ANNUAL REPORT 14

vlsci
LIFE SCIENCES COMPUTING

VLSCI is funded by the Victorian Government and contributing institutions and is hosted by the University of Melbourne.

This petascale facility delivers expertise and systems for life sciences computing.

From 2010-2014 the first ever IBM Research Collaboratory for Life Sciences was co-located at VLSCI.

CONTENTS

STEERING COMMITTEE
CHAIR'S REPORT

On behalf of the former Steering Committee (the Committee) of the Victorian Life Sciences Computation Initiative (VLSCI), which provided advice to the University of Melbourne during the first five years of operation of the VLSCI, from 2010 to 2014, I am pleased to commend this 2014 Annual Report.

Prior to its disbandment at the end of 2014, the Committee included senior nominees from Melbourne, Monash and La Trobe Universities, the Walter and Eliza Hall Institute of Medical Research (WEHI), Melbourne Health, the National Computational Infrastructure (NCI) and IBM, in addition to the Chair of the VLSCI Scientific Advisory Committee (SAC) Prof. Tony Bacic, who joined as incoming SAC Chair in early 2014, and the VLSCI Director, Prof. Peter Taylor. The Committee was pleased, at the start of the year, to welcome the addition of a nominee from the Victorian Comprehensive Cancer Centre, Prof. David Bowtell of the Peter MacCallum Cancer Centre. At its July meeting, the Committee thanked retiring member, Dr Mark Kosten of La Trobe University, and welcomed Prof. Brian Smith as his replacement at the September meeting. The Committee was grateful for the sustained involvement of Prof. Liz Sonenberg who provided a host of valuable links and helpful feedback from the host institution, the University of Melbourne.

To fulfil its responsibility for reviewing all aspects of the operation of the VLSCI and for providing recommendations and strategic advice to the host institution, through the Deputy Vice Chancellor (Research), Prof. James McCluskey, the Committee met four times in 2014, in February, July, September and December. With the official end of the initial five-year grant period, the December meeting was thus the last formal meeting of the Committee in its original form.

With a well-managed budget, relatively low levels of downtime, high levels of user satisfaction, a growing list of Life Sciences Computation Centre (LSCC) subscriptions and an active outreach and skills development program, the main focus of the Committee during 2014 was on achieving long-term sustainability for VLSCI. The Business Plan 2014 identified the tasks involved, with an important challenge being achievement of firm commitments from existing and potential new stakeholders for cash contributions to VLSCI operations through 2015-16 as the essential foundation for development of a long-term funding strategy, including through demonstration of the key role of VLSCI in the overall national research infrastructure strategy. At its July meeting, the Committee was pleased to receive very strong endorsement from Dr Ajay Royyuru, IBM, for the scope and scale of VLSCI activities to date, as documented in the 2013 Annual Report. Dr Royyuru confirmed IBM's unequivocal support for the VLSCI enterprise and its future potential within an international context. His comments were agreed to and endorsed by the Committee.

The Committee wishes to acknowledge the important advocacy activities undertaken by several Committee members and Victorian University Deputy Vice-Chancellors which contributed to the assurance of funding for 2015-16 operations to sustain VLSCI in the short-term.

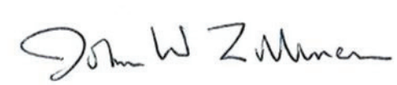
The extensive information assembled in support of the 2015-16 funding strategy strengthened the Committee's view that VLSCI is an extremely important component of life science research infrastructure in Victoria and that its ongoing funding will be essential if Australia is to keep up with the fast-moving international developments in life sciences computing, emerging developments in personalised medicine and the opportunities provided by a rejuvenated biotechnology sector. The Committee urged the University and the VLSCI management team to continue their high-level discussions with partner institutions and stakeholders in order to progress the formulation of an agreed sustainability strategy beyond 2015-16.

The Committee considered that LSCC activities are key to the case for VLSCI funding as part of the long-term national research infrastructure. It was particularly impressed by the example set by successful projects such as the partnership with the University of Queensland in the establishment of the NeCTAR-funded Genomics Virtual Laboratory and the positive reception from EMBL Australia of VLSCI's expression of interest in hosting the next phase of Bioinformatics Resource Australia – EMBL. At the end of the year, this was in the final stage of negotiations and the Committee was hopeful for a positive outcome.

At the time of writing, Prof. Taylor has resigned as VLSCI Director, and returned to Europe to fulfil family and professional commitments. The Committee wishes him well in the future and thanks him for all his fine work in building and sustaining VLSCI through its first five highly productive years.

At the conclusion of this five years of operation, the Committee was satisfied that the first essential stage in securing the long-term funding for VLSCI had been reached with the Victorian Government's commitment to ongoing funding for 2015-16. It saw the immediate tasks ahead as including the establishment of a revised governance structure reflecting the new stakeholder arrangements.

I have greatly appreciated the opportunity to be associated with the rollout of this important piece of Australian research infrastructure and I am sure that all past members of this Committee will be looking forward to watching the future success of VLSCI.



John W. Zillman AO FAA FTSE

SCIENTIFIC ADVISORY COMMITTEE
CHAIR'S REPORT

The SAC met twice in 2014 with a focus on addressing a key aspect of its Terms of Reference, namely to offer strategic advice to the Director and Steering Committee on matters of science and computing technology that inform future directions. More specifically, its task was to review the LSCC activities, propose larger-scale projects and activities, advise on national and international engagement, comment on existing scientific projects running on VLSCI systems and assist with the strategic positioning of VLSCI in relation to the national policy framework.

With the strategic focus for VLSCI being one of ongoing sustainability, the Committee directed its efforts on discussing the future requirements in life sciences computing, noting that all governments will be wanting to address policy problems in agri-food production systems and infectious diseases arising out of economic, demographic and climate pressures. Given that all solutions to these issues require some form of detailed computational analysis, the Committee advised the VLSCI to focus its case for sustainability around this increasing need for computational power and intellectual capital, both already in high demand within Australia.

With the conclusion of the 2010-2014 Grant funding period, this Committee's work has been suspended pending the University's examination of a new governance structure. I thank all Committee members for their enormously generous and valuable contributions of time and ideas over the years and know we all look forward to hearing of a sustainable funding solution for this highly successful and crucial infrastructure, beyond the new funding awarded for 2015-16 by the Victorian Government in October 2014.

Professor Tony Bacic
Personal Chair FAA, Director, Bio21 Molecular Science & Biotechnology Institute, Director, Plant Cell Biology Research Centre (PCBRC), Deputy Director, ARC Centre of Excellence in Plant Cell Walls, School of Botany, University of Melbourne.

DIRECTOR'S REPORT

It is my pleasure to commend to you my fifth VLSCI Annual Report. The growth of the enterprise continues to display its success: starting with 62 projects with 241 people from 11 Institutes as listed in 2010 data, by 2014 this had grown to 169 projects, 742 people and 50 institutes. In addition, 20 subscriptions to the LSCC are now generating a healthy income stream to support our work and they represent some significant new initiatives in life sciences computing such as the Melbourne Genomics Health Alliance, microbial genomics at the Microbiological Diagnostic Unit and clinical genomics at Cancer Council Victoria.

When VLSCI was first established, Dr Ewan Birney, now Associate Director of the EMBL-European Bioinformatics Institute (EMBL-EBI) had emerged from early work on the Human Genome Project and work on a number of large-scale genomics projects and was engaged as an early advisor to VLSCI, having been co-opted to the Scientific Advisory Committee. It is worth quoting him then, from the ECCB14 Conference in France in September 2014, where he pointed out that molecular biology is now

> *'a leading example of a data intensive science, with both pragmatic and theoretical challenges being raised by data volumes and dimensionality of the data. These changes are present in both large-scale consortia science and small-scale science, and across now a broad range of applications – from human health, through to agriculture and ecosystems. All of molecular life science is feeling this effect.'*

He went on to describe a shift from the 'blue collar' challenges of data volume to the 'white collar' challenges of interpretation.

My own engagement with this period has been as an expert in high-end computing with a scientific background

in computational chemistry, drafted into the biological sciences to bring that mature knowledge of scientific computing and complex technical procurements to this emerging scientific world of life sciences computing. As I write this, having spent the past five years establishing this unique facility for Australia, I have resigned as Director as of March 2015 to return to those chemistry roots in Europe.

VLSCI is now a mature enterprise, researchers and students are aware of their computing needs and we are meeting their needs. Training continues and grows. We are well equipped to continue to deliver what is needed for Australia's ever-growing demands in life sciences computing, especially in bioinformatics. The future for VLSCI will be in meeting those 'white collar' interpretation challenges mentioned by Ewan.

The most exciting part of the past five years has been to see the way VLSCI has impacted research through the combination of all of its parts – the facility, the experts, the outreach program and Victorian Government support in other ways. A personal favourite has been to see my dear friend from the UK, VESKI innovation fellow Tiffany Walsh, Professor in Bio/Nanotechnology, Institute for Frontier Materials, Deakin University, arrive to set up her lab, bring with her significant overseas funding and start producing some exciting science which is of great interest to industry. At the end of 2014, Prof. Walsh reported she had commenced negotiations for a consultancy with CSL Ltd in Parkville to help develop a knowledge-base to enable the rational design of new therapeutics. I am hopeful that this consultancy will develop into a longer-term partnership. And none of this would have been possible without the high-end computing capacity at VLSCI which lured Prof. Walsh back to Victoria.

The Victorian Government is to be commended for its vision in establishing programs like VESKI, for funding VLSCI in 2009 and in recommitting to its future through additional funding granted in 2014 for continuing in 2015-16.

Having already done so personally, I also wish to restate here my sincere thanks and gratitude to all Committee members for their support, time and energy given to VLSCI over the past five years.

The 2014 Annual Report data once again shows just how far VLSCI reaches beyond its immediate stakeholders and is now taking its place in Australia as a significant centre for life sciences computing. I will look forward to its future development with pride in what has been achieved to date and great interest in its future progress.

Professor Peter R. Taylor
Director

VICTORIAN LIFE SCIENCES COMPUTATION INITIATIVE **ANNUAL REPORT 2014**

01.

VLSCI now

VLSCI is funded by the Victorian Government and contributing institutions and is hosted by the University of Melbourne. This petascale facility delivers expertise and systems for life sciences computing.

ABOUT THE **VLSCI**

The Victorian Life Sciences Computation Initiative (VLSCI) combines collaborative research expertise with high end computing. The critical infrastructure and expertise offered by VLSCI has become essential to local life science research disciplines involving big data such bioinformatics, computational biology, computational imaging, advanced modelling and bioengineering.

What does the VLSCI do?

Empowering the life science research community through access to state-of-the-art resources, centralised computational expertise, know-how and training services, VLSCI:

- provides a world-class computational service that supports the transformation of life sciences research through high end computing
- provides researchers with the capability to address much larger life sciences research problems than previously addressed in Australia
- facilitates greater research collaboration within Victoria, nationally and internationally
- develops skills in computational biology, bioinformatics, advanced simulation and modelling, data management and more generally the application of advanced computing in life sciences
- supports industry development through the uptake of computational research in life sciences
- collaborates with Australia's major computational infrastructure and networking activities such as NeCTAR to support and increase access for researchers across Australia
- works with Australia's other high-end computer centres to promote Australia's capacity in high-end computing and to create standard access processes.

A model of success

The state-of-the-art equipment and high-level experience and expertise enables Australian research to compete globally and attract international funding.

The Peak Computing Facility (PCF) includes the biggest supercomputer dedicated to life science research in the world. Staff offer specialist technical expertise and services to maximise user experience and ensure efficient access to computing resources appropriate to life science research, including hardware and software documentation.

The Life Sciences Computation Centre (LSCC) has built specialist teams to support researchers and drive capacity-building activities. These expert teams have been spread across multiple research institutions to accelerate life sciences computing.

The Outreach and Skills Development Program provides a diverse program of events and activities to engage researchers, students, stakeholders, experts and the public in life sciences computing.

OUR **PEOPLE**

Directorate

Prof. Peter R. Taylor *Director*

Ms Karin Diamond *Business Manager*

Ms Fiona Kerr *Executive Officer*

Ms Claudia Curcio *Reception/Administration Assistant*

Ms Laura Williams *P/T Reception/Administration Assistant*

Communications, Skills and Development

Ms Helen Gardiner *Communications Manager*

Dr Christina Hall *Communications Officer*

Computing Facility

Dr Vera Hansper *Facility Manager*

Mr Bob Danani *HPC Specialist IBM*

Dr Andrew Isaac *Specialist Programmer*

Dr Jeff Tan *HPC Specialist IBM*

Dr Michael Kuiper *Computational Molecular Scientist*

Mr Matthew Wallis *HPC Specialist IBM*

Dr Matthew Hodges *Systems Administrator (to Apr. 2014)*

Dr Bernard Pope *Specialist Programmer*

Mr Chris Samuel *Senior Systems Administrator*

Mr Carl Thomas *Storage and Infrastructure Administrator*

Ms Jin Zhang *Systems Administrator*

Life Sciences Computation Centre

A/Prof. Andrew Lonie *Head, LSCC*

Dr Enis Afgan *Research Scientist*

Ms Charlotte Anderson *Bioinformatician/Research Assistant*

Dr Dieter Bulach *Senior Research Scientist*

Ms Jessica Chung *Bioinformatician/Research Assistant*

Dr Ira Cooke *Research Scientist*

Ms Harriet Dashnow *Research Scientist*

Prof. Gary Egan *Theme Leader, Computational Imaging*

Dr Nuwan Goonasekera *Software Engineer*

Mr Simon Gladman *Research Scientist*

Dr Nathan Hall *Senior Research Scientist*

Dr Chol-hee Jung *Research Scientist*

Dr Itamar Kass *Research Fellow*

Mr Yousef Kowsar *Scientific Software Developer*

Dr Khalid Mahmood *Research Scientist*

Dr Juan Nunez-Iglesias *Research Scientist*

Dr Amanda Ng *Computational Imaging Scientist (to June 2014)*

Dr David Powell *Research Scientist*

Dr Gayle Philip *Research Scientist*

Mr Andrew Robinson *Scientific Programmer*

Dr Torsten Seemann *Senior Research Scientist*

Dr Clare Sloggett *Research Scientist*

Prof. Brian Smith *Theme Leader, Molecular Modelling*

Dr Michael Thomas *Research Fellow*

Dr Fernando Rossello *Research Scientist*

Dr Paul Harrison *Research Scientist*

IBM Research Collaboratory for Life Sciences - Melbourne

Dr John Wagner *Manager and Research Staff Member*

Dr Daniel Oehme *Research Staff Member*

Dr Stephen Moore *Research Staff Member*

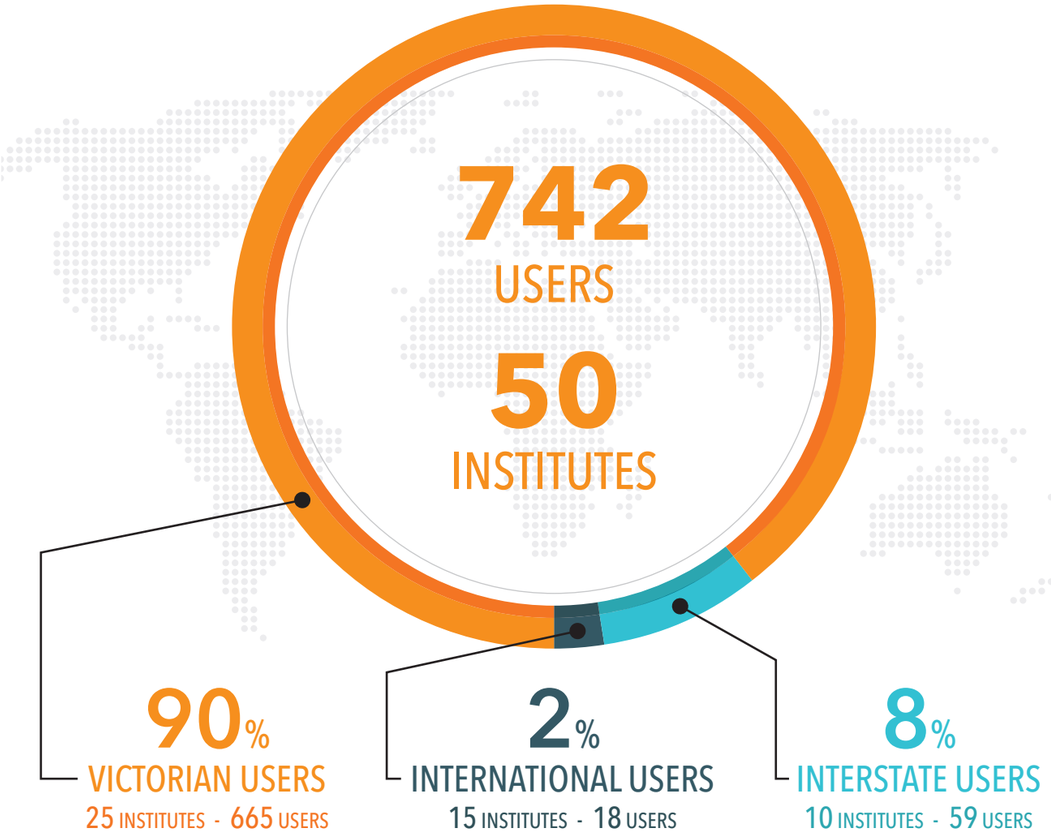
Dr Matthew Downton *Research Staff Member*

02.

2014 Snapshots

Local, interstate and overseas collaborations led to a 13% increase in users, more high quality publications, grant income success and new Victorian jobs in 2014.

RESEARCH **IMPACT**



The 59 interstate users (including those accessing systems through NCMAS) came from ten institutions: the Universities of Adelaide, Curtin, Sydney, Wollongong, New South Wales, Queensland, Sunshine Coast and Western Australia, the Australian National University and another ten were from sundry institutions.

Eighteen users from 15 international institutes accessed VLSCI systems from Denmark, Turkey, Poland, England, Germany, Finland, Sweden and from high profile organisations such as the Life Technologies, the Wellcome Trust Sanger Institute, Imperial College London, University of Oxford, Max Planck Institute for Biochemistry, Georg-August-Universität Göttingen, EVADO eClincial Solutions, and New York University School of Medicine.

Having a very large number of processors enabled us to run hugely parallel jobs. This was particularly beneficial to one part of our project which involved doing molecular docking to find new inhibitors of a membrane protein. Having so many processors allowed for many drug candidates to be examined in a range of conditions, all within a limited space of time.

Publications – Impact

There are many different ways to measure the impact of research publications and all institutions and disciplines are reviewing their methodologies constantly. Journal Impact Factors (JIF) offer one measure to assess VLSCI's success.

In 2012, of the 81 published journal articles generated by VLSCI merit-allocated projects, the JIF ranged between 0.818 and 21.543, with an average impact factor of 3.770.

In 2014, of the 86 published journal articles generated by VLSCI merit-allocated projects, the JIF ranged between 1.119 and 31.477, with an average impact factor of 5.593.

Of the 90 published articles reported, 64 (i.e. 71%) were in journals that are in the top 25% (Q1) of their discipline categories.

For listings of all Publications, go to Active Projects, see pp 78-91.

We are developing custom statistics software to discover novel genomic regions associated with breast cancer and colorectal cancer risk from high dimensional genomics data sets. The software is specifically designed to take advantage of the large-scale parallel computing architecture of the BlueGene/Q (that is, the large number of CPU cores). Importantly, VLSCI has provided us with parallel programming support throughout the existence of the project. This has been extremely valuable and the project would not be nearly as successful without their help.

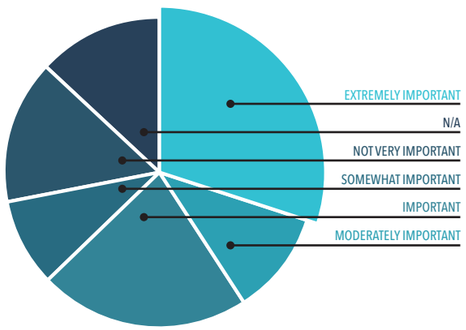
Grant Income

Chief Investigators were asked to nominate what sources of grant income they accessed for their work on VLSCI systems in 2014. This is seen as a measure of the importance of access to the systems to carry out the work funded by the grant, or in attracting the grant in the first instance. In 2014, a total of over $57m in annual grant income funding was supporting VLSCI projects and while the majority of funding was through the ARC, a trend towards more NHMRC funding was observed. This is seen as an indication of the growing data analysis needs of the health and medical research sector.

FUNDING SOURCE FOR 2014	$
International	5,586,667
ARC	32,456,068
NHMRC	18,856,423
Other, Aust	686,559
TOTAL - ALL	**57,585,717**

Note: Approximately $1.44m of grant income was for NCMAS projects outside of Victoria.

63% of Chief Investigators allocated resources on VLSCI systems rated access to VLSCI facilities as somewhat important to extremely important to their **grant funding success**:



Employment

33% of Chief Investigators allocated resources on VLSCI systems reported increased capacity to employ additional staff/students as a result of their 2014 VLSCI project:

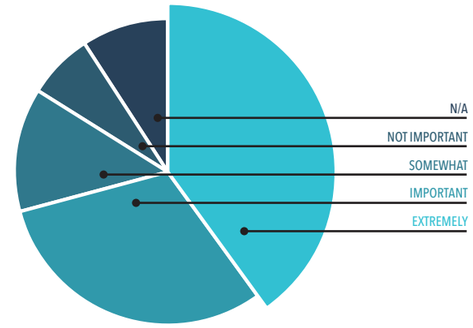
Undergraduate.....22
Postgraduate.....36
Post Doctoral.....15
Other.....4

Chief Investigators also reported other direct benefits to their projects through staff and students accessing outreach opportunities:

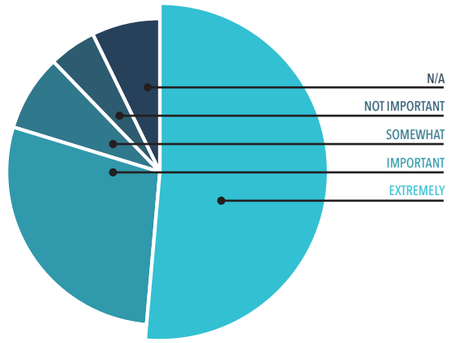
UROP student.....6
Seminars.....43
Travel/conference grants.....19
PhD top ups.....6
Internships.....10
Sponsoring of own conference.....8

Without VLSCI, we would not have been able to attempt working on such an ambitious model, because, even though access to computational resources could have been acquired elsewhere in principle, it would be impossible to carry out such extensive ad hoc prototyping work in that mode. The exploratory prototyping work was essential to make this project work.

Most Chief Investigators allocated resources on VLSCI systems reported that access to the systems was somewhat important to extremely important in **starting a new project**.

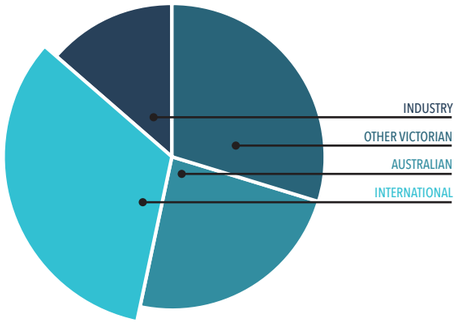


Most Chief Investigators allocated resources on VLSCI systems reported that access to the systems was somewhat important to extremely important in **carrying out an existing project**.



COLLABORATIONS

Chief Investigators allocated resources on VLSCI systems reported on the extent of their connectedness to other research teams via collaborations. The host institutes are reported on p 38. Of the 100 respondents, 66 reported they were working on projects with collaborators from other institutions. Of those 66, 58% were with other Victorian institutions, 45% with institutions in other Australian States, 64% with international groups and 26% were industry collaborations.



Before Avoca (BlueGene/Q) became available, it was not possible for the Australian part of the collaboration to contribute in this task.

