meso- and Macro Scale Permeability Simulations on the Pan Cluster". eResearch NZ 2015, Queenstown, New Zealand, Mar 2015.
17. **Clarke RJ, Finn MD, MacDonald M,** "Hydrodynamic Persistence within Very Dilute Two-Dimensional Suspensions of Squirmers". Proceedings of the Royal Society of London: Mathematical, Physical and Engineering Sciences, 470 (2167), 2014.
18. **R Miller, H Jiang, A Kolipaka, R Mazumder, M Nash, B Cowan, A Young,** "Determining Anisotropic Myocardial Stiffness from Magnetic Resonance Elastography: A Simulation Study". 8th International Conference, FIMH 2015, Maastricht, The Netherlands, Jun 2015.
19. **ATT Tran, MM Hyland,** "Modeling of Micrometre-Sized Molten Metallic Droplet Impact on a Solid Wall". 8th International Conference on Computational and Experimental Methods in Multiphase and Complex Flow, Valencia, Spain, Apr 2015.
20. **MC Stein, C Wild, A Scott,** "Approximating the Full Likelihood for Marginal2 x J Contingency Tables and Case-control Data". 60th World Statistics Congress, ISI2015. Rio de Janeiro, Jul 2015.
21. **C Zhang, SJ Zarrouk, R Archer,** "Development of a Fully Coupled Flow-geomechanics Simulator for Flow in Saturated Porous Media". The 6th International Conference on Computational Methods, Auckland, Jul 2015.
22. **S Yasin, M Miandeh, RP Orense, R Das,** "Simulation of the Screw Driving Sounding (SDS) Test in Sandy Soil Using Smoothed Particle Hydrodynamic Method in Abaqus". The 6th International Conference on Computational Methods, Auckland, Jul 2015.
23. **Tunnicliffe J, Fuller I, Eaton B, Peacock D, Marden M,** "Reconstructing the Sediment Dynamics of an Overloaded Gravel Bed River, East Cape". To appear in 11th International Symposium on Ecohydraulics, Melbourne, Australia, Feb 2016.
24. **Billac T, David M, Battley M, Thomson R, Kindervater C, Das R,** "Multi-terrain Impact Simulations of a Crashworthy Composite Helicopter Subfloor". 29th Congress of the International Council of the Aeronautical Sciences, St Petersburg, Russia, Sept 2014.
25. **Billac T, Battley M, Das R, Thomson R,** "Water Impact of Helicopter Subfloor Panels". 71st Annual Forum of the Americal Helicopter Society, Virginia Beach, VA, May 2015.
26. **R Leonhardt, D Vogt,** "3D-printed Dielectric Helical THz Waveguides" . IRMMW-THZ Conference. Hong Kong, Aug 2015.
27. **A Ashikov, C Clifton, B Belev,** "Behaviour and Design of EBFs for Seismic Actions - the NZ Experience". Paper presented at The XV International Scientific Conference Rzeszw Lviv Kosice, Sept 2015.
28. **C Walter, AG Jones, GA Ryan,** "The Importance of Smoothing Parameters and Starting Models in 3D Inverse Magnetotelluric Modelling: An Example from the Taupo Volcanic Zone, New Zealand". 2nd EM Induction Workshop, Weimar, Germany, 2014.