Victorian Institutions collaborating on VLSCI projects:

- Alfred Hospital
- Baker IDI
- Bio21 Institute
- Burnet Institute
- Deakin University
- IBM Research Collaboratory for Life Sciences-Melbourne
- La Trobe University
- Ludwig Institute for Cancer Research
- Microbiological Diagnostic Unit, Public Health Laboratory
- Monash Institute of Pharmaceutical Sciences
- Monash University *(including Australian Centre for Blood Diseases)*
- National Herbarium of Victoria
- National Vision Research Institute
- Northern Health
- Murdoch Children's Research Institute
- Peter Doherty Institute
- RMIT University
- University of Melbourne
- Victoria University
- WEHI

Australian Institutions collaborating on VLSCI projects:

- ARC Plant Cell Wall Centre of Excellence
- Australian National University, ACT
- Bureau of Meteorology, ACT
- CSIRO
- Curtin University, WA
- Defence Science Technology Organisation
- Garvan Institute of Medical Research
- Office of Environment and Heritage, NSW
- Queensland Institute of Medical Research, QLD
- University of Adelaide, SA
- University of Queensland, QLD (incl. Australian Institute for Bioengineering & Nanotechnology and the Institute for Molecular Bioscience)
- NICTA
- University of New South Wales, NSW
- University of Western Sydney, NSW
- University of Wollongong, NSW
- Victor Chang Cardiac Research Institute, NSW

International institutions collaborating on VLSCI projects:

- Aix-Marseille Universite/CNRS, France
- Allan Herbarium, Landcare, New Zealand
- Alzheimer's Disease Center, NIH-funded, National Institute on Aging, USA
- Autonomous University, Barcelona, Spain
- Barcelona Supercomputing Center, Spain
- Biomedical Simulation Laboratory, University of Toronto, Canada
- The Bionics Institute, Australia
- Children's Hospital of Philadelphia, USA
- Florida Atlantic University, Miami, USA
- Guangzhou Institute of Biomedicine and Health, China
- Imperial College London, UK
- Institute for Biomedical Engineering & Informatics, Technical University, Ilmenau, Germany
- Institut Pasteur, France
- KAUST, Saudi Arabia
- Kinki University, Japan
- MD Anderson Cancer Center, Texas, USA
- Northwestern University, Illinois, USA
- Platform for Advanced Scientific Computing, Switzerland
- Prague Technical University, Czech Republic
- Sandia National Laboratories, California, USA
- Sanger Institute in Cambridge, UK
- Seoul National University, Korea
- University of Canterbury, New Zealand
- University College (Dublin), Ireland
- University at Buffalo, USA
- University of California, Davis, USA
- University of California, San Diego, USA
- University of Exeter, UK
- University of Florida, Miami, USA
- University of Lugano, Switzerland
- University of Malaya, Malayasia
- University of Manchester, UK
- University of Miami, Florida, USA
- University of Missouri, Columbia, USA
- University of Nottingham, UK
- University of Pottsdam, Germany
- University of Wisconsin, Milwaukee, USA
- Wellcome Trust Centre for Human Genetics, University of Oxford, UK
- Wellcome Trust Sanger Institute, University of Oxford, UK
- and sundry collaborators from Switzerland, The Netherlands, USA and Canada.

Industry Collaborations

- Joint Telstra/Swinburne University-funded Brain and Psychological Sciences Research Centre, Radiofrequency Dosimetry Laboratory, Australia
- BlueScope Steel, Australia
- Capsugel, France
- CSL Limited, Australia
- Floragenex, Inc., Portland, USA
- Heidelberg Engineering, Germany
- Haag-Streit Diagnostics, Switzerland
- Medtronic Australasia
- Neurosolutions Limited, Australia
- Servier Australia

MARTIN KRZYWINSKI
MELBOURNE TOUR

9 OCTOBER

ICT for Life Sciences Forum

Approximately 200 people attended Martin's talk titled: What does art have to do with science? There he challenged scientists to consider that the prevalent practice of 'letting scientific data speak for itself' does not necessarily allow it to be communicated – even amongst a small group of peers. And it gives the work no chance of having further impact, creating a wasted opportunity. He challenged those present to consider that ugly data does not necessarily make it more serious or trustworthy and that making it beautiful and approachable, can still mean it is trustworthy. Martin demonstrated ways people respond to visual information, adding that these insights should encourage researchers to respect the fact that their multiple audiences are discerning, visual consumers who are to be given as much consideration as possible in all efforts to communicate science. The talk promoted much discussion which continued on with students, guests and researchers at the informal reception hosted by the ICT Forum.

A pioneer of 21st century biological data visualisation.

WIRED, 6/11/13

One of my goals in life, which I can now say has been accomplished, is to make biology look like astrophysics.

Martin Krzywinski

10 OCTOBER

Masterclass

4 VLSCI PhD top-up students presented their work to an audience of 50 other PhD/Masters students.

Seminar

Over 100 attended a lunchtime talk on communicating science to scientists.

Left to right: Luisa Teasdale, Peter Hickey, Martin K, Brendan Ansell, Bernd Merkel

11-12 OCTOBER

Best student talk: David Budden (UoM0. Best Early Career Researcher talk: Belinda Phipson (MCRI). Presented by Andrew Lonie. Image courtesy of Matthew Wakefield.

ABiC

Martin attended the Australian Bioinformatics Conference with over 180 conference participants, many of whom interacted with Martin.

Co-sponsored by:

illumina

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LIFE SCIENCES COMPUTATION

12-15 OCTOBER

AGTA

Martin delivered an online Illumina webinar to over 200 registrants from Australia and South East Asia at the 2014 Australasian Genomic Technologies Association conference in addition to an Illumina booth presentation.

Left to right: Nick Wong, Adam Kowalczyk, Martin K, Ken Doig.

16 OCTOBER

Martin with a group from Elizabeth Blackburn School of Sciences

Workshops

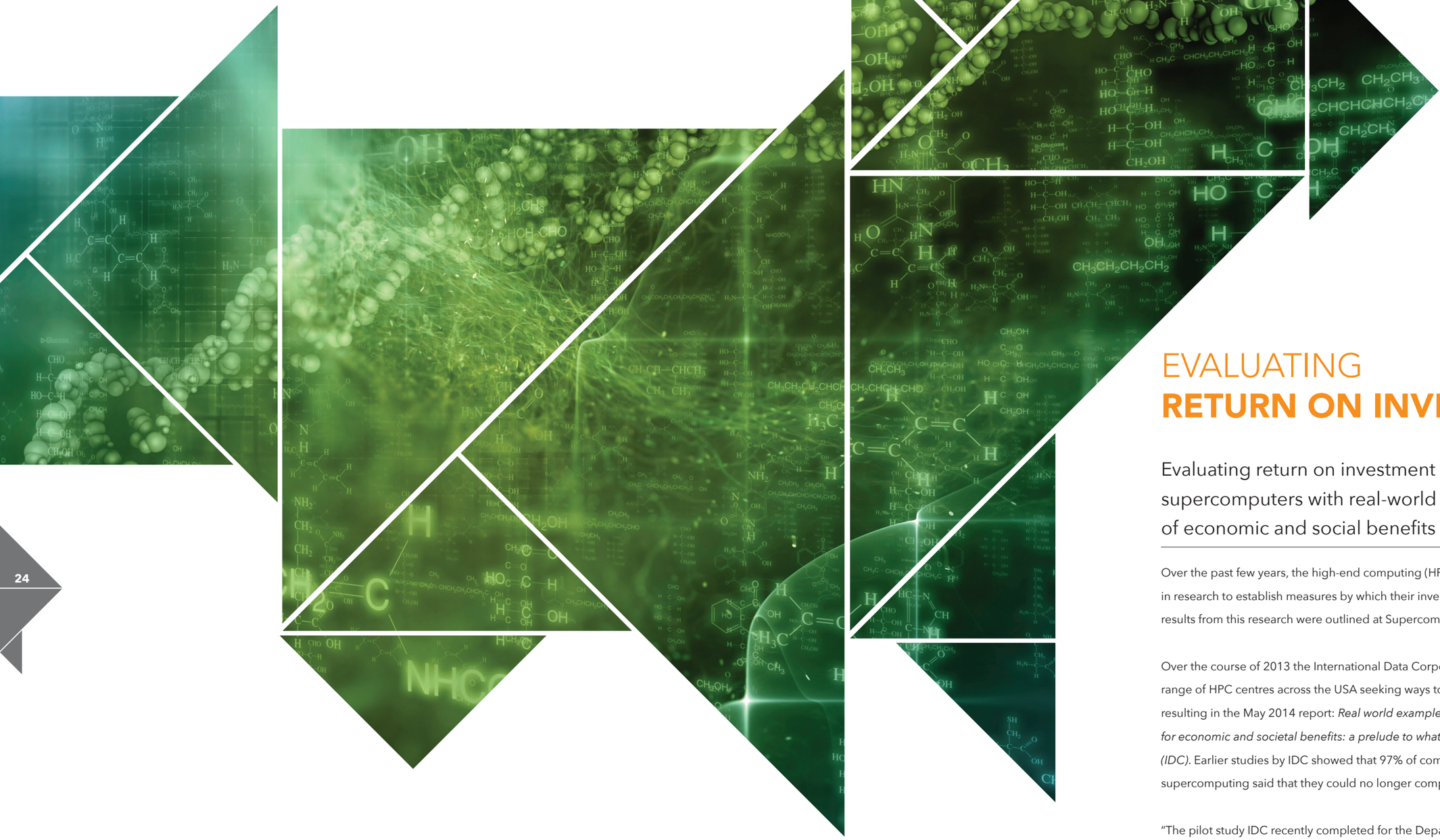
Peter Mac (100 staff and students)

WEHI (8 staff)

17 OCTOBER

Circos Plots - Train the Trainer workshop

20 LSCC staff enjoyed a one day workshop on this genomic visualisation tool as developed by Martin.



The life science expertise and pre-installed software packages are extremely valuable in reducing the workload. In addition, good fast and expansive storage reduces effort and time to produce results when coupled with adequate computing resource.

EVALUATING **RETURN ON INVESTMENT**

Evaluating return on investment (ROI) in VLSCI supercomputers with real-world examples of economic and social benefits

Over the past few years, the high-end computing (HPC) sector worldwide has been engaged in research to establish measures by which their investments may be evaluated. The early results from this research were outlined at Supercomputing 2013 in Denver, Colorado USA.

Over the course of 2013 the International Data Corporation (IDC) interviewed a range of HPC centres across the USA seeking ways to measure return on investment, resulting in the May 2014 report: *Real world examples of supercomputers used for economic and societal benefits: a prelude to what the exascale era can provide (IDC)*. Earlier studies by IDC showed that 97% of companies that had adopted supercomputing said that they could no longer compete or survive without it.

"The pilot study IDC recently completed for the Department of Energy provided further proof that HPC is one of the best investments many companies can make," said Steve Conway, IDC research vice president for HPC. "Successful CIOs will need to acquire this understanding or risk losing ground to competitors that learn how to exploit HPC effectively." Nov 2013.

Evaluating ROI in HPC at VLSCI – three case studies

Adapting some of the IDC high-level categories used to evaluate local HPC investment, these preliminary examples here focus on the rapidly expanding role of supercomputing in life sciences industries and begin to provide good evidence for investment in HPC systems and support in Australia.

By definition, industry return on investment uses the broadest possible definition of 'industry'; including education, health, academic and commercial collaborations and international exchanges.

CASE STUDY 1
Seeking out social networks

What was achieved?

This psychological sciences team, working with computer scientists, developed new methods for interrogating large datasets from social networks on supercomputers which has led to an international collaboration with the Science of Networks in Communities (SONIC) group at Northwestern University, Chicago, a leader in this field. University of Melbourne researchers developed and validated methods on VLSCI systems and a resulting collaboration with Prof. Noshir Contractor and others at the SONIC lab is seeing these methods applied to their much bigger data networks (eg. Facebook data), on the San Diego Supercomputing Center's (SDSC) systems through XSEDE, the Extreme Science and Engineering Discovery Environment in the USA. This gives Victorian researchers access to much larger data sets which will add further value to their work.

This work examined cultural dynamics and complex contagion; creating and verifying parallelised application for estimating model parameters of networks far larger than previously possible. This has applications not only in sociology, but also in epidemiology and health, for example in understanding the spread of disease.

Associated Organisations

Australia; University of Melbourne, Psychological Sciences and MelNet, a Melbourne-based consortium of universities with significant expertise in social network analysis, which conducts research and training in the theory, methods and applications of social networks.
USA; Northwestern University, SONIC Lab, Chicago, SDSC – system being used by SONIC via XSEDE, University of Illinois, lead institution for XSEDE, Chicago and the **UK**; University of Manchester, Mitchell Centre for SNA.

Industries

Health - medical and psychological, ICT, big data, engineering, education.

Innovation enabled

Traditionally social research has been limited in scale to thousands of face-to-face interviews, however online social networks generate tens of millions of interactions which can be analysed to produce new insights into how people interact in these networks. This information is of interest to a range of commercial and academic, health and medical, social and computer science researchers. Designing ways to interrogate such big and novel data collections requires smart algorithms and high performance computing, both of which have been successfully trialled on VLSCI systems.

Type of ROI

- generated intellectual capital
- increased Australia's reputation for social network research through a collaboration with an internationally renowned group in this field
- enhanced the reputation of Prof. Garry Robins, already an internationally-respected leader in his field, and his team
- improved institutional capacity to attract high-calibre students to work in Melbourne
- created an opportunity for Dr Alex Stivala, post-doctoral fellow, to work in the USA
- retained activity in Victoria, Australia and got access for Melbourne researchers to bigger facilities and funded projects in the USA
- opened a further collaboration in Switzerland.

Associated Income

- ARC, $414,444 over 3 years
- NHMRC/ARC Research Grant Support Scheme, $33,176 over 1.5 years

Outputs

Several papers are in preparation.

Broader Impact

Cultural transformation is required to meet many challenges such as climate change, accelerated globalisation, and the changing balance of economic, political, and military powers. Questions arise. How can we steer the course of our cultural transformation, so that future generations can inherit a sustainable world? How can we effectively analyse very large social networks to this end? How do cultural dynamics interact with social structure?

As well as the publications, collaborations and overseas supercomputer access (via collaborations), our work using VLSCI has led directly to a research grant from the US Air Force Office of Scientific Research (commencing 2015).

CASE STUDY 2

Finding the missing links in Australia's plant and fungi records

What was achieved?

At a time when the botanical world is quickly moving into next generation sequencing (NGS) techniques to extract new knowledge about the plant world, access to systems and expertise at VLSCI has enabled Royal Botanic Gardens Melbourne (RBG) staff to gain bioinformatics skills and develop techniques in population genetics and evolutionary studies. The RBG can now give the most up to date advice to stakeholders, on conservation genetics and taxonomy, something still not done in many other parts of the world. VLSCI has improved RBG's ability to understand Victoria's biodiversity and employ the latest bioinformatics resources to new projects.

With these new skills and established analytical pipelines to access VLSCI's systems, RBG staff are furthering their reputation and recognition, keeping them in the running for competitive grant funding, publications and international collaborations.

New collaborators have been found to extend these newly acquired skills into more projects investigating plant and insect interactions; the evolution and population genetics of Australian flowering plants; and, agricultural grasses and native orchids (a collaboration with Potsdam University, Germany).

Associated Organisations

Australia; Royal Botanic Gardens Melbourne, University of Melbourne, Bio21 and Departments of Botany & Genetics – including supervision of students by RBG staff, Monash University and La Trobe University, Department of Botany in Victoria. University of New South Wales, New South Wales, Australian National University, Canberra and **Germany**; University of Potsdam.

Industries

Horticultural, agricultural, cultural, biotechnology, education, ecology, state and federal government (management of public assets).

Innovation enabled

The Royal Botanic Gardens Melbourne (RBG) undertakes multiple projects studying plant and fungal biodiversity, with a focus on practical conservation outcomes. Several of these projects were advanced during 2013/4, using analyses conducted via VLSCI resources. VLSCI technical staff uploaded specific programs and advised researchers on how to analyse data more rapidly, doing computationally intensive analyses that would have been impractical to run on desktop computers (due to the time needed).

RBG has now increased its data collection and expanded the range and type of molecular biodiversity analyses undertaken and this has deepened advice now provided to State and other agencies.

Type of ROI

- generated intellectual capital with Victorian assets
- increased Australia's reputation for botanical and mycological research
- enhanced the reputation of RBG staff
- improved RBG's capacity to attract high-calibre staff and students
- strengthened collaborative ties with Australian universities
- created an opportunity for overseas collaborations.

Associated Income

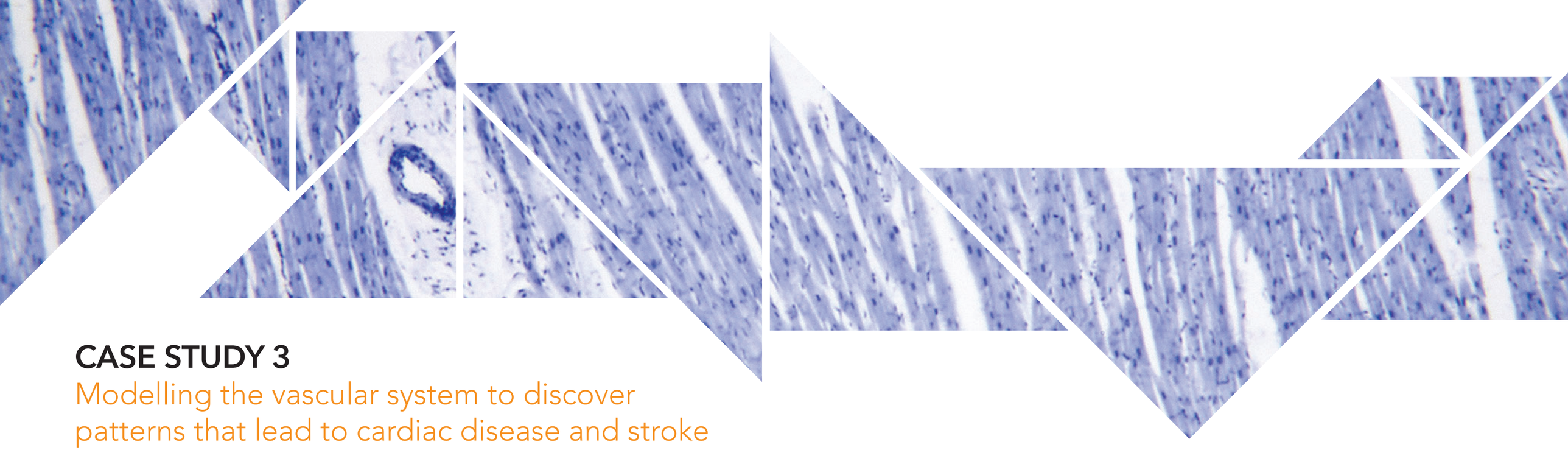
- ABRS Bush Blitz, $358,263 over 3 years
- ARC Discovery Grant, $452,000 over 3 years
- Hanson Construction P/L, $250,000 over 3 years

Outputs

Several papers published or in preparation in fields of biogeography, molecular phylogenetics and evolution, freshwater biology, aquatic botany, conservation genetics and botany.

Broader Impact

Next generation sequencing techniques give the RBG access to a treasure-trove of history, data and as yet identified new assets in the form of genetic information. Getting access to this information is exciting students and researchers, inviting collaborations and suggesting new ways for management to find new income streams for their ongoing work. This new information will also aid decision-making in Victorian natural heritage resources, conservation, and biodiversity which is of benefit of all.



CASE STUDY 3

Modelling the vascular system to discover patterns that lead to cardiac disease and stroke

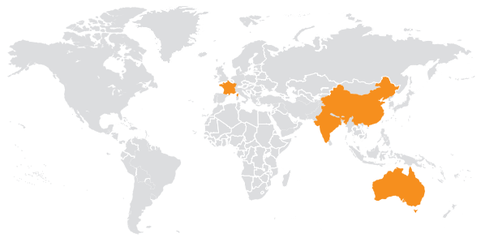
What was achieved?

Fluid dynamic simulation tools were developed to predict whether blood vessel plaques may be vulnerable to rupture by measuring the changes in blood flow patterns around atherosclerosis as well as the structural stresses in the vessel wall. A physiologically relevant computer model simulated the blood flow, the structural stresses and shear stresses around atherosclerotic plaques. At the same time, a large experimental program was implemented using micro-computed synchrotron X-ray tomography to obtain the digitalised artery geometries, atomic force microscopy to measure the anisotropic elasticity properties of the vessels, a vessel chamber set up to study the dynamics of the system and a nanoparticle investigation producing in vivo imaging of plaques.

An international team of engineers, medical researchers, a clinician, physicists, and biologists undertook this comprehensive and complex study, laying the foundations for the new nano- and bio- technologies theme (led by Prof. Kerry Hourigan, Monash University) of the recently established joint South-East University (SEU) - Monash Research Institute at Suzhou, China.

Associated Organisations

Australia; Monash University and Baker IDI / Alfred Hospital, Victoria, **China**; SEU, Suzhou, **France**; CNRS-IRPHE, Marseille, IMFT, Toulouse and **India**; IITB-Monash Research Academy, Mumbai.



Industries

Health and medical research, clinical applications, manufacturing, small technologies, education, preventative medicine.

Innovation enabled

For high performance computing to realise its potential in life sciences research, it requires researchers with big ideas. Prof. Hourigan embraced access to the facility to drive an international, multi-disciplinary program to investigate the mechanisms of cardiovascular disease, from the motion of small cells to the mechanical forces leading to vulnerable plaques, using theoretical, experimental including animal trials, and computational methods. Four major projects are now being formulated for the SEU -Monash Research Institute at Suzhou, China, to develop studies and devices in the area of bio- and nano- technologies.

Type of ROI

- generated intellectual capital with Victorian assets
- increased Australia's reputation in fluid dynamics research
- enhanced the reputation of Monash staff
- attracted ARC funding to Victoria, due to the visionary nature of the project
- strengthened ties with collaborators in France and India and enabled Monash University and the lead researcher to establish an exciting research program in China.

Associated Income

This entire program of work is funded by a series of ARC grants of approximately $1million with a further $3.5m grant for work being carried out at the National Computational Infrastructure in Canberra.

Outputs

Several papers published or in preparation in the Journal of Fluid Dynamics and the Computational and Structural Biotechnology Journal.

Broader Impact

Access to high-end computing was essential to being awarded the Australian Research Council grants. Now, more such interdisciplinary, collaborative projects are in the pipeline, enabled by this important infrastructure. For example, this project is linked to another joint project at the IITB-Monash Research Academy in Mumbai, which is working on the development of more efficient bioreactors, to culture pluripotent stem cells for the mass production of cardiomyocytes to repair tissue damage to the cardiovascular system.

03.

Supercomputer Systems

A world-class petascale facility focussed on the needs of life scientists.

The VLSCI Peak Computing Facility (PCF) is a world class petascale facility with three systems built on two architectures (BlueGene/Q and x86) which are dedicated to life science research. Each system offers varying memory and data-handling capacities to suit the large memory computational resources required by a range of tasks - from genomics through to high capacity processing of computational imaging data. From July 2015 a new system will be operational which is also specified to handle the needs of the bioinformatics and genomics communities (currently specified to be FDR14 with storage nodes connected at QDR (40Gb/s).

IBM Blue Gene/Q - Avoca

- Peak performance of 838.86 teraFLOPS.
- 65,536 PowerPC based 1.6GHz cores.
- A total of 64TB RAM
- Interconnect between compute nodes forms a five-dimensional torus providing excellent nearest neighbour and bisection bandwidth.
- Suitable for large-scale parallel processing.
- Compute nodes run a custom lightweight operating system called Compute.
- Node Kernel (CNK) that is similar to Linux and mostly POSIX compliant.
- The head node runs the RHEL 6 operating system, a variety of Linux.

IBM iDataplex x86 system - Merri

- Peak performance of 7.3 teraFLOPS.
- 688 Intel Nehalem compute cores running at 2.66GHz.
- 36 nodes with 96GB RAM and 8 cores per node.
- 44 nodes with 48GB RAM and 8 cores per node.
- 3 nodes with 1024GB RAM and 16 cores per node.
- Connected to a high speed, low latency QDR Voltair InfiniBand switch for inter-process communications.
- The system runs the RHEL 6 operating system, a variety of Linux.

IBM iDataplex x86 system – Barcoo

- Peak performance - compute nodes currently performing at 20 teraFLOPS - with Xeon Phi cards running nominally at 1 teraFLOPS each
- 1120 Intel Sandybridge compute cores running at 2.7GHz.
- 67 nodes with 256GB RAM and 16 cores per node.
- 3 nodes with 512GB RAM and 16 cores per node.
- 20 Xeon Phi 5110P cards installed across 10 nodes.
- Connected to a high speed, low latency Mellanox FDR14 InfiniBand switch for inter-process communications.
- The system runs the RHEL 6 operating system, a variety of Linux.

EXPERTISE

- HPC Systems Administration
- HPC programming
- Specialist HPC programming – parallelizing of algorithms
- Bioinformatics
- Molecular Modelling and Dynamics

STORAGE INFRASTRUCTURE

- 700TB GPFS Parallel Data Store (shared by Barcoo, Merri and Avoca)
- 1PB HSM tape system, made available through GPFS (shared by Barcoo, Merri and Avoca).

INTERCONNECT

A key feature of HPC systems is the interconnecting network (interconnect) between the computational nodes and also between the computational nodes and storage system. VLSCI supports a high speed (up to 40Gb/s for Merri and Avoca and 56Gb/s for Barcoo) Infiniband interconnect to provide extremely fast communication for data, both to and from storage and for internode communication during calculations.

SOFTWARE

From 'ACG' to 'Zlib' over 220 licensed software applications specific to life sciences are installed on VLSCI's systems, with technical staff available to install and troubleshoot new and customised software via a responsive help ticket system.

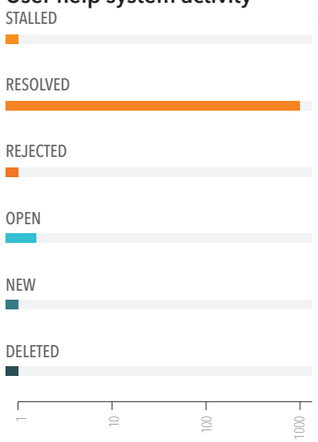
USER SATISFACTION SURVEY
DATA

Systems support services

VLSCI ensures user requests are dealt with promptly and efficiently by using a help request ticketing system.

This chart shows that 1053 help request tickets were dealt with by the PCF staff in 2014. This compares with 1292 in 2013 and 912 in 2012 and generally reflects that users have adjusted to the relatively new job scheduler, SLURM.

User help system activity



Reporting

VLSCI users' quarterly usage reports indicate the amount of 'in-kind' contributions made to the Initiative through the associated work being generated by access to this resource. In-kind contributions for 2014 were 34% over budget for Victorian institutions, with a trend also starting to be seen in interstate contributions. For more information, refer to Financial Reports, pp 100-104. Also, in-kind contributions are fully documented in the *Financial Supplement to the Annual Report 2014*, which is available upon request to the Business Manager.

Software

All backlog requests for generic and specialist life sciences software have been fulfilled and new requests continue to be implemented according to user demand.

Job queuing time

For all jobs that ran for one hour or greater, a measure is taken of how many waited for less than their estimated job time to begin executing. That is, the job remains in a queue for less time than its total estimated run time. While VLSCI aims to achieve 50% or greater, this indicator is consistently much higher.

MACHINE	NAME	2011 (%)	2012 (%)	2013 (%)	2014 (%)
SGI x86	Bruce *	76.0	85.5	91.0	85.5
iDataplex x86	Barcoo **	-	-	82.0	78.8
iDataplex x86	Merri	73.5	86.0	88.0	86.5
BlueGene/Q	Avoca	-	98.0	96.0	85.5
BlueGene/P	Tambo ***	97.5	96.0	-	-

* *Bruce was decommissioned at the end of June 2014*

** *Barcoo came online in late July 2013*

*** *Tambo was decommissioned in mid 2012 with the arrival of Avoca.*

2014 Highlights

The Resource Allocation Scheme (RAS) Round 8, for access to VLSCI systems throughout 2014, received 62 applications. Only one was rejected outright and four were found to be outside of the life sciences.

Round 9 was a special invitation-only round offered once funding for 2015-16 had been guaranteed. Existing users representing 9 projects (seven from Round 7 and two from Round 8) were invited to apply for further resources.

A major development project to upgrade the account management software (Karage) used by VLSCI and a number of specialist centres across Australia, was initiated in the second half of 2014. The Django specialist company, CommonCode, was commissioned to redevelop Karaage, originally developed by VPAC (now V3 Alliance). The project aims to improve the maintenance and updating of the software and to introduce new features to both improve the user experience and give system administrators and business managers valuable administration and reporting tools. VLSCI, working closely with V3 Alliance, aims to develop and license its use to HPC and specialist facilities.

With 15% of Avoca made available at the national level through the National Computational Merit Allocation Scheme (NCMAS), a total of 17 projects were approved from 18 applications.

A series of essential software updates were performed on all systems at the beginning of November, with minimal disruption to service.

Bruce was decommissioned at the end of June. The hardware was donated to the Melbourne NeCTAR node to provide spare capacity and its replacement was included in the 2015-16 budget submitted to the Victorian Government and secured in October. This replacement hardware (to be purchased in mid 2015) is for both this system and Merri, which will be decommissioned mid-2015.

As at November 2014, Avoca was ranked No. 76 in the Top500, No. 46 in the TopGreen500 and equal 7th in the Graph500. This list is updated twice a year, in June and November, and is avidly followed by high performance computer enthusiasts. The peak performance is measured using the LINPACK Benchmark – regarded as the industry benchmark for high end computing.

As at 31 December 2014 VLSCI's Avoca remained the fastest computer on the TOP500 list dedicated to life sciences computing.

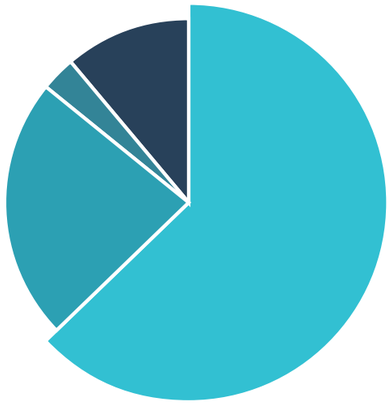
Refer to pp 78-91 for all projects running on VLSCI systems in 2014.

Operating at the petascale since July 2012

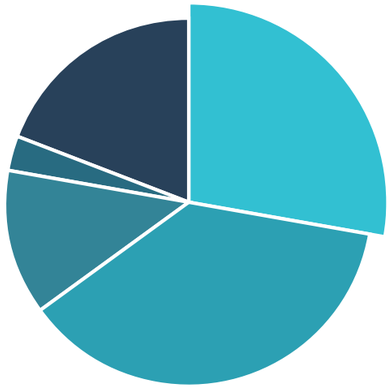
Communication Channels

Among the 100 respondents, overall user satisfaction remained very high and expert staff committed to this important initiative continues to be the key reason for this by Chief Investigators.

EMAIL HELP

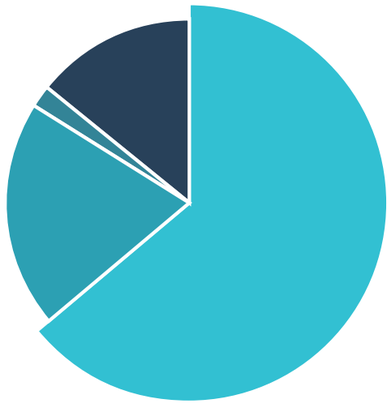


WEB CONTENT FOR TECHNICAL HELP

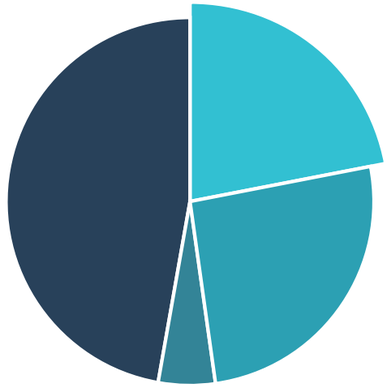


COMMUNICATION CHANNELS

SUPPORT STAFF



TRAINING AND EDUCATION

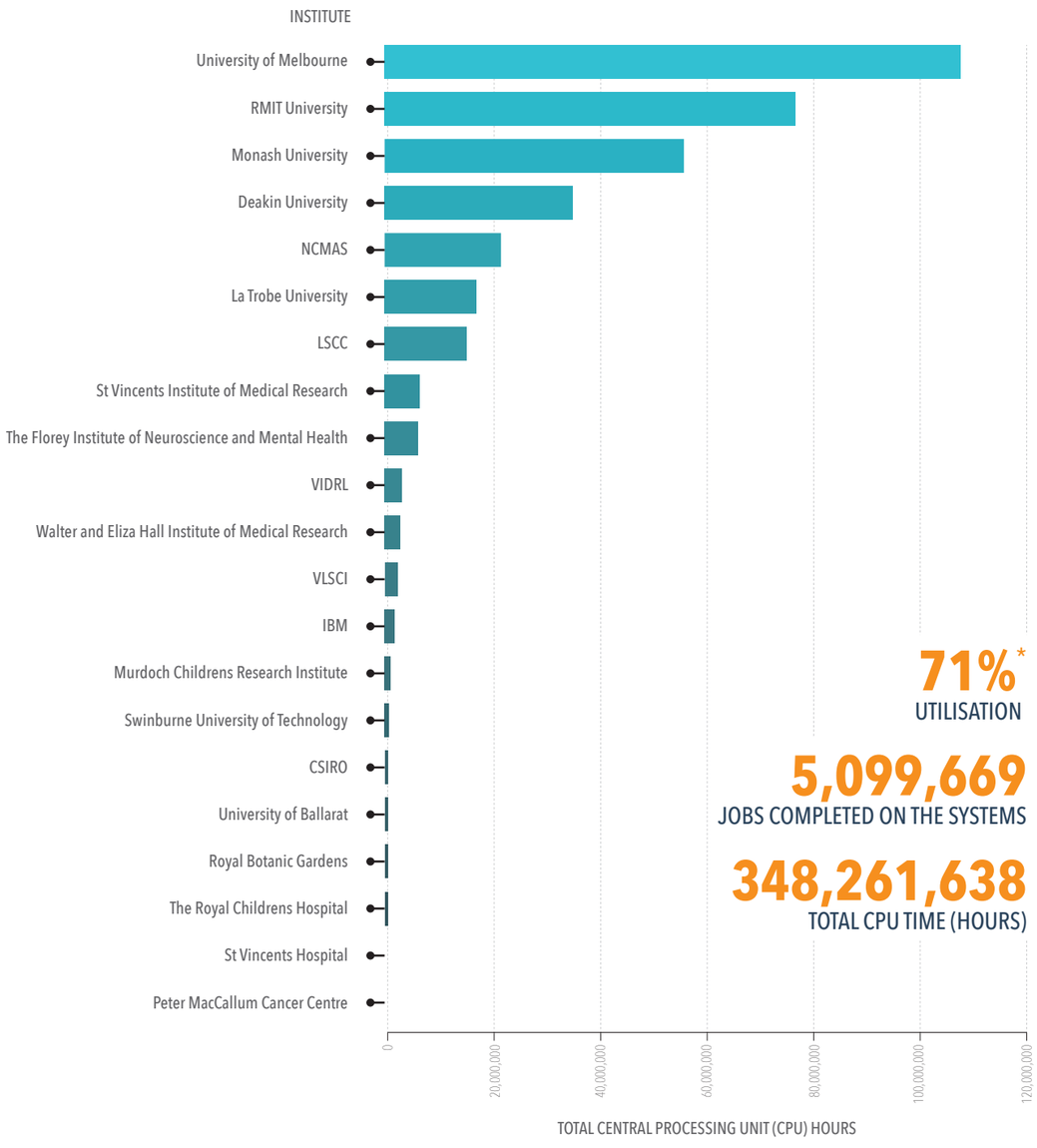


VERY GOOD GOOD ADEQUATE POOR VERY POOR N/A

Dr Marta Enciso, LIMS, and Mr Tamir Dingjan, MIPS, at the VLSCI RAS Presentation Day.

SYSTEM **USAGE**

The distribution of usage across project host institutes (in Victoria or via NCMAS) for the period 1 January to 31 December 2014.



71% *
UTILISATION

5,099,669
JOBS COMPLETED ON THE SYSTEMS

348,261,638
TOTAL CPU TIME (HOURS)

* *Utilisation is derived by dividing actual usage by the amount of resources (CPU hours) allocated. This figure is an average of the two types of systems – BG/Q and x86. The BG/Q utilisation dominates the overall system utilisation as capacity of that system is 10 times greater than that of the x86 systems. The projects which use the BG/Q necessarily require more complex algorithms to make the best use of the architecture. VLSCI finds that a nearly 72% utilisation figure for this system, and overall, is highly acceptable.*

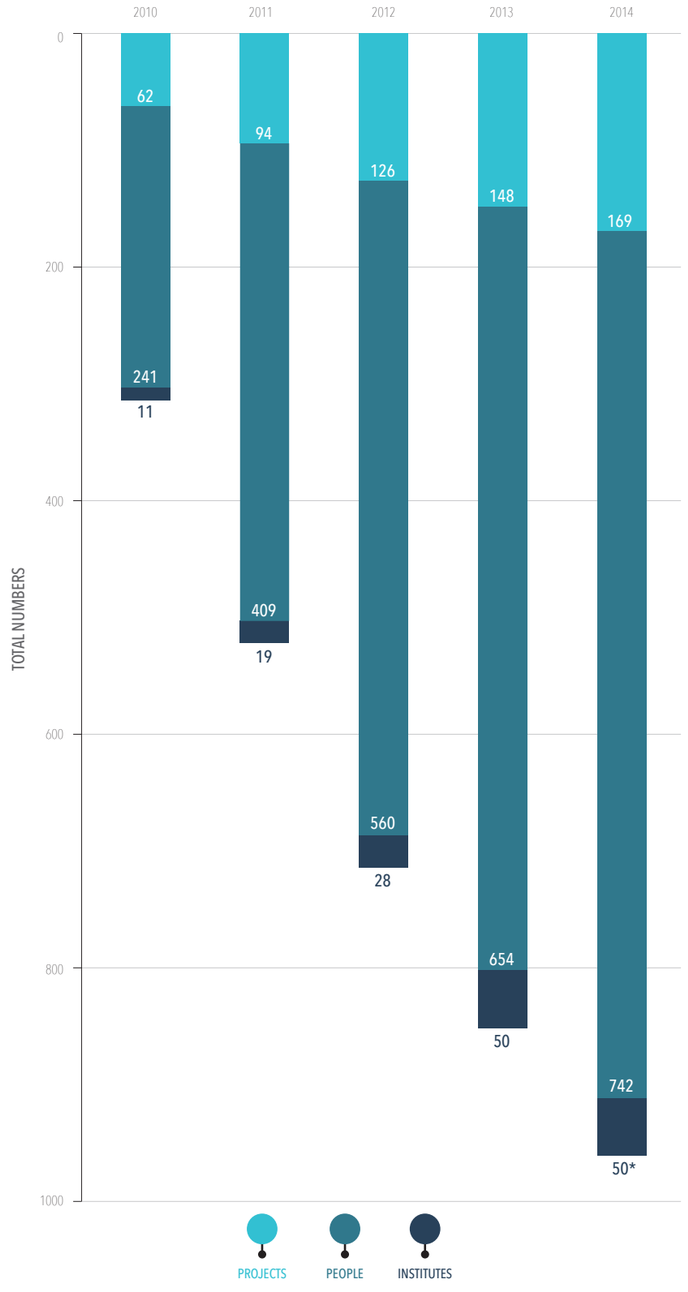
In addition to access to state-of-the-art high-performance computing, we have a long-standing project collaboration with VLSCI bioinformaticians resulting in joint bioinformatics pipeline development.

The RAS Committee is a peer review Committee which awards compute resources based upon merit to Victorian users. NCMAS users are awarded through that national scheme. Over 2014, projects ranged across broad discipline areas of Molecular Modelling & Dynamics, Cardiac Modelling, Device Design, Neuroscience, Cancer Genomics, Applied Modelling, Genomcis, Computational Bioimaging and BioEngineering.

Dr Vera Hansper
PCF Manager

Growth in Activity 2010-2014 - Projects, People, Institutes

The actual number of users accessing VLSCI systems continued to grow in 2014 by 13%.



* *25 were Victorian, 25 interstate and overseas, some via NCMAS*

04.

Life Sciences Computation Centre

A dedicated team of bioinformaticians and computational biologists offering expertise and system access for complex data analysis and modelling.

The LSCC team divide their time between research, training and platform development. Each of these activities attract funding from multiple sources and this creates extra capacity to continue to take on new projects. In 2014, LSCC staff were almost fully allocated to subscriber projects, with the rest of their time spent contributing to community capacity building activities and software development.

As projected at the beginning of the year, income for 2014 from both projects and subscriptions was almost $2 million. The growth in subscriptions reflects the effectiveness of the unique LSCC, where the management and analysis of large data sets is well-handled locally, the intermittent staffing requirements are leveled out and direct access to high end compute resources is assured, with subscribers not having to apply through the merit allocation scheme. Subscribers are building their local skills, capabilities and work pipelines to handle the growing quantities of data being generated by larger, more complex research programs with LSCC staff as collaborators, now with especially well-developed bioinformatics expertise, particularly in cancer, microbial and clinical genomics.

With funding from NeCTAR and the Australian National Data Service (ANDS), and in partnership with the University of Queensland (UQ), the very successful development and roll-out of the Genomics Virtual Laboratory (GVL), along with the development of training materials by LSCC staff, has enabled researchers to conduct their own complex data analysis on the Australian research cloud. The platform is in demand as a training tool and increasingly the team is undertaking to support teams across the globe to use the platform for their own training sessions. This has secured a place for LSCC expertise in the national research infrastructure landscape, now acknowledged through success in winning grants for new national initiatives.

Access to the VLSCI facilities has enabled us to do truly ground-breaking research and push the boundaries of what is possible in our field.

LSCC **HIGHLIGHTS**

- At the end of 2014 and following lengthy negotiations, VLSCI was well-placed to extend its current activities nationally through a new contract to host EMBL Australia's Bioinformatics Resources Australia – European Molecular Biology Laboratory (BRAEMBL) hub. This will see some of the successful training and development activities established through the LSCC rolled out across the Australian research community and will attract funding to further support these initiatives.

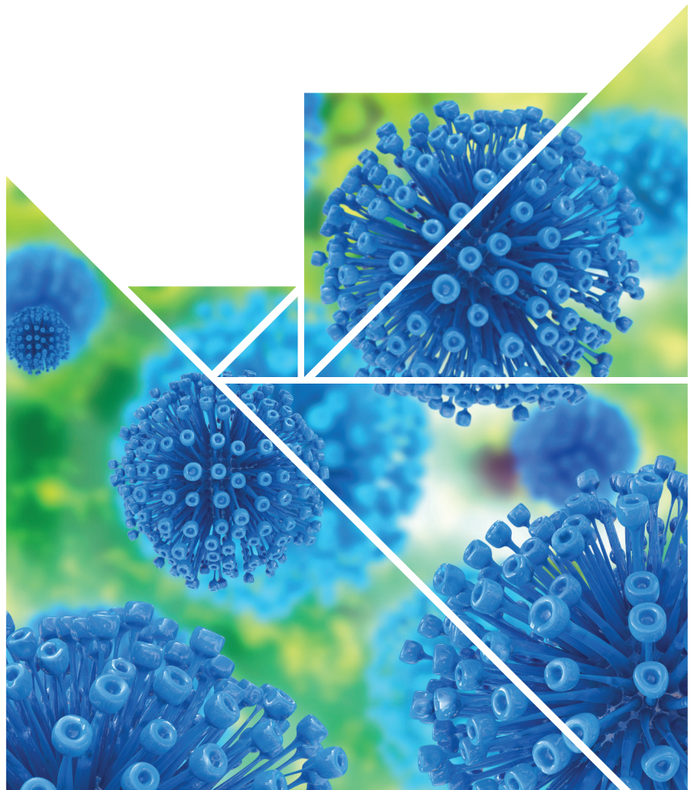
- Throughout 2014, staff were assigned training workshops to deliver and almost 1000 students and early career researchers attended these (for full details see pp 74-75). All workshops were evaluated and the overall level of satisfaction was excellent. Staff were also on the teaching team for the Australian Mathematical Sciences Institute's annual BioInfoSummer 2014 held in early December and based on the GVL.

- New funding was awarded through both NeCTAR and ANDS for two major infrastructure projects to roll out in 2015 in collaboration with the Research Computing Centre at UQ, with a total value of $350,000.

- The GVL training materials developed by LSCC staff continued to deliver outcomes, with workshops being held across Australia but also in the USA and India, where the Australian Genome Research Facility used the GVL to deliver a large Next Generation Sequencing (NGS) workshop for attendees from ten Indian institutions. Also in South Africa, the GVL Galaxy server was used to deliver the NGS variant detection tutorial to molecular biology students at the University of the Witwatersrand, Johannesburg.

- The GVL is now a mature platform, drastically reducing the price of entry to a legitimate genomics analysis environment. It has already been successfully implemented at Peter Mac for use by their bioinformaticians. Others to follow include the Universities of Western Australia, Sydney and Tasmania.

- VLSCI sponsored the inaugural Australian Bioinformatics Conference (ABiC 2014) in October and LSCC staff Torsten Seeman, Matthew Wakefield and Clare Sloggett were all on the program. Visiting VLSCI guest Martin Krzywinski (see report pp 22-23) was also included in the program and VLSCI awarded the following prizes: Best student talk - David Budden (UoM) and Best Early Career Researcher talk - Belinda Phipson (MCRI). Being the first significant conference dedicated to practising bioinformaticians to be held in Australia, the organisers delivered a popular event with which VLSCI was happy to be associated. One attendee commented that it worked because it delivered "Bioinformatics for bioinformaticians by bioinformaticians". Conference organisers were focussed on making the event representative of the community, and women were well represented both in the program and among the attendees (65% male, 35% female). With 78% of attendees being practising bioinformaticians, this investment in their careers is well-placed. Given most have already undertaken a minimum of five years of tertiary training along with more years working in a laboratory, there has already been a significant investment in their education and VLSCI is very focused on ensuring they stay supported in this industry.



Finding ways to diagnose lethal metastatic prostate cancer

Melbourne researchers are part of a world-wide effort to better understand prostate cancer through the use of next generation sequencing technologies and analysis of clinical data in collections around the world. One project, Australian Prostate Cancer Research Centre @ Epworth (APCRC@EPWORTH) has subscribed to the LSCC for one aspect of the research program. Dr Clare Sloggett, Bioinformatician and Research Fellow, LSCC, with research interests in statistical methods and machine learning, next-generation sequencing analysis, and cancer genetics, is helping to investigate lethal metastatic prostate cancer and expression signatures of high-grade prostate cancer. She is working with other bioinformaticians to develop software pipelines for whole-genome sequence analysis and transcriptome analysis, which are being used to determine the origin of these cancer types.

Dr Sloggett's access to VLSCI systems allows this complex analysis of large datasets to be done at the speed required to keep up with outputs for significant publications and at the end of 2014 some significant journal articles were in preparation for publication in 2015.

This world-wide research effort involves, in Victoria, UoM, NICTA, VLSCI, Peter MacCallum Cancer Centre, Monash University, Victorian Cancer Agency, VTCB, TissuPath, Australian Prostate Cancer Research, Cancer Council Victoria, La Trobe Institute for Molecular Science, in New South Wales, the Garvan Institute, AGRF, Australian Prostate Cancer Research, NSW, and internationally, Bar-Ilan University, Israel, Katholieke University, Belgium, Cambridge Research Institute and Wellcome Trust Sanger Institute, UK, University of Toronto and Vancouver Prostate Centre, Canada, and The Cancer Genome Atlas, Illumina and Memorial Sloan Kettering Cancer Center, USA.

Streamlining virus modelling processes at the Victorian Infectious Diseases Reference Laboratory

Drawing upon the pool of growing talent in the molecular modelling and dynamics community in Victoria, Mitchell Bartolo, Honorary Medical Scientist at VIDRL, was employed by VLSCI in 2014 to develop scripting methods to streamline the simulation and analysis of human enterovirus species and produce final models representing novel virus capsid structures for publication and future research. Under the direct supervision of Dr Jason Roberts, VIDRL, whose enterovirus (including polio) modelling on VLSCI systems has been well documented over the past five years, Mitchell's role in the project was to tidy up and automate the processes of building biologically relevant models for simulation, allowing future jobs to be launched quickly and without error. This work has been documented for use by others in the molecular modelling community across Victoria and beyond.

LSCC **SUBSCRIPTIONS**

The subscription model of engagement with LSCC which provides expert bioinformaticians and direct access to HPC systems continued to grow in 2014, from two subscribers in 2013 to 20 in 2014. A range of institutions and programs access our experts and systems to work on a range of community capacity building projects and large-scale research projects.