Posters

1. **VSC Canela, HJ Carmichael,** "Production of Sub-Poissonian Light of High Photon Number". 71st Scottish Summer School in Physics. Jul 21 -Aug 2015, Uni of Strathclyde, Glasgow, UK.
2. **VSC Canela, HJ Carmichael,** "Production of Sub-Poissonian Light of High Photon Number: A Quantum Trajectory Computer Simulation". NZIAS-MPIPKS Return Tandem Workshop, Rotorua, New Zealand, Feb 2015..
3. **MC Edwards, R Meyer, N Christensen,** "Bayesian Semiparametric Spectral Density Estimation with Applications in Gravitational Wave Data Analysis". 10th Conference on Bayesian Nonparametrics, Raleigh, North Carolina, Jun 2015.
4. **A Keane,** "Delay Differential Equations". Short Thematic Program on in Physical Sciences and Engineering, Fields Institute, Toronto, Canada, May 2015.
5. **HJ Carmichael, R Gutierrez-Jauregui,** "On Dissipative Quantum Phase Transitions in Light-Matter Interactions: Response to Counter-Rotating Term". AsiaPacific Conference and Workshop on Quantum Information Science National Cheng-Kung Uni, Taiwan, Dec 2014.
6. **Sathar S, Trew ML, Cheng LK,** "The Role of the ICC Myenteric Plexus Network in the Anisotropic Propagation of Intestinal Slow Wave Activity". Joint Meeting of the Federation of European Physiological Societies and the Hungarian Physiological Society, the FEPS, Budapest, Hungary, Aug 2014.
7. **A Gavryushkin, D Welch, T Heath, AJ Drummond, T Stadler,** "The Fossilised Birth-death Process Applied to the Total-evidence Approach for Dating with Fossils". Smbe, Vienna, Jul 2015.
8. **R Miller, H Jiang, A Kolipaka, R Mazumder, M Nash, B Cowan, A Young,** "Determining Anisotropic Myocardial Stiffness from Magnetic Resonance Elastography: A Simulation Study". 8th International Conference, FIMH 2015, Maastricht, The Netherlands, Jun 2015.
9. **R Miller, H Jiang, R Mazumder, B Cowan, MP Nash, A Kolipaka, A Young,** "Determining Anisotropic Myocardial Stiffness from Simulated Magnetic Resonance Elastography with Gaussian Noise". Cardiac Physiome Workshop, Auckland, Apr 2015
10. **Davies, B,** "Simulating Mobility, Place Use, and the Distribution of Stone Artefacts at Rutherfords Creek, Western New South Wales". Australian Archaeological Association Annual Meeting, Cairns, QLD, Australia, Dec 2014.
11. **C Zhang, SJ Zarrouk, R Archer,** "Thermo-Hydro-Mechanical Simulation in Porous Media with FEniCS". FENICS '15, Imperial College London, Jul 2015.
12. **B Curran,** "Transcript Comparison of Pseudomonas Syringae pv. Actinidia Genes Expressed in Vitro and in Planta", PSA Symposium, Bologna, Jun 2015.
13. **ATM Daniel, R Johannes,** "A Correlation between Experimental pKa's and Their Corresponding Proton Affinities as calculated Using DFT: A Possible Prediction Tool". Conference of School of Chemical Sciences Centenary Celebration, Mar 2015.
14. **ATM Daniel,** "A Correlation between Experimental pKa's and Their Corresponding Proton Affinities as calculated Using DFT: A Possible Prediction Tool". First year PhD presentation.
15. **Cooling MT, Nosies,** "A Case-study in Constraining Model Behaviour". 8th International CellML Workshop, Waiheke Island, Auckland, NZ, 2014.
16. **SJ Masson, S Parkins,** "Generation of Extreme Spin Squeezing in the Steady State of a Generalised Dicke Model". 14th Int Conference on Squeezed States and Uncertainty Relations, Gdansk, 29 Jun–3 Jul 2015.
17. **SJ Masson, S Parkins,** "Generation of Extreme Spin Squeezing in the Steady State of a Generalised Dicke Model". 71st Scottish Summer School in Physics. Glasgow, 21 Jul -2 Aug 2015.
18. **S Beier, JOrmiston, M Webster, J Cater, S Norris, P Medrano-Gracia, A Young, BCowan,** "Coronary Bifurcation 3D Flow Accessed with Dimensionally Scaled ex vivo PC-MRI and CFD - A Comparison for Idealized, Stented and Patient Specific Geometries". Cardia Physimoe Workshop, Auckland, Apr 2015.
19. **AN Hinton, P Murrell,** "The Conduit Package" . The UseR! 2015 Conference, Aalborg, Denmark, Jun-Jul 2015.

Other

1. **JE Cater,** Project title: "Modeling Airflow through the Vocal Tract Using Computational Fluid Dynamics". Supported collaborative research for: 1) Michael Hanks & James Hou of Engineering Science. And, 2) Data sharing and processing between Richard Clarke, Catherine Watson using the vocal tract.
2. **Support project completion for Reynisson J, Wright LJ, Dalebrook A,** Project title: "Density Functional Calculations of the Electronic Structure and Reactions of Organometallic Metallabenzene Complexes".
3. **Support project completion for Michael G. Gardiner,** "Density Functional Studies of Multistep Reductive Reaction Paths in Palladium (II) Chemistry. Manuscripts in preparation detailing results with experiments.
4. **Snell R G,** Project title: "Using High Performance Computing to Investigate Human Genomic Information for Human Health". Extended research collaboration with additional clinicians at ADHB and University of Otago.
5. **Snell RG,** Project title: "Using High Performance Computing to Investigate Human Genomic Information for Human Health". Community engagement through Minds for Minds Newsletter to over registrands within New Zealand.
6. **S Beier,** "Study of Coronary Arteries". Featured in the national Engineering News Magazine Women in Engineering, Nov 2014.
7. **S Beier,** "CT Fluid Dynamics in Stent Assessment". Keynote speaker at the Annual Scientific Meeting of the Cardiovascular Society (CSANZ), June 2015.
8. **S Beier,** "Our Changing World". Featured in NZ Radio, Jul 2015
9. **S Beier,** Received $5,000 "Publication Bursary Award", 2015.