INSTITUTION	2014 SUBSCRIBER
Australian National University and Murdoch Children's Resesarch Institute	Prof. Simon Eastel
Cancer Council Victoria and Department of Pathology, UoM (2 projects)	Prof. Graham Giles Prof. Melissa Southey
Eastern Hill Precinct (St Vincent's Institute, St Vincent's Hospital, CERA)	Prof. Mark Cook
Melbourne Genomics Health Alliance	A/Prof. Clara Gaff
Monash Institute of Medical Research	A/Prof. Neil Watkins
Monash University, Central Clinical School	A/Prof. David Curtis
Monash University, Department of Anatomy and Developmental Biology	A/Prof. Jose Polo
Monash University, Department of Psychology	Prof. Nellie Georgio-Karistianis
Monash University, School of Biomedical Sciences: Biochemistry	Dr Traude Beilharz
NeCTAR Endocrine Virtual Laboratory	Prof. Richard Sinnott
NeCTAR Genomics Virtual Laboratory (3 projects)	A/Prof. Andrew Lonie
Royal Melbourne Hospital, Department of Surgery	A/Prof. Chris Hovens
University of Melbourne, Dental School	Prof. Eric Reynolds
University of Melbourne, Department of Microbiology and Immunology	A/Prof. Tim Stinear
University of Melbourne, Microbiological Diagnostics Unit	Prof. Ben Howden
University of Melbourne, School of Population Health: MEGA	Prof. John Hopper
Walter and Eliza Hall Institute, Stems Cells and Cancer Division	A/Prof. Clare Scott

LSCC **CAPACITY BUILDING PROJECTS**

In addition to formal subscriptions, LSCC bioinformaticians work with researchers to ensure their complex data analysis is timely and of high quality. Those teams to have benefitted from their help in 2014 were:

PROJECT TITLE	RESEARCHER	INSTITUTE
AGRF (various projects)	Ms Lavinia Gordon	AGRF
Interaction between boron nitride nanotubes and biological structures	Dr Tamsyn Hilder	ANU
Genetic and epigenetic effects of L-sulforaphane	Dr Tom Karagiannis	Baker IDI
Cancer methylation genomics	Dr Gianluca Severi	CEC
Eye disease genomics	Prof. Paul Baird	CERA
Quantum monte carlo method development	Dr Amanda Barnard	CSIRO
Modelling HIV proteins	Prof. Johnson Mak	Deakin
Network modelling	A/Prof. Mahdu Chetty	FedUni
Abalone transcriptomics	Dr Jan Strugnell	La Trobe
Calculating the pKa of 'superbase' molecules	Dr Peter Barnard	La Trobe
Dictoselium	Prof. Paul Fisher	La Trobe
Epigenomics	Prof. Emma Whitelaw	La Trobe
Fungal pathogens	Dr Kim Plummer	La Trobe
Modelling of *E. coli* AG43 autotransporter protein	Dr Begona Heras	La Trobe
Molecular modelling	Prof. Brian Smith	La Trobe
Self assembly of β-peptides into superstructures	Dr Adam Mechler	La Trobe
MCRI genomics	Dr Alicia Oshlack	MCRI
Oral Health CRC genomics	Various researchers	MDS
MHTP genomics	Various researchers	MHTP
3 RNAseq	Dr Traude Beilharz	Monash
Bacterial genome assembly and annotation	Dr Torsten Seemann	Monash
Clinical genomics school, general	Various researchers	Monash
High content screening	Prof. Bryan Williams	Monash
High content screening	Prof. Christophe Marcelle	Monash
Molecular animations of pore forming toxins	Dr Michelle Dunstone	Monash
RNA / genomics	Dr Traude Beilharz	Monash
Spiny Mouse genomics	Dr Hayley Dickinson	Monash
Transcriptomics and epigenetics of iPS cells	A/Prof. Jose Polo	Monash
Mollusc phylogenetics	Dr Adnan Moussalli	MuseumVic
Breast cancer exomes	A/Prof. Ian Campbell	Peter Mac
Ovarian cancer genomics	Prof. David Bowtell	Peter Mac
Sarcoma genomics	Prof. David Thomas	Peter Mac
TCGA melanoma genomes	A/Prof. Tony Papenfuss	Peter Mac
Transposable elements in intestinal cancer	Prof. Rob Ramsay	Peter Mac
Prostate cancer genomics	A/Prof. Chris Hovens	RMH
Elucidation of the transition pathway between open and closed states of GLIC, a ligand gated ion channel	A/Prof. Toby Allen	RMIT
Endometriosis	Prof. Peter Rogers	RWH

PROJECT TITLE	RESEARCHER	INSTITUTE
Metagenomic analysis of intestinal bacterial communities	Dr Leah Hickey	RWH
ADAR1	Dr Carl Walkley	SVI
Adenocarcinoma genomics	Dr Gavin Wright	SVI
Bone marrow transplant genomics	Dr Kathy Traianedes	SVI
EMPathy project	Prof. Erik Thompson	SVI
Genomics & immunology	Dr Mark Chong	SVI
Immunogenetics	Dr Tom Brodnicki	SVI
Mechanism of Type 1 diabetes	Prof. Tom Kay	SVI
Pore forming toxins of *Clostridium perfringens*	Prof. Michael Parker	SVI
Breast cancer genomics	Prof. Melissa Southey	UoM
Clinical genomics - general	A/Prof. Andrew Lonie	UoM
CO2CRC metagenomics	Dr John Moreau	UoM
Comparative genomics to define mammalian evolution	A/Prof. Andrew Pask	UoM
Drosophila metagenomics	Prof. Ary Hoffmann	UoM
Endocrine Virtual Laboratory	Prof. Richard Sinnott	UoM
Epilepsy genomics	Prof. Terry O'Brien	UoM
Evolution of pathogenic bacteria	A/Prof. Tim Stinear	UoM
Fungal genomics	A/Prof. Alex Andrianopoulos	UoM
Fungal genomics	Prof. Barbara Howlett	UoM
Genomic medicine	Prof. Graham Taylor	UoM
Glioblastoma genomics	Dr Theo Mantamadiotis	UoM
High content screening development	Dr Juan Nunez-Iglesias	UoM
Interactions of albumin with the neonatal FcRn receptor	Prof. Norman Saunders	UoM
Modelling antifreeze proteins at the ice water interface	Dr Angus Gray-Weale	UoM
Parasite genomics	Prof. Robin Gasser	UoM
Polymorphism mapping in parasitic nematodes	Prof. Robin Gasser	UoM
Population genomics of eucalyptus	A/Prof. Gerd Bossinger	UoM
Prion protein modelling	Prof. Andrew Hill	UoM
Public health microbiology	Prof. Ben Howden	UoM
Tammar wallaby genome	Prof. Marilyn Renfree	UoM
Walachia genomics	Prof. Ary Hoffmann	UoM
Whole genome breast cancer analysis	Prof. John Hopper	UoM
Cancer Genome Atlas analysis	Dr Gordon Smyth	WEHI
Colorectal cancer genomics	Dr Oliver Sieber	WEHI
Docking and pharmacophore modelling of inhibitors of BAK	Dr Guillaume Lessene	WEHI
Gating in potassium channels	Dr Jacqui Gulbis	WEHI
High content screening	Prof. Tony Burgess	WEHI
Melbourne Genomics Health Alliance	A/Prof. Clara Gaff	WEHI

Expert Working Group Activity

During 2014 the team established regular expert working group meetings where researchers (with or without subscriptions) now discuss and plan their experiments, work through data to be analysed, get advice on progress or just troubleshoot. These groups explored the following topics in 2014:

MICROBIAL & DE NOVO GENOMICS

21 Projects ranging from Acinetobacter resistance to Oral, Obesity and Asthma Microbiomes.

CLINICAL EXOME/GENOME ANALYSIS

14 projects ranging from the ALLOCATE project (Ovarian cancer) to the Endocrine Virtual Laboratory and the Mesothelioma Genome project.

EPIGENOMICS INTEGRATIVE ANALYSIS

13 projects ranging from bladder, breast and prostate cancer to investigating developmental changes in bone-bone marrow development.

RNA-SEQ & DE NOVO ASSEMBLY

24 projects ranging from HIV, Leukemia, stroke and diabetes to the Axolotl transcriptome.

MICROSCOPY

3 projects investigating colon cancer, mitotic chromosomes and spinal injury recovery in zebrafish embryos.

Software Development

The following open source projects had significant input into their design and implementation from VLSCI staff:

Annokey. Gene-based search for key-terms in the NCBI gene database and associated PubMed abstracts. http://bjpop.github.io/annokey/. Published in *Source Code for Biology and Medicine, 2014*. http://www.scfbm.org/content/9/1/15. Collaboration with GEL lab, Department of Pathology, UoM.

Rover. Read-pair overlap considerate variant-calling software for PCR-based massively parallel sequencing datasets. https://github.com/bjpop/rover. Simple, low-cost, modular targeted DNA sequencing technology. Supported by NHMRC project grant APP 1025879. Published in *Source Code for Biology and Medicine, 2014*. http://www.scfbm.org/content/9/1/3. Collaboration with the GEL lab, Pathology, UoM. Part of the Hi-Plex project: http://www.hiplex.org/.

FAVR. Filtering and Annotation of Variants that are Rare. https://github.com/bjpop/favr. Published in *BMC Bioinformatics, 2013*. http://www.biomedcentral.com/1471-2105/14/65/abstract. Collaboration with GEL lab, Department of Pathology, UoM.

Rubra. A bioinformatics pipeline. https://github.com/bjpop/rubra. Presented at the Bioinformatics Open Source Conference, 2013 (BOSC2013). Used by many bioinformatics projects at VLSCI.

Bpipe. A bioinformatics pipeline. https://github.com/ssadedin/bpipe. Published in *Bioinformatics 2012*. http://bioinformatics.oxfordjournals.org/content/early/2012/04/11/bioinformatics.bts167.abstract. Collaboration with MCRI.

SRST2. Short Read Sequence Typing for Bacterial Pathogen. https://github.com/katholt/srst2. Accepted for publication in *Genome Medicine, 2014*. Collaboration with UoM researchers Dr Kat Holt and Dr Mike Inouye.

HiTIME. High-resolution Twin-Ion Metabolic Extraction. https://github.com/bjpop/HiTIME. Submitted for publication in 2014. Collaboration with Department of Chemistry, UoM.

Methpat. A program for summarising CpG methylation patterns. https://github.com/bjpop/methpat. Poster presented at the Australian Bioinformatics Conference, 2014. Collaboration with the Ludwig Institute for Cancer Research.

Degust. A web tool to help analyse, visualise and fully appreciate Differential Gene Expression data from RNA-seq experiments. http://www.vicbioinformatics.com/software.degust.shtml. Collaboration with VBC, Monash.

Prokka. A software tool for the rapid annotation of prokaryotic genomes. http://www.vicbioinformatics.com/software.prokka.shtml. Published in *Bioinformatics, 2014*. Collaboration with VBC, Monash.

A/Prof. Andrew Lonie
Head, LSCC

05.

IBM Research Collaboratory for Life Sciences - Melbourne

From 2010 – 2014 IBM established the first IBM Research Collaboratory for Life Sciences in Melbourne. It was co-located with VLSCI. From 2015 its operations moved to the offices of IBM Research Australia.

2014 IN REVIEW
REFLECTING ON FIVE YEARS TOGETHER

As the IBM Research Collaboratory for Life Sciences-Melbourne (the Collaboratory) came to a close at the end of 2014, IBM and the University of Melbourne (UoM) had much to look back on with pride, having accomplished all that the two organisations aspired to when their partnership began. In addition to forming the basis for the expanding partnership that has developed since, the VLSCI and the Collaboratory have been the focal point for many great accomplishments in education, training and research.

Perhaps the biggest research accomplishment for 2014 was the deepening and progression of the Collaboratory's work with all three nodes of the ARC Centre of Excellence in Plant Cell Walls. This work involves computational investigations of plant cell wall polysaccharide synthesis, interactions and degradation. The last year saw great progress in building and simulating molecular models of cellulose synthase like (CSL) proteins in collaboration with Dr Monika Doblin at the UoM node; modelling of cellulose microfibrils and microfibril-microfibril interactions, in collaboration with Prof. Tony Bacic at the UoM node and Prof. Mike Gidley at the University of Queensland node; and on the molecular modelling and dynamics investigations into the evolutionary adaptation of substrate specificity in b-glucanases with Prof. Geoff Fincher at the University of Adelaide node. This work led to the acceptance of a second paper to the journal Plant Physiology, one of the two top journals for plant science, as well as the preparation of a third manuscript for publication in 2015. The Collaboratory also progressed to publication a project begun a year ago with Prof. Frances Separovic

IBM's John Wagner and Mathias Reumann (bottom left) help to kick off a major project led out of Prof. John Hopper's (Melbourne School of Population and Global Health) in 2012. In 2014 Prof. Hopper's team announced their new DEPTH algorithm which maximises the VLSCI systems and machine learning tools to get more out of genome- and epigenome-wide association studies. Their intention is to apply this hypothesis-generating tool to many of the vast data resources which have been generated through publicly funded research projects over many years to aid in cancer investigations.

VLSCI was the first choice for high-performance computing resource because the current ARC Linkage project is a joint project with IBM. More importantly, Dr. Stephen Moore's (IBM Collaboratory) experience in medical imaging modalities and computational fluid dynamics simulations of arterial flow has been essential for our team to kick start this project. Approval of a clinical procedure or a clinical device is a long process that involves multiple tiers of numerical tests before clinical studies in animals and humans. VLSCI has kindly provided an enormous amount of service units that are essential to this fundamental work.

Prof. Andrew Ooi, Associate Dean (Academic), Melbourne School of Engineering, University of Melbourne.

and Daniel Weber, characterising the lipid-binding site of the pore-forming protein toxin, Equinatoxin II, in micelles. Combining high-resolution solution state NMR to map the lipid-binding site through chemical shift perturbations with atomistic-level calculations of the protein-lipid interactions underlying the binding events has yielded great insight into these important toxins.

Finally, the Collaboratory continued to build on the many other research programs begun over the last few years. For example, our continuing collaboration with A/Prof. Ross Bathgate and Dr Daniel Scott at the Florey Institute of Neuroscience and Mental Health, and Prof. Stan Skafidas, UoM, has produced significant data from Dr Natalie Gunn's small angle x-ray scattering (SAXS) work using the Australian Synchrotron; and produced two additional papers for submission in early 2015. Collaboratory researchers continued to be involved in many of the large-scale projects allocated resources on VLSCI systems through the peer review process. These projects include VR0003, VR0082, and VR0276, and those with IBM Chief Investigators. They are documented in the ACTIVE PROJECTS table on pp 78-91. Collaboratory staff also continued with a wide range of teaching, skills development, student mentoring and supervision, and communications and outreach activities at VLSCI, as detailed in this report.

No doubt the most significant achievement, however, has been the lasting relationships and collaborations which have formed from working together side by side to build and grow not only the world class VLSCI, but also the high performance life sciences computing ecosystem across Parkville and beyond.

This is precisely what the University of Melbourne and IBM set out to accomplish five years ago, and this is precisely what has been achieved together during that time.

Collaborators in the Bionic Vision Australia research project include researchers at UoM, NICTA, UNSW and the National Vision Research Institute. Project Lead Prof. Tony Burkitt reported:

This work would not be feasible without access to VLSCI systems which were useful in handling the finite element problem that required a large amount of memory. Purchasing dedicated hardware for our group would have been costly, and would also have been wasteful, as the bottleneck in our work is the model design and setting-up time. Moreover, the parallel processing capabilities of VLSCI facilities sped up our calculations considerably. In practical terms, this means that we would not have otherwise been able to attempt working on such an ambitious model. Even though access to computational resources could have been acquired elsewhere in principle, it would be impossible to carry out such extensive ad hoc prototyping work in that mode. The exploratory prototyping work was essential to make this project work. Moreover, this work has led to new international collaborations through introductions to IBM's T.J. Watson Lab in New York, for which ongoing access to VLSCI facilities will be essential.

In the Community

IBM staff contributed to partner institution the University of Melbourne through the following roles:

John Wagner. Senior Fellow. Department of Electrical and Electronic Engineering, School of Engineering, 20 February 2012 to 8 July 2014.

John Wagner. Honorary Fellow. Department of Mathematic and Statistics, Faculty of Science, 2 August 2010 to 31 December 2014.

John Wagner. IBM-University of Melbourne Partnership Committee.

John Wagner. Scientific Committee Member. Centre for Neural Engineering, August 2011 to August 2014.

In addition to publications/presentations associated with Active Projects (pp 78-91), the following list documents additional work contributed to the research community by Collaboratory staff:

O. Creado, B. Srinivasan, P. Le, J. Tan. The ideal computing system framework - a novel security paradigm. The SIJ Transactions on Computer Science Engineering & its Applications, 2(3):35-44 (2014).

O. Creado, P. Le, J. Tan. An explicit trust model towards better system security in Fourth International Conference on Computer Science and Information Technology, Sydney, Australia, February 2014.

S.K. Kannam, Computational modelling of biosensors in Melbourne Meeting of Molecular Modellers, Melbourne, Australia, February 2014.

S.K. Kannam, S.C. Kim, P.R. Rogers, N. Gunn, J. Wagner, S. Harrer and M.T. Downton. Sensing of protein molecules through nanopores: A molecular dynamics study. Nanotechnology, 25(15):155502, 2014.

S.C Kim, S.K. Kannam, S. Harrer, S. Moore, M.T. Downton, J. Wagner. Geometry dependence of conductance drop in nanopore in the presence of a particle. Physical Review E, 89(4):042702, 2014.

J. Korte, K.J. Layton, B. Tahayori, P.M. Farrel, S.M. Moore, L.A. Johnston. Encoding chemical shift with rabi modulated continuous wave excitation in International Symposium on Magnetic Resonance in Medicine, Milan, Italy, 2014.

S.M. Moore, R.L. McIntosh, S. Iskra, A.W. Wood, Are RF exposure limits appropriate for adverse environmental conditions and the wearing of protective clothing? in BioEM2014, Cape Town, South Africa, 2014.

A.N. Simonov, W. Grosse, E.A. Mashkina, B. Bethwaite, J. Tan, D. Abramson, G.G. Wallace, S.E. Moulton, A.M. Bond. New insights into the analysis of the electrode kinetics of flavin adenine dinucleotide redox centre of glucose oxidase immobilized on carbon electrodes. Langmuir, 30(11):3264-3273 (2014).

D. Weber, S. Yao, G. Anderluh, T. Lybrand, M. Downton, J. Wagner, F. Separovic. Modelling the interactions of equinatoxin II with micelles in Biophysical Society, San Francisco, February 2014.

John Wagner, PhD
Manager and Research Staff Member
IBM Research Collaboratory for Life Sciences-Melbourne

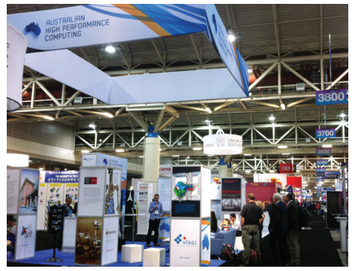
06.

Australian HPC at Supercomputing 2014

Australian high-end computing capacity and expertise on show at the world's largest supercomputing conference.

VLSCI Communications, with assistance from NCI, iVEC (Pawsey) and V3 Alliance, planned, coordinated, implemented and staffed the Australian HPC booth at Supercomputing 2014 (SC14) held in New Orleans, Louisiana, USA from 17-20 November. Other HPC Centres represented at the booth were MASSIVE, QCIF, Swinburne and CSIRO, joining in this unique opportunity to exchange expertise with over 10,000 participants.

This conference showcases what is new in high end computing and offers an extensive program of technical talks for our system experts. With three publicly-funded petascale facilities now in Australia - NCI in Canberra, Pawsey in Perth and VLSCI in Melbourne – the Australian HPC booth has for three years shown the rest of the world that Australia is a significant presence in high-end computing and has unique capabilities. At the booth there were formal talks about Australian science and systems, staff fielded enquiries from students and researchers looking for study and work opportunities in Australia and booth staff hosted the team of 25 staff attending from Australian facilities. Booth staff connected with colleagues from other institutions to share experiences and ideas.



Christopher Bording (Pawsey) and Vera Hansper (VLSCI) were both on the program committee for the *1st International Workshop on HPC User Support Tools (HUST-14)*. This successful workshop was established to build greater collaboration between HPC support teams all around the world, where system administrators, user support team members, tool developers, policy makers and end users discussed common issues and ways they might cooperate to solve them.

Elsewhere VLSCI's Senior Systems Administrator, Chris Samuel, presented a site report at the SchedMD booth outlining VLSCI's hardware, software and use of SchedMD's Slurm workload manager software.

The Communications team once again participated in an informal session entitled: *High Performance Communication for High Performance Computing (hpc-hpc)*, with Helen Gardiner sharing her work on applying some aspects of the IDC 'return-on-investment' methodology to the three VLSCI case studies (pp 25-31).

A highlight for visiting students from the John Monash Science School this year was the arrival at the booth of HPC legend, Chester Gordon Bell, to hear their presentations (top right: C.Gordon Bell chats with student, Anirudh Mittal). This generated some important social media activity also.

With the SC14 Top500 announcements, Avoca remained in the Top500. It now ranks 76th and is 46th in the Top Green500. Avoca also retained its equal 7th ranking in the Graph 500, the official benchmark for data intensive supercomputers as required for life sciences computing.

07.

Interactions

An extensive outreach program continues to deliver a slow and steady increase in visibility interstate and overseas.

Showcasing Research

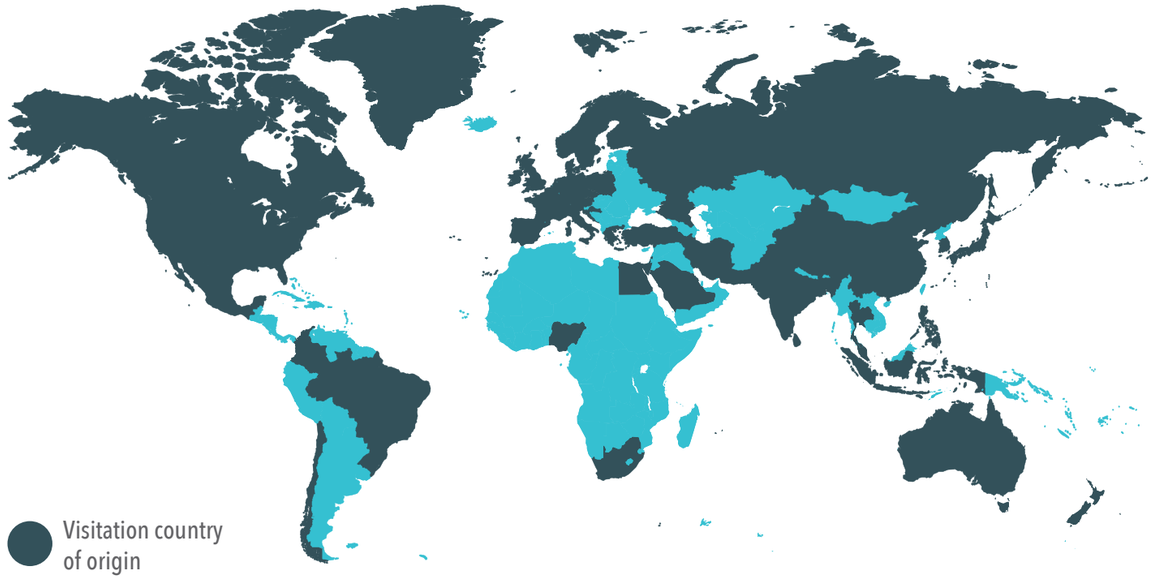
Forming part of Melbourne Knowledge Week, the **Superscience in Supercomputers** forum was held on 28 October. The event was designed to share stories that demonstrated how 'the world's largest supercomputer devoted to life science research is driving major advances right here in Melbourne' with a broad audience, which included Victoria's Lead Scientist, Ms Leonie Walsh.

The event was opened with a speech by the Chair of Knowledge City for the City of Melbourne, Cr Jackie Watts. The audience then heard how four of VLSCI's biggest users are using supercomputing to accelerate their research:

- **A/Prof. Tiffany Walsh** *(Institute for Frontier Materials, Deakin University)* finds ways to copy nature's building blocks to make new nano-materials.
- **Dr Michael Kearney** *(Department of Zoology, University of Melbourne)* models how animals might be affected by future climate scenarios.
- **Prof. Ingrid Winship** *(Melbourne Health / University of Melbourne)* uses complex data analysis techniques to characterise what defines an individual's predisposition to common cancers.
- **Dr Torsten Seemann** *(Victorian Bioinformatics Consortium, Monash University/LSCC)* uses microbial genomics techniques to investigate infectious disease outbreaks.

Superscience in Supercomputers speakers: Michael Kearney, Tiffany Walsh, and Torsten Seemann.

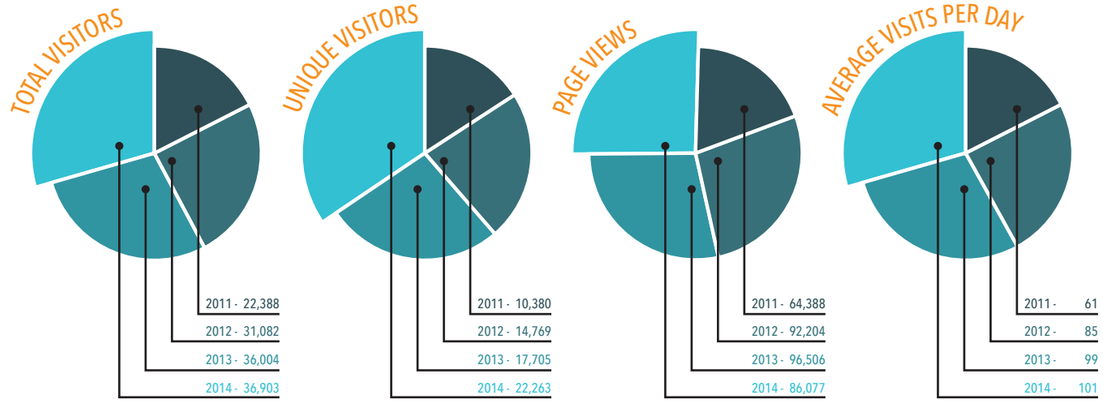
On 6 November, the VLSCI Resource Allocation Scheme Committee Presentation Day was held at the Woodward Conference Centre, Melbourne Law. This annual event provides the opportunity for RAS grant recipients to interact directly with the RAS Committee, hear how their peers are using VLSCI resources, and network with other researchers engaged in life sciences computation. More than 50 attendees and Committee members spent the whole day participating in a range of cross-disciplinary talks, posters and discussions.



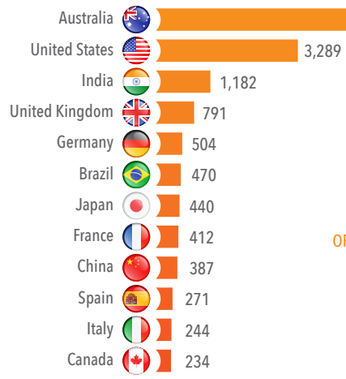
Visitation country of origin

160 COUNTRIES
138 DIFFERENT LANGUAGES

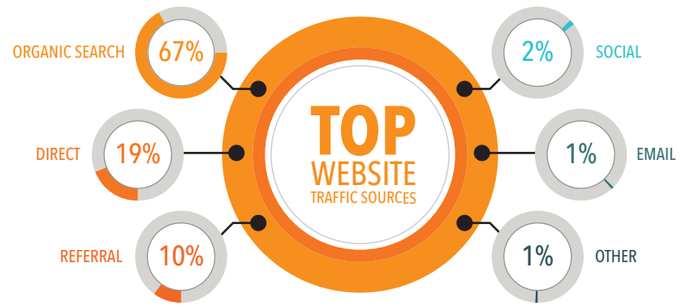
A pleasing trend over the past three years has been the gradual increase in international visitors to the website. As visitor numbers continue to rise overall, the percentage of visitors from countries other than Australia has increased from 25% in 2012, to 30% in 2013, and 36% in 2014. Notable increases in overseas visitors were from the USA, India, Brazil, Japan and France.

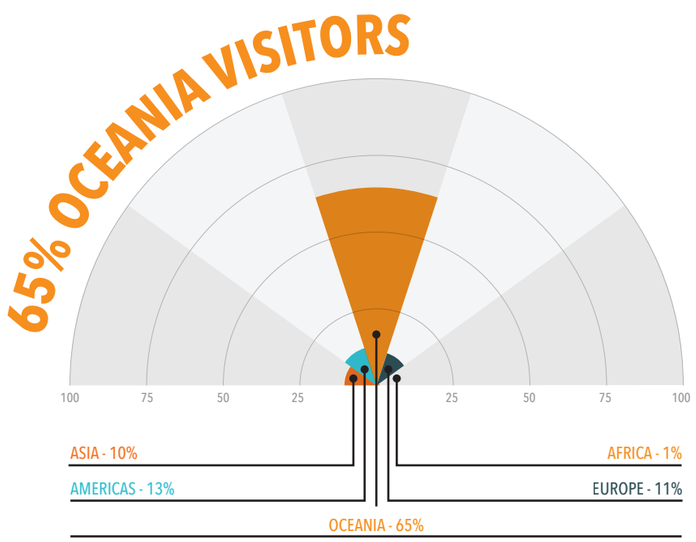


TOP 5 WEBPAGE VISITS
283,589 WEBSITE PAGE VIEWS
FROM 1 OCTOBER 2011 TO 31 DECEMBER 2014

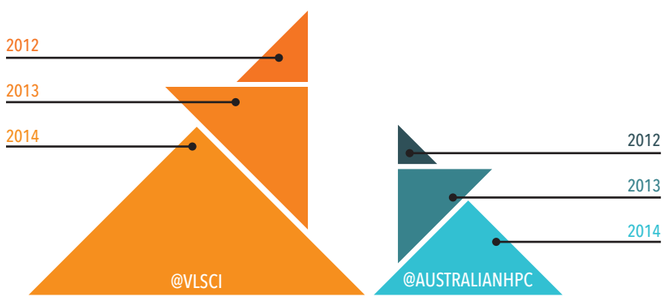


36,930 WEBSITE VISITORS
FROM 1 JANUARY 2014 TO 31 DECEMBER 2014





333% INCREASE in TWITTER
ACTIVITY ON THE @VLSCI TWITTER ACCOUNT BETWEEN 2012 AND 2014



The VLSCI twitter account, @vlsci, now has 400 followers (up from 120 in 2012 and 240 in 2013) and is one of the many ways users get up to date systems news as well as learn about outreach opportunities. As part of activities for the Australian HPC booth at Supercomputing 2014, VLSCI also hosts and maintains the @australianhpc twitter account.

Subscribers now include students, researchers, industry people and the high-end computing community across Australia and overseas.

IN THE **NEWS**

The growing public and media interest in the potential for precision and personalised medicine keeps VLSCI in the news. In 2014 the media strategy was focused on industry engagement, advocacy for funding and celebration of the part VLSCI played in several significant scientific achievements made by Victorian researchers.

ESTIMATED MEDIA VALUE	$
National television	100,000*
Major daily newspapers	174,500
National radio	26,400
Industry news	68,100
TOTAL	**369,000**

* *These figures are calculated according to media monitoring conventions that take the cost of buying the equivalent media space and applying a conservative multiplier of three to arrive at an approximate editorial equivalent value. This calculation does not consider whether people acted on such information but it also does not incorporate a measure of the extended coverage VLSCI stories received through associated social media and internet activity generated by the original stories.*

A highlight was the coverage of veski Innovation Fellow (now) Prof. Tiffany Walsh's work in Bio/Nanotechnology at the Institute for Frontier Materials at Deakin University. Prof. Walsh's high profile work covers a range of cutting edge technologies and is of interest to both the medical and defence industries.

Prof. Walsh's research into invisibility 'cloaking' received significant media attention early in the year with an ABC radio interview and newspaper and online coverage.

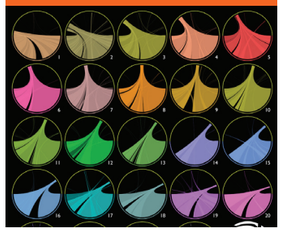
Photo courtesy of Star News Group

Prof. Walsh's work was also selected for inclusion in Stories of Australian Science 2014, 10000 copies of which are printed and sent to the Department of Industry in Canberra, to Tokyo to accompany Questacon's Science Circus tour of Japan, to Australian and international journalists including contacts at Nature, Scientific American, Science News, Reuters, the BBC, New York Times, Wall Street Journal, Asahi Shimbun and the Financial Times; to all Federal MPs and Ministers; science agency leaders; Australian embassies and consulates; foreign embassies in Canberra; science educators and students; and the broader science community.

VLSCI once again sponsored The Graeme Clarke Oration, delivered on 5 June by Dr Donald Ingber, Director, Wyss Institute for Biologically Inspired Engineering at Harvard University. Media and brand exposure was extensive via social media and interviews on ABC Radio – PM on 3 June, Revolutions with Jon Faine on 4 June and ABC Radio Adelaide on 6 June, and COSMOS Magazine. Refer p 77 for event data.

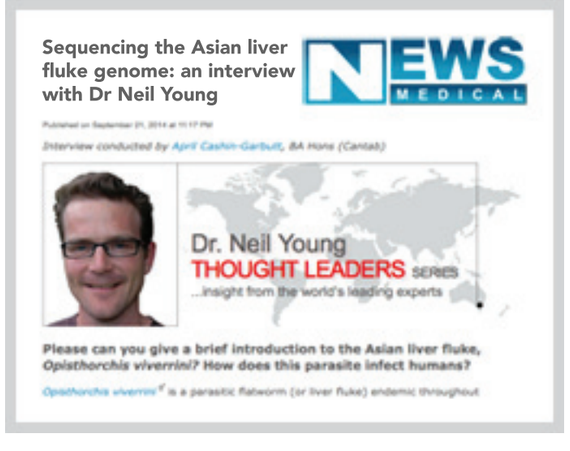
On 7 July the 2014 Scientific American Worldview measuring biotechnology innovation around the world reported Australia had moved from 7th position in 2013 to 4th position in 2014 with VLSCI claiming some part in boosting Australia's profile in this industry.

As highlighted on pp 22-23, the VLSCI/Illumina sponsored tour to Melbourne by data visualisation expert Martin Krzywinski created an opportunity to reach out beyond the life sciences computation community to the growing community of data visualisation researchers and students via traditional media and social media outlets.



Prof. John Hopper's new DEPTH algorithm, which is attracting cancer researchers around the world, received international exposure through a special feature in research media's journal, *International Innovation*.

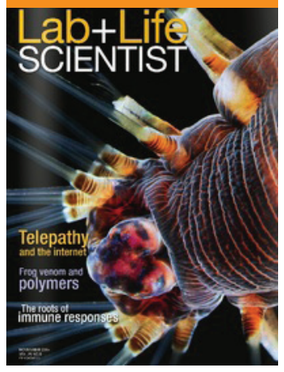
VLSCI prize donated to Kyabram library network for the best Neural Knitworks exhibit held as part of National Science Week.



HPC wire
Since 1986 - Covering the Fastest Computers in the World and the People Who Run Them

The Victorian Government announcement of renewed funding for VLSCI was well covered in the general and IT media.

Additional media included in particular, articles in the biotechnology industry journal *Australasian Biotechnology*, *Forbes Asia* online, *The Scientist* and *Australian Life Scientist* and *ABC Science* online.



INDUSTRY ENGAGEMENT

Ausbiotech *member, VLSCI has featured in articles in both Australasian Biotech and Australian Life Sciences journals*

Australian Bioinformatics Network *member*

Australian HPC Community *Australian HPC booth at Supercomputing 2014, New Orleans, Louisiana, USA in November*

Australian National Data Storage *LSCC project collaborations*

AMSI *collaborating to provide internships for post-graduate Mathematicians and Computer Scientists*

BioMedVic *Biomedical Research Victoria (was Bio21 Cluster) cooperation on events and sponsorship of UROP program*

BioMelbourne Network *member, VLSCI staff and associates attended a range of Network events throughout the year*

Bioplatforms Australia *delivering training and sundry programs*

COMBINE *Australian bioinformatics student collective, major sponsor*

eResearch Australasia 2014 *VLSCI staff attended conference in Melbourne in October*

HPC500 *High Performance Computing industry body accepted as member*

ICT for Life Sciences Forum *(now Convergence Science Network) sponsor of Forum and Graeme Clark Oration*

INCF *Victorian node co-sponsor*

ISC2014 *International Supercomputing Conference 2014 Facility Manager attended, Leipzig, Germany in June*

MGHA *Melbourne Genomics Health Alliance contributing bioinformaticians and computer systems for pilot programs*

NCMAS *15% of IBM Blue Gene/Q made available to Australian research community via this Scheme*

NeCTAR-funded Genomics Virtual Laboratory and Research Cloud *partnering to deliver these to the community*

Research Data Storage Infrastructure *LSCC project collaborations*

Victorian Government's Technology Voucher Program *registered provider*

Victorian Platform Technologies Network *member*

Dr Damjan Vukcevic, MCRI, presenting his research at the VLSCI RAS Presentation Day.

08.

Career Development for Computational Biologists

Supporting skills development in students and sharing expertise amongst research groups is central to VLSCI activities.

- *PhD top-ups – supporting 25 exceptional students with annual stipends*
- *MSc (Bioinformatics) - providing student bursaries to high achieving students*
- *Internships – employing talented postgraduates over their Summer recess*
- *Undergraduate Research Opportunities Program (UROP) - co-sponsoring the Program from 2012-2014 and providing direct stipend support from 2010-2014 to computaoinal biology projects for Victorian undergraduates*
- *Sponsorship of conferences and meetings*
- *Travel and conference grants for career development*
- *Extensive workshop program and teaching through VLSCI staff in University appointments.*

Chief Radiographer at The Florey Institute of Neuroscience and Mental Health, Austin campus, and part-time PhD student at Monash University, Shawna Farquharson, has won the VLSCI 1st prize award in the category Computational, Neuroengineering and Neuroimaging at the 2013 & 2014 Students of Brain Research conferences, Melbourne. Her principal research interest is in diffusion MRI and the application of white matter fibre tractography techniques to neurosurgical and epilepsy patient populations of clinical and neuroscience interest.

The annual Students of Brain Research Student Symposium is supported by VLSCI. The 2014 SoBR Student Symposium was held on 30 October 2014 at the Melbourne Brain Centre.

"The VLSCI travel awards have directly helped support my travel to conferences such as the International Society for Magnetic Resonance in Medicine (ISMRM) to present my work to the wider neuroscience community. Awards at recent conferences include the President's Award for most outstanding proffered paper in Salt Lake City, and 3rd prize in Toronto for outstanding research at the 22nd & 24th Annual Meetings for Section of Magnetic Resonance Technologists (SMRT) at ISMRM."

PHD TOP-UPS,
SUMMER INTERNSHIPS, UROP

STUDENT	HOST INSTITUTION	PRIMARY SUPERVISOR/S	PROJECT
PHD TOP-UP STUDENTSHIPS			
Brendan Ansell	UoM, Veterinary Science	Aaron Jex Malcolm McConville	Investigating mechanisms of drug resistance in Giardia
Woldeamanuel Birru	Monash, MIPS	Colin Pouton	Molecular dynamics simulations of lipid drug delivery systems
Daniel Brown	UoM, Pathology	Theo Mantamadiotis	Investigating signalling pathways in glioma stem cells
Daniel Cameron	UoM, WEHI	Tony Papenfuss Terry Speed	Detecting somatic indels and other structural variants using high-throughput genomic sequencing
Thomas Coudrat	Monash, MIPS	Patrick Sexton Denise Wootten	Development of methods for G-Protein Coupled Receptors (GPCRs) conformation modelling and investigation of the structural determinants for their activity
Sarah Diepstraten	La Trobe, Genetics	Adam Hart	A new experimental model for analysis of human globin gene switching during embryonic stem cell differentiation
Samuel Forster	Monash, Faculty of Medicine	Paul Hertzog	Systems biology of the Type 1 IFN response
Monther Al Hamdoosh	La Trobe, Computer Science	Dianhui (Justin) Wang	Regulatory motifs identification using machine learning techniques.
Peter Hickey	UoM, WEHI	Terry Speed Peter Hall	The statistical analysis of data from high-throughput assays for studying DNA methylation
Emma Hodges	Monash, Chemical Engineering/ Engineering	Ravi Jagadeeshan	Mesoscopic simulations and experimental observations of cell adhesion in hydrodynamic flow
Danielle Ingle	UoM, Microbiolology & Immunology	Roy Robins-Browne Kathryn Holt Marija Tauschek Timothy Stinear	Virulence within atypical enteropathogenic *E. coli*
David Kaplan	UoM, Florey	Steven Petrou	The dynamic action potential clamp as a tool for investigating anti-epileptic drugs.
Stefano Mangiola	UoM, Veterinary Faculty	Robin Gasser	Design and application of advanced bioinformatic tools to explore the parasitic worms system biology
Bernd Merkel	UoM, MDHS	Patricia Desmond Nicola Lautenschlager Matthias Guenther Christopher Steward	Investigation of white matter changes with MRI in older adults at risk of Alzheimer's Disease
Ehtesham Mofiz	UoM, WEHI/MDHS	Tony Papenfuss	Scabies mite genome project
James Pham	UoM, Bio21	Stuart Ralph Matt Perugini Ren Dobson	Cysteinyl-tRNA synthase as a potential antimalarial target
Cyril Reboul	Monash, Biochemistry & Molecular Biology	James Whisstock Ashley Buckle	Structural aspects of the pore-forming protein, Perforin
Nafise (Nina) Erfanian Saeedi	UoM, Electrical & Electronic Engineering	David Grayden	Neural network model of auditory perception
Simon Sadedin	UoM, MCRI	Alicia Oshlack Terry Speed Andrew Sinclair	Improving detection of disease causing variants in targeted NGS data
Jeffrey Spencer	UoM, Electrical & Electronic Engineering	David Grayden Neil McLachlan	A neurobiologically plausible computation model of sound and speech recognition

STUDENT	HOST INSTITUTION	PRIMARY SUPERVISOR/S	PROJECT
Luisa Teasdale	Museum Vic, Terrestrial Invertebrates, Sciences	Adnan Moussalli	Using 'next generation' sequencing to resolve deep phylogenetic relationships in the land molluscs (Panpulmonata)
Jian D.L Yen	Monash, Faculty of Science	Ralph Mac Nelly	Thermodynamic ecology: theoretical and empirical approaches.
MSC(BIOINFORMATICS) BURSARY RECIPIENTS			
Dharmesh Dinesh Bhuva (VLSCI bursary)	Eng, UoM	Edmund Crampin	Cofactor identification in cancer
Adrian Hecker (Peter Mac bursary)	Peter Mac	Kaylene Simpson Juan Nunez-Iglesias	Unsupervised clustering of high-content screen images to discover off-target phenotypes
Tiane Ryman (VLSCI bursary)	Eng UoM	Melissa Davis	Identification and analysis of molecular interaction networks driving metastasis in diverse cancers
Ryan Wick (VLSCI bursary)	UoM	Kathryn Holt Justin Zobel	Analysing genes of interest in a set of microbial metagenomic sequencing reads
Luke Zappia (VLSCI bursary)	UoM	Fred Hollande Arthur Hsu	Human circulating tumour cells: from biology to biomarkers
VLSCI SUMMER INTERNS 2014-2015			
Simon Belluzzo	La Trobe	Ira Cooke	Easy deployment of tools with complex dependencies using Docker and Galaxy on the Cloud
Emanuel Birru	VLSCI	Michael Kuiper	Molecular dynamics workflow
Andres Chaves	Zoology, UoM/ VLSCI	Michael Kearney Andrew Isaac	Improving efficiencies and generality of code used to compute animal and microclimate heat budgets
Steffi Cheung	VLSCI	Dieter Bulach	Development of techniques for the de novo assembly of genomes from metagenomic samples
Hugh Ford	Eng, UoM	Edmund Crampin Andrew Lonie	Spatiotemporal models of calcium dynamics within heart cells: a nuclear focus
Jordan Holland	La Trobe	Brian Smith	Determining the relative stability of protein helices
Tane Hunter	MCRI	Alicia Oshlack Andrew Lonie	Diagnosis of childhood syndromes by analysis of clinical exome data.
Diego Montufar	La Trobe	Brian Smith	Development of a web resource for analysing helices in proteins
Susmita Saha	VLSCI	Juan Nunez-Iglesias	Feature selection for clustering of high throughput microscopy images
Jumana Yousef	Pathology, UoM/ VLSCI	Melissa Southey Chol-Hee Jung	Assessment of normalisation methods for DNA methylation microarray data
Luke Zappia	VLSCI	Andrew Isaac Bernard Pope	Analysis of mass spectrometry data, metabolomics and high performance computing
GOOGLE SUMMER OF CODE INTERNSHIP			
Vighnesh Birodkar	Monash LSCC	Juan Nunez-Iglesias	Implementing region adjacency graphs in scikit-image
UROP STUDENTS			
Henry Chiu	ARMI	Mirana Ramialson	Developing and using the Trawler_web software to discover regulatory DNA motifs

STUDENT	HOST INSTITUTION	PRIMARY SUPERVISOR/S	PROJECT
Louis Dang	ARMI	Mirana Ramialson	Identification of novel non coding sequences responsible for heart disease
Douglas Eager	Monash	Minna-Liisa Anko	Mapping of splicing factor RNA binding sites based on CLIP-seq data
Derrick Futschuk	WEHI	Andrey Kan	Computational immunology
John Gilbertson	UoM	Nicholas Geard	Computational Simulation and mathematical modelling of infectious disease dynamics
John Gray	MIPS	David Chalmers	Molecular modelling of ligand binding to G protein-coupled receptors (GPCRs)
Soroor Hediyah	Eng, UOM	Melissa Davis	Indentifying the molecular networks commonly disrupted in metastisising carcinoma
David Hughes	MIMR	Ross Chapman	Factors Regulating the expression of Interferon regulated genes; data mining of the INTERFEROME database
Jan Jarosz	Eng, UOM	Vijay Rajagopal Edmund Crampin	Using 3D models of heart cells to understand how cell structure affects cell function
Preethi Jeeva	Monash	Sheena McGowan	Molecular simulation of the PlyC phage lysin, a novel antimicrobial scaffold
Roger Li	VLSCI	Danny Park Bernie Pope Tu Nguyen-Dumont	Development of a massively parallel sequencing assay for epimutation testing
Dominic Long	Monash	Natalie Borg	The transfer of ubiqitin to a cellular substrate
Michael Milton	Eng, UOM	Melissa Davis	Creating cell type specific signalling reaction networks in models of breast cancer
Damian Pavlyshyn	WEHI	Andrey Kan	Computational immunology
Kristin Ribye	MBC	Michael Hildebrand	Exploring Somatic Mutation in Focal Epilepsies
Nick Rosa	CSIRO	Janet Newman	Thermal melt curves as predictors of crystallisation
Jessica Tran	WEHI	Shalin Naik	Determining the transcriptomes of individual dendritic cell progenitors
Felix Yuen	Monash	Minna-Liisa Anko	Mapping of splicing factor RNA binding sites based on CLIP-seq data
Tony Jialun Wei	RCH	Morgan Sangeux	Muscle activity during walking for children with cerebral palsy
Daniel Williams	UoM	Christos Pantelis	Development of a gene based classifier for the diagnosis of schizophrenia
BEST UROP PRESENTATION IN COMPUTATIONAL BIOLOGY PRIZE WINNER			
James Nguyen-Tran	MIPS	David Chalmers Colin Poutin Dallas Warren	Investigating the partition coefficient LogP through Molecular Dynamics
WORK EXPERIENCE STUDENTS			
Kushargra Khare	John Monash Science School	Michael Kuiper	
Angus Morten	John Monash Science School	Michael Kuiper	
Theresa Wang	Presbyterian Ladies College	Matthew Downton (IBM)	
Ben Harper	Elizabeth Blackburn School of Sciences - University High School	Michael Kuiper Andrew Hill (Bio21)	Year 11 research project (year long): Simulations of prion proteins
RHD STUDENTS WITH VLSCI SUPERVISION			
Fiona Durand	PhD, La Trobe	Ira Cooke Nick Hoogenraad	Differential expression of membrane proteins under heat shock
Shane Gordon	PhD, La Trobe	Matthew Downton (IBM) John Wagner (IBM)	Investigations into binding modes of substrates and small molecules to bacterial dihydrodipicolinate synthase
Shakira Johnson	PhD, La Trobe	Nathan Hall Kim Plummer	Genomics and transcriptomic studies of Venturia host-pathogen responses

STUDENT	HOST INSTITUTION	PRIMARY SUPERVISOR/S	PROJECT
Brett Shiel	PhD, La Trobe	Nathan Hall Ira Cooke Jan Strugnell	Understanding of abalone heat stress through transcriptomics
Sara Alaei	PhD, Monash	Fernando Rossello Jose Polo	IPS reprogramming pathway
Saad Alsunbal	PhD, Monash	Jeff Tan (IBM)	Secure network and protocol architecture
Mark Creado	PhD, Monash	Jeff Tan (IBM)	Basic security primitives for operating systems
Kieren Marini	PhD, Monash	Fernando Rossello Neil Watkins	Mechanisms of platinum chemoresistance in lung cancer
Tom Stent	PhD, Monash	Dieter Bulach Julian Rood	Clostridial necrotic enteritis
Dan Brown	PhD, UoM	Andrew Lonie Theo Mantamadiotis	Genomic characterisation of Glioblastoma multiforme (GBM) subtypes
Andrew Buultjens	PhD, UoM	Torsten Seemann Tim Stinear	Tracking the source of myocbacterim ulcerans in Victoria
Kian Ho	PhD, UoM	Michael Kuiper Rao Kotagiri	Computational substrate querying and topology prediction of the beta-sheet
Sehrish Kanwal	PhD, UoM	Andrew Lonie Richard Sinnot	Informatics platforms for clinical genomics
Shabnam Khatibi	PhD, UoM	John Wagner (IBM)	TGF-Beta and IL-6 signalling in cancer
James Korte	PhD, UoM * Intern at IBM Watson Research Center, NY USA	Stephen Moore (IBM) John Wagner (IBM)	Continuous waveform MRI
Jason Kwong	PhD, UoM	Torsten Seemann Ben Howden	Genomics for public health microbiology
Ehtesham Mofiz	PhD, UoM	Torsten Seemann Tony Papenfuss	Scabies mite genome
Camelia Quek	PhD, UoM	Chol-Hee Jung Andrew Hill (Bio21)	Implication of small transcriptome in exosomes during Prion disease
Sabrina Rodriguez	PhD, UoM	Andrew Lonie Richard Huggins	Predicting Phenotypes through pathway analysis using conditional independence and central subspaces
Melissa Yeow	PhD, UoM	Dieter Bulach Melissa Southey	Using a high throughput sequencing strategy to detect microbial agents (viral or bacterial) associated with prostate cancer
Gourav Singhai	MSc, La Trobe	Nathan Hall Matthew Perugini	Predicting lysing inhibition in bacterial DHDPS enzymes
Adrian Hecker	MSc(Bioinf), UoM	Juan Nunez-Iglesias Kaylene Simpson	Clustering of high content screen images
Helen Mitchell	MSc(Bioinf), UoM	Simon Gladman Stuart Dashper	Oral microbiome metagenomics
Erica Plummer	MSc(Bioinf), UoM	Suzanne Garland Dieter Bulach	Effect of probiotic supplementation on microbiota of preterm infants
Serene Siah	MSc(Bioinf), UoM	Torsten Seemann, Tim Stinear	Genomic analysis of a novel marine mycobacterium
Agnes Tan	MSc(Bioinf), UoM	Jimmy Twin	A study of incident Bacterial Vaginosis
Yu Wan	MSc(Bioinf), UoM	Eric Joo Chol-Hee Jung	Breast cancer epigenome-wide association study
Nikeisha Caruana	BSc(Hons), La Trobe	Ira Cooke Nathan Hall Jan Strugnell	Proteomics and transcriptomics of squid toxins
Elizabeth Lieschke	BSc(Hons), UoM	Matthew Wakefield Clare Scott	Premalignant Analysis of high-grade serous ovarian cancer genetically engineered mouse models
Brooke Whitelaw	BSc(Hons), La Trobe	Ira Cooke Jan Strugnell	Proteomics and transcriptomics of blue ringed octopus and octopus kaurna

INTERNSHIPS 2013-2014

Adrian Hecker, Characterising and predicting effects of nsSNPs on protein structure.