10. **S Beier,** "Three Minute Thesis (3MT®)" Runner-up at the University of Auckland, 2014
11. **A Bilge,** "Implementing Hamiltonian Monte Carlo for Effcient Bayesian Evolutionary Analysis". AWC Summer Scholarship Report. Apr 2015.
12. **A Bilge,** T Vaughan, AJ Drummond, "Efficient Bayesian Evolutionary Analysis Using Hamiltonian Monte Carlo". Poster published in FigShare, the University of Auckland 2015.
13. **E Bretscher.** "Fast and Economical Small Displacement Monohull Vessels". For PhD provisional defence registration seminar, Auckland, Mar 2015.
14. **S van Hove,** Callaghan Innovation Doctoral Study award.
15. **AN Hinton,** "Helping People to Connect with Data". Technical report, UoA Statistics Technical Blog 2015.

Thesis

1. **S Widyanti,** "Numerical Model of the Deep Hydrothermal Convection in the Taupo Volcanic Zone, New Zealand". Master thesis completed in June 2015.
2. **IS Zeng,** "Statistical Methods In Clinical Proteomic Studies -A Protein Concerto", PhD thesis completed in 2014.
3. **Chen XJ,** "A Spatiotemporal Modeling Study of a GnRH Neuron". The University of Auckland Completion 2014.
4. **VV Dighe,** "Modelling Smart Wind Turbine Blades". ME Thesis 2015.
5. **R Storey,** "Large Eddy Simulation of Dynamically Controlled Wind Turbines", PhD Thesis awarded, Dean's List 2015.
6. **B Liu,** "Influence Analysis on Phylogeny Inference". MSc thesis completed on Nov 2014.
7. **X Lu,**" CFD of the Vocal Tract ". PhD thesis, submitted 2015.
8. **C Walter,** " Three-dimensional Magnetotelluric Modelling of the Taupo Volcanic Zone, New Zealand". PhD thesis, submitted 2015
9. **Tu, Tai-Yin, Tom,**" Computational Fluid Dynamic Study of Dynamic Stall Behaviour of the NREL S814 Aerofoil at Low Reynolds Number ". Master thesis, submitted 2014.
10. **Chen Yu,** "Effect of Hydrogen Supplementation on Performance, Knock Behaviour, and Emissions of an SI Engine Operating at Lean Air-fuel Ratios". PhD thesis, submitted 2015.
11. **O'Byrne K,** "Mathematical Modelling of Airway Smooth Muscle". PhD Thesis, submitted 2015.
12. **Onundi YB,**" Oxidation of Bisphenol A, Triclosan and 4-Nonylphenol by Fe-B* Activated Peroxide". PhD thesis, submitted 2015.
13. **C Liu,** Title: "An Abstract Micro Simulation of Gentrification: A case of Point Chevalier, Auckland". PhD Thesis, submitted 2015.

Software package

1. **Stanway, J Eldridge,** "BPASS: Binary Population and Spectral Synthesis V2.0". Submitted 2015. Available in bpass.auckland.ac.nz with a companion instrument paper to explain the results.
2. **J Eldridge, Stanway, Xiao, McClelland, Bray, Izzard,** A new updated version of stellar population models for use by the astrophysical community.

Grant

1. **Cater JE, MV Hove, Sibyile CC, Maxwell P. Jackson T, Javaremi AN, J Storey.** Project title: "Modelling CO2 Concentrations in the Upper Airways". Funded by MBIE Smart Ideas. Proposal: PROP-37861-SIP1-UOA, Sept 2014.
2. **John Edward Cater,** "Smart Patient Simulators for Next Generation Respiratory Therapy". MBIE Grant $860k.
3. **P Medrano-Gracia, J Ormiston, M Webster, B Cowan, S Beier, A Young, C Ellis,** "Statistical Atlas of the Anatomy of Coronary Arteries" Awarded $200,000 Senior Fellowship by Green Lane Fund, Oct 2014.
4. **J Sneyd,** "Multiscale Modeling of Saliva Secretion". NIDCR Grant renewed for 2015 (2R01DE019245-06A1)

Patent

1. **French Patent Application 1457862 under project title:**" Scaled Normalisation of Uncertain Databases". (c. Aug 2014).

Book/Book chapter

1. **ATT Tran, MM Hyland,** "Modeling of Micrometre-Sized Molten Metallic Droplet Impact on a Solid Wall". Computational Methods in Multiphase Flow VIII", page 375-386.

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