The internship was invaluable to my career and study. As somebody about to commence the Master of Bioinformatics program, the internship provided a great opportunity to both gain some experience working on a Bioinformatics project and make some contacts in the community.

All the staff at the VLSCI were very welcoming and helpful and created a positive environment for the interns to work in. It was also fantastic to be given a great deal of responsibility and independence working on the project.

Yuri Benovitski, Visualising MRI Scans on a Virtual Environment (CAVE2).

Jocelyn Penington, BioPPSy / Solubility: An extensible program for calculating parameters to predict solubility (or other things)

Luke Shillabeer, Design and analysis of primers within a high-plex PCR protocol.

Working alongside a VLSCI supervisor and collaborators from the University of Melbourne GEL laboratory, the aim of my internship was to improve existing bioinformatics software systems used by my collaborators for human cancer research. My VLSCI internship was a tremendously positive experience. I have taken away from it a network of colleagues, supervisors and collaborators to work with during my Master of Science (Bioinfo), interest in research areas I did not previously know existed and a significantly increased interest in continuing my academic career into a PhD.

SKILLS DEVELOPMENT

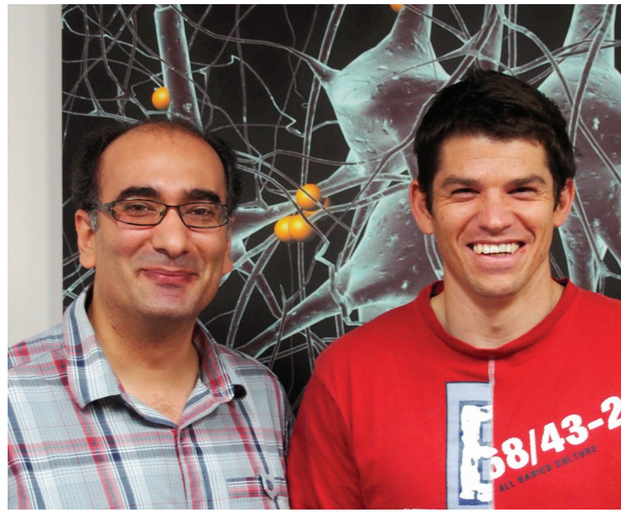
The diverse training opportunities offered by VLSCI through involvement at all levels of the research community are taken up by hundreds of aspiring young researchers each year. From work experience for high school students and lectures for undergraduate university students through to professional placements of new graduates in short term internships and hands-on workshops for early career researchers, VLSCI builds the careers of computational life scientists. Yousef Kowsar's (on left) professional journey is a great example of how VLSCI can assist a motivated researcher to redirect their career and follow their passion. The broad skills he has built on his journey now also benefit others through his employment now at VLSCI where he is working to find new tools for genomics researchers.

Yousef's university degree in Software Engineering led to seven years of industrial experience in Iran as senior software developer and product manager. The opportunity to undertake further study at the UoM's Department of Computing and Information Systems provided him with the chance to also take some subjects from the MSc (Bioinformatics) course, which is coordinated by VLSCI's LSCC Head, A/Prof Andrew Lonie. It opened up a whole new area to Yousef, where he could apply his skills to his interests to solve new problems.

'How the human body works and the complexity of biology has always fascinated me. Studying bioinformatics showed me the role computer science can play in important developments in biology, like the future of personalised medicine.'

While writing up his experimental Masters research project on 'Finding the shortest path in a dynamic network,' Yousef undertook a VLSCI internship on orchestrating cloud resources for bioinformatics tools. Fortunately, cloud and distributed computing expert, Dr. Enis Afgan (on right), had relocated to Australia to work with VLSCI for 15 months, strengthening international collaborations and supervising projects including Yousef's.

The resulting research into the provision of an on-demand big data analysis platform for bioinformaticians to leverage available cloud resource for analysing genomics data resulted in a publication and VLSCI offered Yousef a student travel grant to present the work at an international conference. The experience inspired this early career researcher further:



'It provided me an amazing insight into how important cloud technologies are used in other research areas. The ability to design an easy to use and on-demand resource to researchers attracted me to continue my career in building cloud platforms for bioinformaticians.'

Since completing his studies, Yousef has become an enthusiastic VLSCI team member, supervising a UROP student, leading hand-on workshops, and actively collaborating with researchers to find better computing solutions.

'Genomics is a big data problem: storing, accessing and archiving data is a burden for the end user. It's my job to find smarter ways to leverage cloud resources for better research outcomes.'

MSc (**BIOINFORMATICS**) GRADUATES

STUDENT	HOST INSTITUTION	SUPERVISOR/S	RESEARCH PROJECT
James Harrison	NICTA	Geoff MacIntyre	Comprehensive annotation of human transcription start sites using machine learning and data integration approaches
Xin Liu	SVI	Mark Chong	RNA processing and degradation
Erica Plummer	RWH	Suzanne Garland Dieter Bulach	Effect of probiotic supplementation on microbiota of preterm infants
Serene Siah	UoM VLSCI	Tim Stinear Torsten Seemann	Genomic analysis of a novel marine mycobacterium
Anna Trigos	Peter Mac	David Goode	Gene expression patterns between tumour cells and eukaryotes
Yu Wan	UoM VLSCI	Eric Joo Chol-Hee Jung	Breast cancer epigenome-wide association study
Jumana Yousef	Peter Mac	Maria Doyle	Developing novel methods to distinguish somatic from constitutional germline DNA variants in tumour sequencing data in the absence of a control sample
Damian Zammit	Bio21	Kathryn Holt	Microbial genomics
Michael Zhang	CERA	Paul Baird	Variants associated with eye diseases

VLSCI STAFF CONTRIBUTIONS TO UNIVERSITY TEACHING

COURSE	YEAR LEVEL	FACULTY, UNIVERSITY	LECTURER/S
MSc(Bioinformatics)	Postgraduate	MGSS, UoM	Andrew Lonie (Coordinator), various LSCC staff
Algorithms for Functional Genomics	Graduate / Postgraduate	Computing & Information Systems, UoM	Clare Sloggett (Coordinator), Simon Gladman, Matthew Wakefield, Harriet Dashnow
Foundations of Computing	Undergraduate	Computing & Information Systems, UoM	Bernard Pope (Coordinator)
Cluster and Cloud Computing	Graduate / Postgraduate	Computing & Information Systems, UoM	Chris Samuel
Introduction to Bioinformatics	Undergraduate	Medicine, Nursing & Health Sciences, Monash	Dieter Bulach
Genetics	Undergraduate	La Trobe	Nathan Hall

Celebrating 14.10.14

ADA LOVELACE DAY

An international celebration of the achievements of women in science, technology, engineering and maths.

"THOUGH I SEE NOTHING BUT VAGUE & CLOUDY UNCERTAINTY IN the FOREGROUND OF OUR BEING, YET I fancy I DISCERN A VERY BRIGHT LIGHT A GOOD WAY FURTHER ON, and THIS MAKES ME CARE much LESS ABOUT THE CLOUDINESS & INDISTINCTNESS WHICH is NEAR."
ADA LOVELACE

Ada worked on Charles Babbage's early mechanical general-purpose computer, the Analytical Engine and is said to have developed the first algorithm for its use. She is often described as the world's first computer programmer. More information at findingada.com

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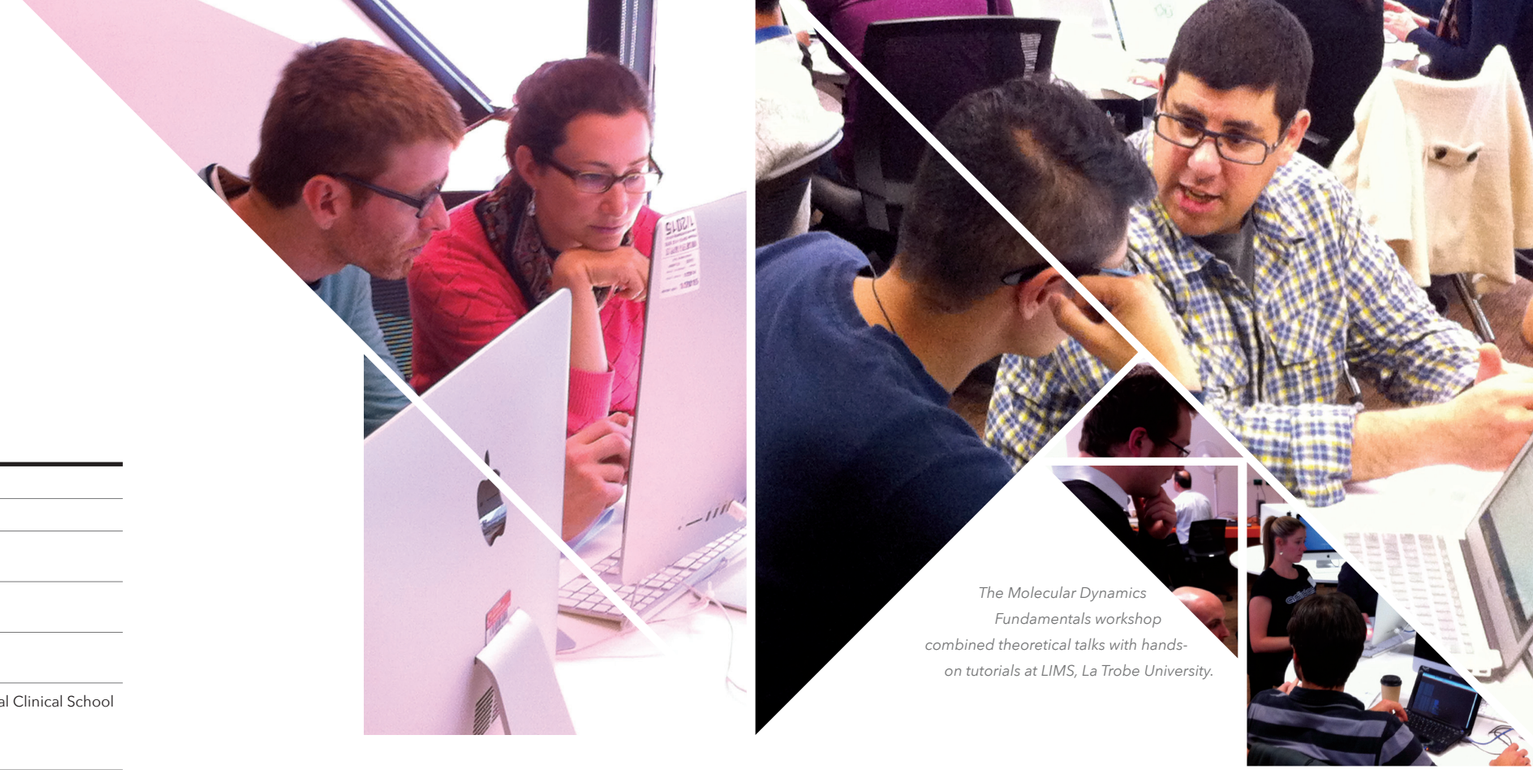
INVITED SEMINARS
AND PRESENTATIONS

EVENT	SUBJECT	PERSONNEL	LOCATION	DATE
Lorne Conference on Protein Structure and Function	Computational Biology session Co-chair	Peter Taylor	Melbourne, Victoria	February
Ludwig Institute	The power of Medical Genomics	Nathan Hall	Melbourne, Australia	February
JAMS TOAST	Microbial Genome Assembly	Torsten Seemann	Sydney, Australia	February
AusBioTech 2014	The Life Sciences Computation Centre	Andrew Lonie	Melbourne, Australia	February
BHP Billiton Science & Engineering Awards	Life Sciences Computation	Michael Kuiper	Melbourne, Australia	February
Bioinformatics Focus on Analytic Methods 2014 (CSIRO)	Genomics Virtual Laboratory	Andrew Lonie	Melbourne, Australia	March
Galaxy Australia Workshop 2014	Genomics Virtual Laboratory	Andrew Lonie	Melbourne, Australia	March
La Trobe University Genetics Departmental Seminar	Backup your Precious Data. Avoiding the data dragons	Andrew Robinson	Melbourne, Australia	March
NorduGrid 2014	Life sciences and HPC Downunder	Vera Hansper	Helsinki, Finland	May
St Vincents Institute seminar series	Genomics resources in Victoria	Andrew Lonie	Melbourne, Australia	May
La Trobe University LIMS Seminar	Resistance Becoming Refractory - Selection or Mutation	Matthew Wakefield	Melbourne, Australia	June
WEHI Bioinformatics Seminar	AmBiVErT - A self contained program for variant calling in amplicon sequencing	Matthew Wakefield	Melbourne, Australia	June
Eastern Hill Precinct Planning Day	Bioinformatics and the VLSCI	Andrew Lonie	Melbourne, Australia	June
CSIRO Experimentalists and Molecular Simulation Workshop	MD projects at VLSCI	Michael Kuiper	Melbourne, Australia	June
American Society for Mass Spectrometry Conference	Proteogenomics as a crucial tool in the search for short secreted proteins	Ira Cooke	Baltimore, USA	June
International Conference on Computational Science 2014	Genomics on the Cloud	Andrew Lonie	Cairns, Australia	June
SciPy 2014	Clustering of high-content screen images to discover off-target phenotypes	Juan Nunez-Iglesias	Austin, TX, USA	July
Galaxy Community Conference 2014	The Australian Genomics Virtual Laboratory	Andrew Lonie	Baltimore, USA	July
Galaxy Community Conference 2014	Test-driven Evaluation of Galaxy Scalability on the Cloud	Nuwan Goonasekera	Baltimore, USA	July
Galaxy Community Conference 2014	Training with Galaxy: a Genome Assembly Example	Simon Gladman	Baltimore, USA	July
Australian Society for Microbiology Annual Conference	FriPan: visualising pan genomes	Torsten Seemann	Melbourne, Australia	July
IMB Winter School	Genome assembly	Torsten Seemann	Brisbane, Australia	July
Genomics Australia/ BioPlatforms Australia meeting	Using the Genomics Virtual Laboratory	Andrew Lonie	Melbourne, Australia	July
Westmead Public Health Genomics Meeting	Public health genomics on the cloud	Torsten Seemann	Sydney, Australia	July
University of Melbourne 3D Printing Expo	3D printing molecules	Michael Kuiper	Melbourne, Australia	July
Molecular Modelling 2014 Conference	AMMA Medal Lecture Chair	Brian Smith	Queensland, Australia	August
Omics Week@Bio21	Genomics on the Cloud	Andrew Lonie	Melbourne, Australia	August
PyCon-AU 2014	Clustering of high-content screen images to discover off-target phenotypes	Juan Nunez-Iglesias	Brisbane, Australia	August
PyCon-AU 2014	Python for Bioinformatics	Clare Sloggett	Brisbane, Australia	August
La Trobe University LIMS Seminar	HPC best-practice and hints for scientists	Andrew Robinson	Melbourne, Australia	August
UK Genome Science 2014	Rapid characterisation of bacterial outbreaks	Torsten Seemann	Oxford, UK	September
UK Midlands Microbiology Meetings	Fast bacterial core genome SNP trees from 100s of bacterial short read data sets	Torsten Seemann	Birmingham, UK	September
Balti Bioinformatics: On Air	Parallel computing in bioinformatics	Torsten Seemann	Birmingham, UK	September
Bio21 Innovation Forum	Genomics on the Cloud	Andrew Lonie	Melbourne, Australia	September
WEHI Molecular Medicine Division Seminar	Degust - visualizing RNA-Seq	David Powell	Melbourne, Australia	September
eResearch Australasia 2014	Genomics Virtual Laboratory at work	Andrew Lonie	Melbourne, Australia	October
Australian Bioinformatics Conference 2014	Xenomapper: mapping reads in a mixed species context	Matthew Wakefield	Melbourne, Australia	October
Australian Bioinformatics Conference 2014	IPython Notebook for Research and Teaching	Clare Sloggett	Melbourne, Australia	October
BioInfoSummer 2014	Genomics Virtual Laboratory	Andrew Lonie Simon Gladman Clare Sloggett	Melbourne, Australia	November
SC2014 - SchedMD session	VLSCI Site Report	Christopher Samuel	New Orleans, USA	November
International Conference on Utility and Cloud Computing	Data Interlocking: Coupling Analytics with the Data	Yousef Kowsar	London, England	December
RACI Congress: Chemistry in Health	Computer aided drug design/ Biomolecular modelling symposium Chair	Brian Smith	Adelaide, Australia	December

TRAINING WORKSHOPS

WORKSHOP TITLE	DATE	VLSCI PRESENTER/S	ATTENDANCE	LOCATION
Using Unix Effectively (3hr)	4 March	Bernard Pope	12	VLSCI
Introduction to HPC at VLSCI (3hr)	11 March	Andrew Isaac	12	VLSCI
Introduction to Molecular Dynamics (3hr)	12 March	Mike Kuiper Michael Thomas	10	VLSCI
Intermediate/Advanced Molecular Dynamics (3hr)	18 March	Mike Kuiper Michael Thomas	9	VLSCI
Software carpentry - Python for bioinformatics (3hr)	26 March	Harriet Dashnow	10	UoM
Variant Detection (6hr)	27 March	Dieter Bulach Simon Gladman Andrew Lonie Gayle Philip	11	Monash Central Clinical School
Galaxy on the Cloud: the Genomics Virtual Lab (3hr)	1 April	Simon Gladman Clare Sloggett Nuwan Goonasekera	25	ITS, Unimelb
Galaxy on the Cloud: the Genomics Virtual Lab - part 2 (3hr)	3 April	Simon Gladman Clare Sloggett Nuwan Goonasekera	25	ITS, Unimelb
Introduction to Git and GitHub (3hr)	10 April	Juan Nunez-Iglesias Simon Gladman	10	VLSCI
Genomics for SVI postgrads (3hr)	28 May	Gayle Philip	5	SVI
Introduction to Unix (3hr)	June	Nathan Hall Ira Cooke Andrew Robinson	20	La Trobe
Training with Galaxy: a Genome Assembly Example (2.5hr)	30 June	Simon Gladman Andrew Lonie	30	Galaxy Community Conference 2014, Baltimore, USA
Image analysis in Python with SciPy and scikit-image (4hr)	6 July	Juan Nunez-Iglesias	85	SciPy Conference, Austin, TX, USA
Tools for microbial informatics (4hr)	6 July	Dieter Bulach Torsten Seemann	78	ASM Annual Conference, PDI
The Genomics Virtual Laboratory for BPA staff (6hr)	17 July	Andrew Lonie Simon Gladman Clare Sloggett	12	VLSCI
Using Unix Effectively (3hr)	12 August	Bernard Pope	15	VLSCI
Introduction to Galaxy on the GVL (3hr)	13 August	Simon Gladman Juan Nunez Iglesias	15	VLSCI
Introduction to Galaxy on the GVL (3hr)	14 August	Juan Nunez-Iglesias Gayle Philip	15	VLSCI
Introduction to HPC at VLSCI (3hr)	19 August	Andrew Isaac	13	VLSCI
Variant calling Basic (2hr)	20 August	Charlotte Anderson Khalid Mahmood Harriet Dashnow	8	VLSCI
Introduction to Git and GitHub (3hr)	21 August	Juan Nunez-Iglesias Ira Cooke	10	VLSCI
Introduction to molecular modelling & visualisation for life sciences (3hr)	26 August	Michael Kuiper	8	VLSCI
Introduction to Bioinformatics (4hr)	27 August	Dieter Bulach	10	Monash Central Clinical School
RNA-Seq Differential Expression with Galaxy (3hr)	27 August	Nathan Hall Gayle Philip Juan Nunez-Iglesias	11	VLSCI



The Molecular Dynamics Fundamentals workshop combined theoretical talks with hands-on tutorials at LIMS, La Trobe University.

WORKSHOP TITLE	DATE	VLSCI PRESENTER/S	ATTENDANCE	LOCATION
Differential Gene Expression (4hr)	1 September	David Powell Simon Gladman Dieter Bulach	19	Monash
RNA-Seq Differential Expression with Galaxy (3fr)	2 September	Juan Nunez-Iglesias Jessica Chung Chol-hee Jung	10	VLSCI
Variant calling Advanced (3hr)	3 September	Harriet Dashnow Khalid Mahmood	8	VLSCI
Advanced RNA-Seq (3hr)	10 September	Juan Nunez-Iglesias Chol-hee Jung Matthew Wakefield	9	VLSCI
Software Carpentry Bootcamp (8hr)	15 and 22 September	Clare Sloggett Juan Nunez-Iglesias	45	UoM
Molecular Dynamics Fundamentals (all day)	1 October	Itamar Kass Michael Kuiper	22	LIMS
Postgraduate Masterclass: Better Data Presentation (3hr)	10 October	Martin Krzywinski	28	MBC
Introduction to Proteomics in Galaxy (3hr)	12 November	Ira Cooke	20	La Trobe
Pythonic Python - COMBINE Symposium (2.5hr)	27 November	Clare Sloggett	40	Monash, Parkville Campus
Image analysis with Python - COMBINE Symposium	27 November	Juan Nunez-Iglesias	40	Monash, Parkville Campus
GVL Workshop - BioInfoSummer 2014 (3.5hr)	3 December	Simon Gladman David Powell Clare Sloggett Andew Lonie Jessica Chung Paul Harrison	40	BioInfoSummer 2014, Monash
GVL Workshop - Bioinfosummer 2014 (3.5hr)	5 December	Simon Gladman Clare Sloggett Gayle Philip Andew Lonie Jessica Chung Paul Harrison	40	BioInfoSummer 2014, Monash
Open source science using Git and GitHub (3hr)	11 December	Juan Nunez-Iglesias	12	VLSCI

CONFERENCE
AND TRAVEL GRANTS

GRANT RECIPIENT	POSITION	INSTITUTION	DESTINATION
Apana Elangovan	Postgraduate student	UoM	22nd Annual International Conference on Intelligent Systems for Molecular Biology (ISMB)
Eric Treml	Research Fellow	UoM	International Marine Conservation Congress, UK
Marek Cmero	Postgraduate student	RMH / UoM	International Conference on Bioinformatics 2014, Sydney, Australia
Andrew Lonsdale	Postgraduate student	COMBINE	International Conference on Bioinformatics InCoB2014, Sydney
Jane Hawkey	Postgraduate student	UoM	Molecular Evolution and Phylogenetics Workshop, Woods Hole, US
Govinda Poudel	Postdoctoral researcher	Monash	NeuroEng 2014: Australian Workshop on Computational Neuroscience, Adelaide, Australia
Marta Enciso	Postdoctoral researcher	La Trobe	Gordon Research Conference: Computational Chemistry, West Dover, VT USA
Jessica Holien	Postdoctoral researcher	SVI	Molecular Modelling 2014, Queensland, Australia
Trayder Thomas	Postgraduate student	MIPS	Molecular Modelling 2014, Queensland, Australia
Tamir Dingjan	Postgraduate student	MIPS	Molecular Modelling 2014, Queensland, Australia
Camelia Quek	Postgraduate student	Bio21	EMBL PhD Symposium (Germany), Wellcome Trust Sanger Computational RNA Biology Confence (Cambridge), EBI NGS Workshop (UK)
Cyril Reboul	Postgraduate student	Monash	Pore-forming Toxins 2014, Italy
Scott Ritchie	Postgraduate student	UoM	Australian Genomic Technologies Association 2014 Conference & Australian Bioinformatics Conference, Melbourne Australia
Thomas Coudrat	Postgraduate student	MIPS	European Conference on Computational Biology 2014 & European Student Council Symposium 2014, Strasbourg, France
Andrey Kan	Postdoctoral researcher	WEHI	Gene Regulatory Networks for Development course, Marine Biological Laboratory, Boston, USA
Anas Sultan	Postgraduate student	Deakin	International Union of Pure and Applied Biophysics Congress 2014, Brisbane, Australia
Kurt Drew	Postgraduate student	Deakin	International Union of Pure and Applied Biophysics Congress 2014, Brisbane, Australia

Right: Facilitators of the International Workshop on Quantitative Biology (L-R): Dr Marcus Kranz, Humboldt University, Germany; Dr Noriko Hiroi, Keio University, Japan; Dr Akira Funahasi, Keio University, Japan; and Dr Sarah Boyd, SBI Australia. The workshop was held at VLSCI in September 2014, in conjunction with the International Conference on Systems Biology. The workshop was organised by Sarah Boyd, SBI Australia, and Noriko Hiroi, Keio University, Japan, and focused on cell imaging processing techniques to extract quantitative information from microscopy images.

SPONSORSHIPS OF
MEETINGS & CONFERENCES

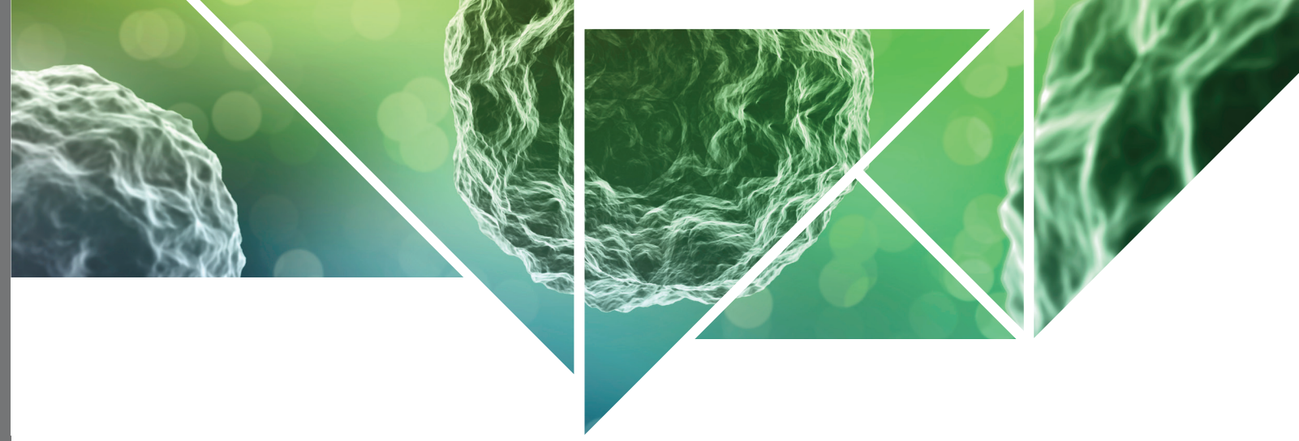
DATE	ACTIVITY (LOCATION)	TYPE OF SPONSORSHIP	TOTAL PARTICIPANTS
9-13 February	39th Lorne Conference on Protein Structure and Function *(Mantra, Lorne)*	Primary sponsor, represented via booth and in program	389 delegates (54% Victorian)
24 April	Code Masters Challenge *(Computing & Information Systems, UoM)*	Sponsored event	62 high school students from 22 schools
5 June	Graeme Clark Oration activities *(Melbourne Convention and Exhibition Centre)*	Sponsored event, hosted a group of students at Oration and Oration Dinner.	1400 Oration attendees
10-12 June	The International Conference on Computational Science *(Cairns, Australia)*	Sponsored event, represented via booth and in program	245 delegates from 31 countries
6 July	GVL Workshop, Australian Society for Microbiology Annual Scientific Meeting *(PDI, UoM)*	Sponsored event, supported Galaxy workshop	78 workshop participants
10 July	13th Melbourne Protein Group Student Symposium *(Bio21)*	Sponsored poster prizes	103 attendees from 10 organisations
23 July	Computing & Information Systems Doctoral Symposium *(UoM)*	Sponsored and judgedprizes	122 students, academics and industry guests
24 July	UROP Conference Day *(MBC)*	UROP sponsorship, plus judging and prize for Best Computational Biology Presentation	120 students, academics and industry guests
31 July-2 August	Molecular Modelling 2014 Conference *(Queensland)*	Sponsored event	111 (main conference), 51 (student symposium)
27-29 August	Genomics Research Symposium, Omics Week *(Bio21)*	Sponsored event	180 registrants each day (3)
13 September	International Workshop on Quantitative Biology	Sponsored and hosted workshop	12 international participants
9-17 October	Melbourne tour by Martin Krzywinski	Co-sponsored and hosted with Illumina	Various, including >200 at public talk, >100 at talk for scientists
11-12 October	Australian Bioinformatics Conference	Sponsored event and supported student attendances	185 attendees from 60 organisations
24-26 October	HealthHack2014 *(Thoughtworks, Melbourne)*	Provided 3 staff to assist with access to GVL and VLSCI systems	100 participants in Melbourne and Sydney
30 October	Students of Brain Research Student Symposium 2014 *(MBC)*	Sponsored oral presentation prize	156 attendees from 14 organisations

Ms Helen Gardiner

Communications Manager

09.

Active Projects in 2014



All projects allocated resources through the Research Allocation Scheme (RAS) Committee process which were allocated for use and active in 2014 are listed here (some roll over from 2013, some continue through to 2015, refer Current Research on the VLSCI website for exact dates for each).

Chief Investigators are asked to list their top 5 publications and/or presentations.

TABLE LEGEND

* Presentation

[ ] Journal Impact Factor

Refer Glossary (p 105) for all abbreviations used in all tables in this Report.

PROJECT ID	PROJECT TITLE	CHIEF INVESTIGATORS	INSTITUTE	VLSCI SERVICE UNITS	ALLOCATION TYPE
VR0003	**Computational Neuroscience: Modelling the brain at microscopic, mesoscopic and macroscopic levels**	David Grayden Anthony Burkitt Mark Cook	UoM UoM UoM	352400	RAS 8
	PUBLICATION/PRESENTATION				
	O'Sullivan-Greene, E., Mareels, I., Kuhlmann, L., and Burkitt, A., Observability limits for networked oscillators, Automatica. [3.132]				
	O'Sullivan-Greene, E., Mareels, I., Limits of Observability in Large-Scale Linear Networked Clocks, Proceedings of IFAC World Congress, Capetown, South Africa.*				
	Erfanian Saeedi, N., Blamey, P. J., Burkitt, A. N., and Grayden, D. B., The effect of stimulation field spread on cochlear implant users' pitch ranking performance: A model-based investigation, 13th International Conference on Cochlear Implants and Other Implantable Auditory Technologies (CI), Munich, Germany.*				
VR0004	**Computational drug formulation**	David Chalmers Colin Pouton	Monash Monash	2100000	RAS 8
	PUBLICATION/PRESENTATION				
	Chalmers, D.K., Birru, W.A., Warren, D.B. and Pouton, C.W., Computational modelling of lipid phase behaviour for drug formulation and delivery, MM2014, Queensland, Australia.*				
VR0007	**Parasite Genomics and Genetics Program**	Robin Gasser	UoM	760000	RAS 8
	PUBLICATION/PRESENTATION				
	Tang *et al*. (Gasser), Genome of the human hookworm *Necator americanus*, Nature Genetics (46, 261-269 doi: 10.1038/ng.2875). [29.648]				
	Jex *et al*. (Gasser), Genome and transcriptome of the porcine whipworm *Trichuris suis*, Nature Genetics (46, 701-706. doi: 10.1038/ng.3012.) [29.648]				
	Young *et al*. (Gasser), The *Opisthorchis viverrini* genome provides insights into life in the bile duct, Nature Communications (5, 4378, doi: 10.1038/ncomms5378). [10.742]				
	Hagen *et al*. (Gasser), Omega-1 knockdown in *Schistosoma mansoni* eggs by lentivirus transduction reduces granuloma size in vivo, Nature Communications (5, Article number: 5375, doi:10.1038/ncomms6375). [10.742]				
	Zhu *et al*. Genetic blueprint of the zoonotic pathogen *Toxocara canis*, Nature Communications (In Press at time of submission). [10.742]				
VR0009	**Toxin binding to membrane proteins: Towards novel treatments in neuropathology**	Andrew Hung David Adams	RMIT RMIT	1800000	RAS 8
	PUBLICATION/PRESENTATION				
	Chhabra, S., Belgi, A., Bartels, P., Robinson, S.D., Kompella, S.N., Hung, A., Adams, D.J. *et al*., Dicarba analogues of α-conotoxin RgIA: Structure, stability and activity at potential pain targets, Journal of Medicinal Chemistry. [5.48]				
	Kompella, S.N., Hung, A., Adams, D.J. *et al*., Alanine scan of α-conotoxin RegIIA reveals a selective α3β4 nicotinic acetylcholine receptor antagonist, Journal of Biological Chemistry. [4.6]				
	Kompella, S.N., Hung, A., Adams, D.J. *et al*., Species difference in α-conotoxin RegIIA inhibition of nAChRs: molecular basis for differential sensitivity, Australian Physiological Society, Australia.*				
	Suresh, A., Hung, A., Adams, D.J., Computational Identification of Structural and interaction properties of GID α-conotoxins at the α7 and α4β2 nicotinic receptor, Wellcome Trust Nicotinic Receptors Conference, United Kingdom.*				

PROJECT ID	PROJECT TITLE	CHIEF INVESTIGATORS	INSTITUTE	VLSCI SERVICE UNITS	ALLOCATION TYPE
VR0010	**Cytoadhesive dynamics of parasitized red blood cells**	Ravi Jagadeeshan Brian Cooke	Monash Monash	800000 1200000	RAS 7 RAS 8
	PUBLICATION/PRESENTATION				
	Jain, A., Sasmal, C., Hartkamp, R., Todd, B.D., and Prakash, J.R, Brownian dynamics simulations of planar mixed flows of polymer solutions at finite concentrations, Chemical Engineering Science 121 (2015) 245–257. [2.613]				
	Ramesh, K.V., Thaokar, R.M., Prakash, J.R., and Prabhakar, R., Significance of thermal fluctuations and hydrodynamic interactions in receptor-ligand mediated adhesive dynamics of a spherical particle in wall bound shear flow, Physical Review E (submitted 2014). [2.326]				
VR0011	**A multi-scale quantitative model of solute regulation and blood flow in a rat kidney**	Edmund Kazmierczak Linda Stern	UoM UoM	22000 10200	RAS 7 RAS 8
VR0021	**Modelling pore forming toxins**	Michael Parker	SVI	2800000	RAS 8
	PUBLICATION/PRESENTATION				
	Wade, K.R., Hotze, E.M., Kuiper, M.J., Morton, C.J., Parker, M.W., and Tweten, R.K., An intermolecular electrostatic interaction controls the prepore to pore transition in a cholesterol-dependent cytolysin, PNAS. [9.809]				
	Feil, S.C., Ascher, D.B., Kuiper, M.J., Tweten, R.K. & Parker, M.W., Structural studies of *Streptococcus pyogenes* streptolysin O provides insights into the early steps of membrane penetration, Journal of Molecular Biology. [3.959]				
	Parker, M.W., Cholesterol-dependent cytolysins: from water-soluble state to membrane pore, The 5th Venoms to Drugs meeting, Kingscliff, NSW, October 2014, Australia.*				
VR0023	**Shear induced platelet aggregation: characterising shear forces in in-vitro geometries**	Kris Ryan Josie Carberry Elizabeth Gardiner Robert Andrews	Monash Monash Monash Monash	4234000	RAS 8
VR0024	**Computational modelling of G protein-coupled receptors**	Patrick Sexton Arthur Christopoulos	Monash Monash	1600000	RAS 8
	PUBLICATION/PRESENTATION				
	Keov, P., *et al*., Molecular mechanisms of bitopic ligand engagement with the M1 muscarinic acetylcholine receptor, Journal of Biological Chemistry. [4.600]				
	Abdul-Ridha, A., *et al*., Molecular determinants of allosteric modulation at the M1 muscarinic acetylcholine receptor, Journal of Biological Chemistry. [4.600]				
	Abdul-Ridha, A., Mechanistic Insights into Allosteric Structure-Function Relationships at the M1 Muscarinic Acetylcholine Receptor, Journal of Biological Chemistry. [4.600]				
VR0025	**Exploiting unique mechanical responses of cells for disease diagnosis and management**	Gregory Sheard	Monash	285000	RAS 8
VR0028	**Protein self-assembly on nano surfaces and interfaces: a friend or foe of bionanotechnology**	Nevena Todorova Irene Yarovsky	RMIT RMIT	920000	RAS 8
	PUBLICATION/PRESENTATION				
	Todorova, N., Chiappini, C., Mager, M., Simona, B., Patel, I.I., Stevens, M.M., and Yarovsky, I., Surface presentation of functional peptides in solution determines cell internalization efficiency of TAT conjugated nanoparticles, Nano Letters. [12.940]				
	Andresen, H., Mager, M., Grießner, M., Charchar, P., Todorova, N., Bell, N., Theocharidis, G., Bertazzo, S., Yarovsky, I., and Stevens, M.M., Single-step homogeneous immunoassays utilizing epitope-tagged gold nanoparticles: On the mechanism, feasibility, and limitations, Chemistry of Materials. [8.535]				
	Makarucha, A.J., Todorova, N., and Yarovsky, I., Effects of graphitic nanomaterials in the dissociation pathway of amyloidogenic peptide dimer, IEEE International Conference on Nanoscience & Nanotechnology, Adelaide, Australia.*				
	Todorova, N., Chiappini, C., Mager, M., Simona, B., Stevens, M.M., and Yarovsky, I., Grafting density and colocation affect cell internalization of peptide decorated nanoparticles: when less is more!, The 39th Lorne Conference on Protein Structure and Function, Australia.*				
	Todorova, N., Yarovsky, I., Atomistic insights into the peptide layer structure of bioresponsive nanoparticle systems, ICONN 2014, Australia.*				
VR0030	**Computer aided drug discovery**	Brian Smith	La Trobe	3040000	RAS 8
VR0031	**In silico modelling of protein dynamics and drug design**	David Wilson	La Trobe	2000000	RAS 8
	PUBLICATION/PRESENTATION				
	O'Brien, N.J., Brzozowski, M., Wilson, D.J.D., Deady, L.W. and Abbott, B.M., Synthesis and biological evaluation of substituted 2-anilino-7H-pyrrolopyrimidines as PDK1 inhibitors, Tetrahedron. [2.817]				
	O'Brien, N.J., Brzozowski, M., Wilson, D.J.D., Deady, L.W. and Abbott, B.M., Synthesis and biological evaluation of substituted 3-anilino-quinolin-2(1H)-ones as PDK1 inhibitors, Bioorganic & Medicinal Chemistry. [2.951]				
	Brzozowski, M., O'Brien, N.J., Wilson, D.J.D., and Abbott, B.M., Synthesis of substituted 4-(1H-indol-6-yl)-1H-indazoles as potential PDK1 inhibitors, Tetrahedron. [2.817]				
	Abbott, B.M., and Wilson, D.J.D., Development of inhibitors of protein kinases, RACI National Convention, Australia.*				

PROJECT ID	PROJECT TITLE	CHIEF INVESTIGATORS	INSTITUTE	VLSCI SERVICE UNITS	ALLOCATION TYPE
VR0052	**Algorithms for vision testing**	Andrew Turpin	UoM	40000	RAS 8
	PUBLICATION/PRESENTATION				
	Chong, L., McKendrick, A.M., and Turpin, A., Targeted spatial sampling using GOANNA improves detection of visual field progression, Ophthalmic and Physiological Optics. [2.664]				
	McKendrick, A.M., Denniss, J., and Turpin, A., Response times across the visual field: empirical observations and application to threshold determination, Vision Research. [2.381]				
	Denniss J., Turpin, A., and McKendrick, A.M., Individualised Structure-Function Mapping for Glaucoma: Practical Constraints on Map Resolution for Clinical and Research Applications, Investigaive Ophthalmology and Visual Science. [3.661]				
	Gog, S., Moffat, A., Culpepper, J., Turpin, A., and Wirth, A., Large-scale pattern search using reduced-space on-disk suffix arrays, IEEE Trans. Knowledge and Data Engineering. [1.815]				
	Denniss, J., Turpin, A., Tanabe, F., Matsumoto, C., and McKendrick, A.M., Structure-Function Mapping: Variability and Conviction in Tracing Retinal Nerve Fibre Bundles and Comparison to a Computational Model, Investigative Ophthalmology and Visual Science. [3.661]				
VR0056	**Neuroanatomical changes in childhood-onset epilepsy**	David Abbott Graeme Jackson	Florey Florey	40000	RAS 8
	PUBLICATION/PRESENTATION				
	Curwood, E., Pedersen, M., Abbott, D., Carney, P., Berg, A., and Jackson, G., Structural brain networks are altered in Childhood Absence Epilepsy, 20th Annual Meeting of the Organisation for Human Brain Mapping, Germany.*				
	Curwood, E., Pedersen, M., Abbott, D., Carney, P., Berg, A., and Jackson, G., Abnormal fronto-temporal cortex in Childhood Absence Epilepsy: a cortical thickness connectivity study, ME@MBC, Australia.*				
	Curwood, E., Pedersen, M., Abbott, D., Carney, P., Berg, A., and Jackson, G., Abnormal fronto-temporal cortex in Childhood Absence Epilepsy: a cortical thickness connectivity study, 28th Annual Scientific Meeting of the Epilepsy Society of Australia, Australia.*				
VR0069	**Molecular dynamics simulation of enteroviruses associated with acute flaccid paralysis**	Jason Roberts Bruce Thorley Andrew Hung	VIDRL VIDRL RMIT	2046100	RAS 8
	PUBLICATION/PRESENTATION				
	Thorley, B.R., Roberts, J.A., Poliovirus: a model virus. From eradication to simulation, Virology Seminar, ICPMR, Westmead, Sydney, Australia.*				
	Thorley, B.R., Roberts, J.A., Poliovirus: a model virus. From eradication to simulation, Doherty Institute Seminar, Melbourne, Australia.*				
	Thorley, B.R., Roberts, J.A., Detection, and 3-Dimensional Reconstruction of a Novel Enterovirus Associated with a Case of Acute Flaccid Paralysis, Australian Society of Microbiology General Meeting, Melbourne, Australia.*				
	Thorley, B.R., Roberts, J.A., Detection, Characterisation and 3D Molecular Modelling of Enteroviruses from Cases of Acute Flaccid Paralysis, Public Health Night and ASM Victorian State General Meeting, Melbourne, Australia.*				
	Thorley, B.R., Roberts, J.A., Discovery and in-silico reconstruction of a novel virus identified from a patient suffering paralysis, 4th Melbourne meeting of the Association of Molecular Modellers of Australasia, Melbourne, Australia.*				
VR0071	**Understanding the role of protein dynamics at the immunological synapse**	Natalie Borg	Monash	6150000	RAS 8
	PUBLICATION/PRESENTATION				
	Kass, I., Buckle, A.M., and Borg, N.A., Understanding the Structural Dynamics of TCR:pMHC interactions, Trends in Immunology. [12.031]				
VR0082	**Population genomics of bacterial pathogens**	Kathryn Holt Tim Stinear Michael Inouye	UoM UoM UoM	464000	RAS 8
	PUBLICATION/PRESENTATION				
	Inouye, M., Dashnow, H., Raven, L., Schultz, M.B., Pope, B.J., Tomita, T., Zobel, J., and Holt, K.E., SRST2: Rapid genomic surveillance for public health and hospital microbiology labs, Genome Medicine. [4.942]				
	Stinear, T.P., Holt, K.E., Chua, K., Stepnell, J., Tuck, K.L., Coombs, G., Harrison, P.F., Seemann, T., Howden, B.P., Adaptive Change Inferred from Genomic Population Analysis of the ST93 Epidemic Clone of Community-Associated MRSA, Genome Biology & Evolution. [4.532]				
	Hamidian, M., Holt, K.E., and Hall, R.M., The complete sequence of Salmonella genomic island SGI2, Journal of Antimicrobial Chemotherapy. [5.439]				
	Holt, K.E., Genomic studies of bacterial pathogen transmission, evolution & resistance, International Conference on Systems Biology, Australia.*				
	Holt, K.E., Detection of antimicrobial resistance genes, plasmids and IS from raw genomic data, International Society for Plasmid Biology Conference, Australia.*				
VR0089	**Dynamics, docking and allostery in DHDPS**	Matthew Perugini Matthew Downton	La Trobe IBM	3015000	RAS 8

PROJECT ID	PROJECT TITLE	CHIEF INVESTIGATORS	INSTITUTE	VLSCI SERVICE UNITS	ALLOCATION TYPE
VR0138	**Stimulation strategies for the bionic eye**	Anthony Burkitt Hamish Meffin David Grayden Nigel Lovell Socrates Dokos	UoM UoM UoM UNSW UNSW	180000	RAS 8
	PUBLICATION/PRESENTATION				
	Meffin, H., Tahayori, B., Sergeev, E.N., Mareels, I.M.Y., Grayden, D.B., and Burkitt, A.N., Modeling extracellular electrical stimulation: III. Derivation and interpretation of neural tissue equations, Journal of Neural Engineering. [3.415]				
	Tahayori, B., Meffin, H., Sergeev, E.N., Mareels, I.M.Y., Burkitt, A.N., and Grayden, D.B., Modeling extracellular electrical stimulation: IV. Effect of the cellular composition of neural tissue on its spatio-temporal filtering properties, Journal of Neural Engineering. [3.415]				
VR0164	**Designing new reactions for novel pharmaceutical synthesis**	Carl Schiesser	UoM	300000	Start-Up/ Discretionary
VR0165	**Molecular systematics of Australian plants and fungi**	Daniel Murphy Elizabeth James	RBG RBG	115000 31320	RAS 7 RAS 9
	PUBLICATION/PRESENTATION				
	Birch, J.L., Cantrill, D.J., Walsh, N.G., and Murphy, D.J., Phylogenetic investigation and divergence dating of Poa (Poaceae tribe Poeae in the Australasian Region, Botanical Journal of the Linnaean Society. [2.699]				
	Birch, J.L., Berwick, F.B., Walsh, N.G., Cantrill, D.J. and Murphy, D.J., Distribution of morphological diversity within widespread Australian species of Poa (Poaceae, tribe Poeae) and implications for taxonomy of the genus, Australian Systematic Botany. [1.146]				
	James, E.A., and McDougall, K.L., Spatial genetic structure reflects extensive clonality, low genotypic diversity and habitat fragmentation in *Grevillea renwickiana* (Proteaceae), a rare, sterile shrub from south-eastern Australia, Annals of Botany. [3.295]				
	James, E.A., and Jordan, R., Limited structure and widespread diversity suggest potential buffers to genetic erosion in a threatened grassland shrub *Pimelea spinescens* (Thymelaeaceae), Conservation Genetics. [1.846]				
	Birch, J.L., Walsh, N.G., Cantrill, D.J., and Murphy, D.J., Classical morphology, Sanger and Next-Generation Sequencing to resolve relationships within a recent radiation: a case study focusing on Australian Poa (Poaceae), Australasian Systematic Botany Conference, Palmerston North, New Zealand.*				
VR0191	**Next Generation Sequencing to identify genes involved in abiotic stress or plant cell wall synthesis**	Ute Roessner	UoM	49000	RAS 8
	PUBLICATION/PRESENTATION				
	Lowe, R.G.T, Cassin, A., Grandaubert, J., Clark, B.L., Van de Wouw, A.P., Rouxel, T., and Howlett, B.J., Genomes and Transcriptomes of Partners in Plant-Fungal- Interactions between Canola (*Brassica napus*) and Two Leptosphaeria Species, Plos One. [3.534]				
	Hill, C., Natera, S., Boughton, B.A., Roy, S., and Roessner, U., Identifying novel salinity tolerance mechanisms by spatial analysis of lipids in barley roots, Australian Lipidomics Symposium, Australia.*				
VR0200	**Charged protein-lipid interactions and regulation of ion channel function**	Toby Allen	RMIT	5300000	RAS 8
	PUBLICATION/PRESENTATION				
	Vorobyov, I., Olson, T.E., Kim, J.H., Koeppe R.E. 2nd, Andersen, O. S., and Allen, T.W., Ion-induced defect permeation of lipid membranes, Biophysical Journal. [3.832]				
	Boiteux, C., Vorobyov, I., and Allen, T.W., Ion conduction and conformational flexibility of a bacterial voltage-gated sodium channel, Proceedings of the National Academy of Sciences, USA. [9.809]				
	Boiteux, C., Vorobyov, I., French, R.J., French, C., Yarov-Yarovoy, V., and Allen, T.W., Local anesthetic and anti-epileptic drug access and binding to a bacterial voltage-gated sodium channel, Proceedings of the National Academy of Sciences, USA. [9.809]				
	Boiteux, C., Vorobyov, I., and Allen, T.W., Bacterial models as tools for sodium channel mechanistic discovery, International Union for Pure and Applied Biophysics, Australia.*				
	Boiteux, C., Vorobyov, I., French, R.J., French, C., Yarov-Yarovoy, V., and Allen, T.W., Using bacterial sodium channels to explore ion conduction, inactivation and inhibition mechanisms, French Biophysical Society Congress, Guethery, France.*				

PROJECT ID	PROJECT TITLE	CHIEF INVESTIGATORS	INSTITUTE	VLSCI SERVICE UNITS	ALLOCATION TYPE
VR0202	**Mapping protein-peptide interactions for the development of nanomaterials for biomedical application**	Andrew Christofferson Irene Yarovsky	RMIT RMIT	400000	RAS 8
	PUBLICATION/PRESENTATION				
	Christofferson, A., Yiapanis, G., Ren, J., Qiao, G., Satoh, K., Kamigaito, M., and Yarovsky, I., Molecular mapping of poly (methyl methacrylate) super-helix stereocomplexes, Chemical Science. [8.601]				
	Ren, J., Satoh, K., Goh, T., Blencowe, A., Nagai, K., Ishitake, K., Christofferson, A., Yiapanis, G., Yarovsky, I., Kamigaito, M., Qiao, G., Stereospecific Cyclic Poly (methyl methacrylate) and Its Topology-Guided Hierarchically Controlled Supramolecular Assemblies, Angewandte Chemie International Edition. [11.336]				
	Christofferson, A., Yiapanis, G. Leung, A., Prime, E., Tran, D., Qiao, G., Solomon, D., and Yarovsky, I., Dynamic performance of duolayers at the air/water interface. 2. Mechanistic insights from all-atom simulations, The Journal of Physical Chemistry B. [3.377]				
	Christofferson, A., Herpoldt, K., Makarucha, A., Gormley, A., Stevens, M., and Yarovsky, I., Simulation of Nanomaterials for Virus Detection and Drug Delivery, Nanotechnology & Medicines for Tomorrow, Australia.*				
	Christofferson, A. Yiapanis, G.,Ren, J., Qiao, G., and Yarovsky, I., Molecular rationale for the structure of cyclic poly (methyl methacrylate) stereocomplexes, International Conference on Nanoscience and Nanotechnology 2014, Australia.*				
VR0203	**Structure-function relationships for materials-binding peptides via advanced conformational sampling**	Tiffany Walsh	Deakin	11200000	RAS 8
	PUBLICATION/PRESENTATION				
	Hughes, Z.E., Tomasio, S.M. and Walsh, T.R., Efficient simulations of the aqueous bio-interface of graphitic nanostructures with a polarisable model, Nanoscale. [6.739]				
	Palafox-Hernandez, J.P., Tang, Z., Hughes, Z.E., Li, Y., Swihart, M.T., Prasad, P.N., Walsh, T.R. and Knecht, M.R., Comparative Study of Materials-Binding Peptide Interactions with Gold and Silver Surfaces and Nanostructures: A Thermodynamic Basis for Biological Selectivity of Inorganic Materials, Chemistry of Materials. [8.535]				
	Hughes, Z.E. and Walsh, T.R., Structure of the Electrical Double Layer at Aqueous Gold and Silver Interfaces for Saline Solutions, Journal of Colloid and Interface Science. [3.552]				
	Wright, L.B., Palafox-Hernandez, J.P., Hughes, Z.E., Brown,A., and Walsh, T.R., Investigating Peptide-Materials Adsorption Selectivity at the Bio/Nano Interface using Advanced Molecular Simulation, CECAM conference "Molecular and coarse-grained modelling of interactions at bio-nano interface", Dublin, Ireland.*				
	Drew, K.L.M., Hughes, Z.E., Palafox-Hernandez, J.P., and Walsh, T.R., Strategies for generating versatile peptide-mediated nanoparticle assemblies in 3-D: Combining Modelling and Experiment, NanoBio 2014, Brisbane, Australia.*				
VR0204	**Assessing thermal effects of on people in realistic environmental conditions**	Steve Moore Robert McIntosh Steve Iskra Andrew Woods	IBM Swinburne Swinburne Swinburne	156000	RAS 8
VR0207	**Prediction and imaging of vulnerable plaque evolution and rupture**	Kerry Hourigan Mark Thompson	Monash Monash	780000	RAS 8
	PUBLICATION/PRESENTATION				
	Rao, A., Radi, A., Leontini, J. S., Thompson, M. C., Sheridan, J. and Hourigan, K., A review of rotating cylinder wake transitions, Journal of Fluids and Structures. [2.229]				
	Thompson, M. C., Radi, A., Rao, A., Sheridan, J. and Hourigan, K., Low-Reynolds-number wakes of elliptical cylinders: from the circular cylinder to the normal flat plate, Journal of Fluid Mechanics. [2.294]				
	Rao, A., Radi, A., Leontini, J. S., Thompson, M. C., Sheridan, J. and Hourigan, K., Influence of a wire upstream of a rotating cylinder, 19th Australasian Fluid Mechanics Conference, Melbourne, Australia.*				
	Assemat, P., Siu, K.K., Armitage, J.A., Hokke, S.N., Dart, A., Chin-Dusting, J. and Hourigan, K., Hemodynamical stress in mouse aortic arch with atherosclerotic plaques: preliminary study of plaque, Computational and Structural Biotechnology Journal progression, Computational and Structural Biotechnology Journal.				

PROJECT ID	PROJECT TITLE	CHIEF INVESTIGATORS	INSTITUTE	VLSCI SERVICE UNITS	ALLOCATION TYPE
VR0210	**Optimising blood flow in stented arteries: a fluid mechanics approach incorporating OCT**	Andrew Ooi Eric Poon Peter Barlis Stephen Moore Daniel Chung Cheng Chin	UoM UoM UoM IBM UoM UoM	4040000 10010000	RAS 7 RAS 8
	PUBLICATION/PRESENTATION				
	Poon, E.K.W, Barlis, P., Moore, S., Pan, W-H., Liu, Y., Ye, Y., Xue, Y., Zhu, S.J., and Ooi, A.S.H., Numerical investigations of the haemodynamic changes associated with stent malapposition in an idealised coronary artery, Journal of Biomechanics. [2.496]				
	Zhu, S.J., Poon, E.K.W., Ooi, A.S.H., and Moore, S., Enhanced targeted drug delivery through controlled release in a 3D vascular tree, Journal of Biomechanical Engineering. [1.748]				
	Poon, E.K.W., Barlis, P., Hayat, U., Moore, S., and Ooi, A.S.H., Impacts on hemodynamics of different bifurcation coronary stent configurations, 19th Australasian Fluid Mechanics Conference, Australia.*				
	Chen, W.X., Chan, L., Hutchins, N., Poon, E.K.W., Ooi, A., Direct numerical simulation of pulsatile flow in pipes, 19th Australasian Fluid Mechanics Conference, Australia.*				
	Chen, W.X., Barlis, P., Hutchins, N., Poon, E.K.W, Ooi, A., Fluid mechanics investigation on the effects of stent malapposition inside curved arteries, AOTULE student conference, Australia.*				
VR0212	**Calculating climatic constraints on animals**	Michael Kearney	UoM	400000 400000	RAS 7 RAS 9
	PUBLICATION/PRESENTATION				
	Kearney, M.R., Activity restriction and the mechanistic basis for extinctions under climate warming, Ecology Letters. [13.042]				
	Kearney, M.R., Isaac, A.P., and Porter, W.P., microclim: Global estimates of hourly microclimate based on long-term monthly climate averages, Scientific Data. [TBD]				
	Walker, S., Stuart-Fox, D., and Kearney, M.R., Has contemporary climate change played a role in population declines of the lizard Ctenophorus decresii from semi-arid Australia?, Journal of Thermal Biology. [1.544]				
	Walker, S., Stuart-Fox, D., Kearney, M.R., The Thermodynamic Niche – physiologically based models of climatic constraints on animals, Heteroclim, France.*				
	Walker, S., Stuart-Fox, D., Kearney, M.R., Thermodynamic constraints on distribution and abundance, Gordon Research Conference: Unifying Ecology Across Scales, USA.*				
VR0224	**Enabling next generation drug screening**	Stan Skafidas Ross Bathgate Stefan Harrer	UoM Florey IBM	3020000 808000	RAS 7 RAS 9
	PUBLICATION/PRESENTATION				
	Kannam, S.K., Computational modelling of molecular sensing using nanopores, MM2014: From Biomolecules to Materials, Australia.*				
VR0225	**Molecular modelling of albumin and other plasma proteins for development of brain drug delivery**	Norman Saunders	UoM	1400000	RAS 8
VR0230	**Simulations of prion protein folding in a domain critical for infectious prion formation**	Andrew Hill	UoM	1600000	RAS 8
	PUBLICATION/PRESENTATION				
	Coleman, B.M., Harrison, C.F., Guo, B., Masters, C.L., Barnham, K.J., Lawson, V.A., and Hill, A.F., Pathogenic Mutations within the hydrophobic domain of the prion protein lead to the formation of protease sensitive prions with increased lethality, Journal of Virology. [4.648]				
	Hill, A.F., Research Update, CJD Support Group Annual Conference, Australia.*				
	Hill, A.F., Role of exosomes in neurodegenerative diseases, Asia Pacific Society for Prion Research, Korea.*				
VR0236	**Modelling post operative arrhythmogensis in Tetralogy of Fallot patients**	Andreas Pflaumer Bryn Jones Chris Butler	RCH RCH IBM	2003000	RAS 8
VR0240	**Statistical imputation of HLA and KIR alleles and studies of disease in diverse human populations**	Stephen Leslie	MCRI	1460000	RAS 8
	PUBLICATION/PRESENTATION				
	Leslie, S., Typing Immune System Genes from SNP Array Data, Plenary Talk, American Society for Histocompatibility and Immunogenetics, USA.*				
	Leslie, S., Typing Immune System Genes from SNP Array Data, Invited Talk: Cambridge Institute for Medical Research, UK.*				
	Motyer, A., Factors Affecting HLA Allele Imputation from SNP Genotypes, Bioinformatics Seminar, Walter and Eliza Hall, Australia.*				
	Vukcevic, D., Efficient And Accurate Imputation Of KIR Types From SNP Variation Data, ACS/IMS Conference, Australia.*				
	Vukcevic, D., Imputation of KIR gene variation from SNP genotypes, Bioinformatics Seminar, Walter and Eliza Hall, Australia.*				

PROJECT ID	PROJECT TITLE	CHIEF INVESTIGATORS	INSTITUTE	VLSCI SERVICE UNITS	ALLOCATION TYPE
VR0250	**Modelling protein-carbohydrate recognition**	Elizabeth Yuriev Paul Ramsland	Monash Burnet	704000	RAS 8
	PUBLICATION/PRESENTATION				
	Agostino, M., Velkov, T., Dingjan, T., Williams, S.J., Yuriev, E., and Ramsland, P.A., The carbohydrate-binding promiscuity of *Euonymus europeaus* lectin is predicted to involve a single binding site, Glycobiology. [3.747]				
	Dingjan, T., Agostino, M., Ramsland, P.A., and Yuriev, E., Antibody-carbohydrate recognition from docked ensembles using the AutoMap procedure, Methods in Molecular Biology (hardcover).				
	Dingjan, T., Agostino, M., Ramsland, P.A.,and Yuriev, E., The role of extended conformational sampling in peptide and carbohydrate docking, Molecular Modelling 2014, Australia.*				
	Dingjan, T., Agostino, M., Ramsland, P.A. and Yuriev, E., Molecular docking: extended conformational sampling of peptides and carbohydrates, RACI National Congress, Australia.*				
VR0251	**Investigation of targeted drug delivery through optimising release position**	Steve Moore Andrew Ooi	IBM UoM	1220000 1600000	RAS 7 RAS 8
	PUBLICATION/PRESENTATION				
	Zhu, S., Poon, E., Ooi, A., and Moore, S., Enhanced Targeted Drug Delivery Through Controlled Release in a 3D Vascular Tree, Journal Biomechanical Engineering. [1.748]				
VR0252	**The hydrophobic effect and protein folding**	Angus Gray-Weale Paul Mulvaney	UoM UoM	300000 300000	RAS 8 RAS 9
	PUBLICATION/PRESENTATION				
	Beattie, J.K., Djerdjeva, A.M., Gray-Weale, A., Kallayc, N., Lützenkirchend, J., Preočaninc, T., and Selmanic, A., pH and the surface tension of water, Journal of Colloid and Interface Science. [3.552]				
	Gray-Weale, A., An explanation for the hydrophobic effect, UWA Seminar, Australia.*				
	Gray-Weale, A., An explanation for the hydrophobic effect, Curtin University, Australia.*				
	Gray-Weale, A., An explanation for the hydrophobic effect, University of Wollongong, Australia.*				
	Gray-Weale, A., An explanation for the hydrophobic effect, Forschungzentrum Juelich, Germany.*				
VR0254	**The genome sequence of the parasitic dinoflagellate Hematodinium**	Sebastian Gornik Thomas Otto Arnab Pain Ross Waller	UoM Sanger KAUST UoM	120000	RAS 8
	PUBLICATION/PRESENTATION				
	Bachvaroff, T.R., Gornik, S.G., Concepcion, G.T., Waller, R.F., Mendez, G.S., Lippmeier, J.C., and Delwiche, C.F., Dinoflagellate phylogeny revisited: Using ribosomal proteins to resolve deep branching dinoflagellate clades, Molecular phylogenetics and evolution. [4.018]				
VR0256	**Molecular simulation of actin dynamics in the malaria parasite: the track of parasite gliding motor**	Jake Baum	WEHI	1800000	RAS 8
VR0257	**Molecular dynamics simulations of the bacteriophage lysin PlyC**	Sheena McGowan	Monash	2000000	RAS 7
VR0258	**Examining the connection between defective mRNA splicing and colon cancer**	Chris Love Joan Heath	WEHI WEHI	57000	Start-Up/ Discretionary
	PUBLICATION/PRESENTATION				
	Badrock, A. Boglev, Y., de Jong-Curtain, T., Doggett, K., Achtman, A., Love, C., Hung, L.L., Verkade, H., Hannan, R., Hannan, K., Sieber, O., Stemple, D., Lieschke, G., Stainier, D., and Heath, J., Loss of Nol8 function results in developmental abnormalities via Tp53-dependent and independent pathways, 6th Strategic Conference of Zebrafish Investigators, USA.*				
	Heath, J.K., Williams, B., Doggett, K., Simkin, J., Keightley, M.-C., Love, C., Sieber, O.M., Gong, Z., and Lieschke, G.J., Targeting essential cellular processes to restrict the growth of proliferating cells, Zebrafish Disease Models, USA.*				
	Badrock, A.P., Boglev, Y., de Jong-Curtain, T., Doggett, K., Achtman, A., Love, C., Verkade, H., Hannan, R.D., Hannan, K.M., Sieber, O., Lieschke, G.J., Stainier, D.Y.R., and Heath, J.K., Loss of Nol8 function in zebrafish results in developmental abnormalities via Tp53-dependent and independent pathways, P53 Workshop, Peter MacCallum Cancer Centre, Melbourne, Australia.*				

PROJECT ID	PROJECT TITLE	CHIEF INVESTIGATORS	INSTITUTE	VLSCI SERVICE UNITS	ALLOCATION TYPE
VR0261	**Co-evolutionary dynamics of culture and complex contagion on social networks**	Alex Stivala Garry Robins Yoshihisa Kashima Michael Kirley	UoM UoM UoM UoM	400000	RAS 8

PUBLICATION/PRESENTATION

Stivala, A., Wang, P., Koskinen, J., Robins, G., and Rolls, D., Ultrametric distribution of culture vectors in an extended Axelrod model of cultural dissemination, Scientific Reports. [5.078]

Stivala, A. D., Koskinen, J. L., Wang, P., Robins, G. L., and Rolls, D., Snowball sampling for estimating exponential random graph models for large networks, Social Networks (under review at time of submission). [2.138]

Stivala, A., Wang, P., Koskinen, J., Robins, G., and Rolls, D., Many snowballs make light work: a technique for large networks, INSNA Sunbelt XXXIV, USA.*

Stivala, A. D., Koskinen, J. L., Wang, P., Robins, G. L., Rolls, D. A. and Lomi, A., Modelling large networks via snowball samples, International Conference on Computational Social Science 2015 (extended abstract submitted), Finland.

PROJECT ID	PROJECT TITLE	CHIEF INVESTIGATORS	INSTITUTE	VLSCI SERVICE UNITS	ALLOCATION TYPE
VR0264	**A longtitudinal study of brain volume and cognitive decline flollowing stroke**	Qi Li Amy Brodtmann Heath Pardoe Toby Cumming Graeme Jackson Geoffrey Donnan	UoM Florey Florey Florey Florey Florey	100000	RAS 8

PUBLICATION/PRESENTATION

Li, Q., Pardoe, H., Lichter, R., Werden, E., Raffelt, A., Cumming, T., Brodtmann, A., Cortical thickness estimation in longitudinal stroke studies: A comparison of 3 measurement methods, Neuroimage: Clinical.

Brodtmann, A., Werden, E., Pardoe, H., Li, Q., Jackson, G., Donnan, G., Cowie, T., Bradshaw, J., Darby, D., and Cumming, T., Charting cognitive and volumetric trajectories after stroke: Protocol for the Cognition And Neocortical Volume After Stroke (CANVAS) Study, International Journal of Stroke. [4.029]

Cumming, T., Li, Q., Werden, E., Raffelt, A., Lichter, R., Pardoe, H., and Brodtmann, A., Cognition early after stroke correlates better with regional brain volume than white matter hyperintensity volume, International Cognitive Neuroscience Conference, Australia.*

Cumming, T., Werden, E., Raffelt, A., Lichter, R., Li, Q., and Brodtmann, A., More physical activity is associated with better cognition at 3 months post-stroke, Stroke Society of Australasia Conference, Australia.*

Veldsman, M., Cumming, T., and Brodtmann, A., Hippocampal connectivity in ischaemic stroke patients and age matched controls, International Journal of Stroke. [4.029]

PROJECT ID	PROJECT TITLE	CHIEF INVESTIGATORS	INSTITUTE	VLSCI SERVICE UNITS	ALLOCATION TYPE
VR0272	**Determination of a cell death gene expression signature for zebrafish intestinal mutants**	Joan Heath	WEHI	115000	RAS 7

PUBLICATION/PRESENTATION

Badrock, A., Boglev, Y., de Jong-Curtain, T., Doggett, K., Achtman, A., Love, C., Hung, L.L., Verkade, H., Hannan, R., Hannan, K., Sieber, O., Stemple, D., Lieschke, G., Stainier, D., and Heath, J., Loss of Nol8 function results in developmental abnormalities via Tp53-dependent and independent pathways, 6th Strategic Conference of Zebrafish Investigators, USA.*

Heath, J.K., Williams, B., Doggett, K., Simkin, J., Keightley, M.-C., Love, C., Sieber, O.M., Gong, Z., and Lieschke, G.J., Targeting essential cellular processes to restrict the growth of proliferating cells, Zebrafish Disease Models.*

Badrock, A.P., Boglev, Y., de Jong-Curtain, T., Doggett, K., Achtman, A., Love, C., Verkade, H., Hannan, R.D., Hannan, K.M., Sieber, O., Lieschke, G.J., Stainier, D.Y.R., and Heath, J.K., Loss of Nol8 function in zebrafish results in developmental abnormalities via Tp53-dependent and independent pathways, P53 Workshop, Peter MacCallum Cancer Centre, Melbourne, Australia.*

PROJECT ID	PROJECT TITLE	CHIEF INVESTIGATORS	INSTITUTE	VLSCI SERVICE UNITS	ALLOCATION TYPE
VR0274	**Infectious diseases modelling and simulation**	James McCaw Jodie McVernon Nicholas Geard	UoM UoM UoM	2280000 60000	RAS 7 RAS 9

PUBLICATION/PRESENTATION

Butler, J., Hooper, K.A., Petrie, S.M., Lee, R., Maurer-Stroh, S., Reh, L., Guarnaccia, T., Baas, C., Xue, L., Vitesnik, S., Leang, S.K., McVernon, J., Kelso, A., Barr, I.G., McCaw, J.M., Bloom, J.D., and Hurt, A.C., Estimating the fitness advantage conferred by permissive neuraminidase mutations in recent oseltamivir-resistant A(H1N1)pdm09 influenza viruses, PLoS Pathogens. [8.057]

Cao, P., Yan, A., Laurie, K., Petrie, S., McVernon, J., and McCaw, J.M., A mathematical analysis of influenza virus-induced innate immune responses based on ferret reinfection experiments, 8th Australian New Zealand Mathematics Convention, Australia.*

Yan, A., Cao, P., Guarnaccia, T., Carolan, L., Aban, M., Moss, R., Petrie, S., McVernon, J., Heffernan, J., Laurie, K., and McCaw, J.M., Using mathematical models to examine the role of innate and adaptive immune responses in controlling infection, 10th Australian Influenza Symposium, Australia.*

McCaw, J.M., Guarnaccia, T., Carolan, L.A., Laurie, K.L., Within host influenza infection dynamics: modelling re-infection to understand the role of immunity, Australian New Zealand Industrial and Applied Mathematics Conference, New Zealand.*

PROJECT ID	PROJECT TITLE	CHIEF INVESTIGATORS	INSTITUTE	VLSCI SERVICE UNITS	ALLOCATION TYPE
VR0275	**Free energy simulations of ion channels and transporters**	Serdar Kuyucak	SydneyUni	2000000	RAS 7

PUBLICATION/PRESENTATION

Heinzelmann, G., and Kuyucak, S., Molecular dynamics simulations elucidate the mechanism of proton transport in the glutamate transporter EAAT3, Biophysical Journal. [3.832]

Heinzelmann, G., and Kuyucak, S., Molecular dynamics simulations of the mammalian glutamate transporter EAAT3, PLOS One. [3.534]

PROJECT ID	PROJECT TITLE	CHIEF INVESTIGATORS	INSTITUTE	VLSCI SERVICE UNITS	ALLOCATION TYPE
VR0276	**Diffusion-guided quantitative susceptibility mapping**	Amanda Ng Bernie Pope	Monash VLSCI	40000	RAS 8
VR0277	**Statistical and simulation modelling of emergency animal disease outbreaks**	Caitlin Pfeiffer Simon Firestone	UoM UoM	15000	Start-Up/ Discretionary
VR0278	**Modelling of beta-glucan endohydrolases in barley**	John Wagner Geoff Fincher	IBM UoA	300000	RAS 8
VR0280	**Hosted Hardware: Andrew Turpin**	Andrew Turpin Timothy Baldwin	UoM UoM	140160	Start-Up/ Discretionary

PUBLICATION/PRESENTATION

Chong, L., McKendrick, A.M., and Turpin, A., Targeted spatial sampling using GOANNA improves detection of visual field progression, Ophthalmic and Physiological Optics. [2.664]

McKendrick, A.M., Denniss, J., and Turpin, A., Response times across the visual field: empirical observations and application to threshold determination, Vision Research. [2.381]

Denniss J., Turpin, A., and McKendrick, A.M., Individualised structure-function mapping for glaucoma: Practical constraints on map resolution for clinical and research applications, Investigative Ophthalmology and Visual Science. [3.661]

Gog, S., Moffat, A., Culpepper, J., Turpin, A., and Wirth, A., Large-scale pattern search using reduced-space on-disk suffix arrays, IEEE Trans. Knowledge and Data Engineering. [1.815]

Denniss, J., Turpin, A., Tanabe, F., Matsumoto, C., and McKendrick, A.M., Structure-function mapping: Variability and conviction in tracing retinal nerve fibre bundles and comparison to a computational model, Investigative Ophthalmology and Visual Science. [3.661]

PROJECT ID	PROJECT TITLE	CHIEF INVESTIGATORS	INSTITUTE	VLSCI SERVICE UNITS	ALLOCATION TYPE
VR0284	**Start Up - Understanding the spatio-temporal patterns of human mediated plant invasions**	Mark Burgman	UoM	7960	Start-Up/ Discretionary
VR0285	**Improving non-invasive assessment of aortic coarctation severity**	Jonathan Mynard Joe Smolich	MCRI MCRI	80000	RAS 8
VR0286	**New methods for mapping variation in forest water use in time and space**	Richard Benyon Dominik Jaskierniak George Kuczera Patrick Lane	UoM UoM UoN UoM	100000	RAS 8

PUBLICATION/PRESENTATION

Jaskierniak, D., Kuczera, G., Benyon, R.J., and Lucieer, A., Spatial variation of tree and stand sapwood area in southeastern Australian forests, Remote Sensing. [2.623]

PROJECT ID	PROJECT TITLE	CHIEF INVESTIGATORS	INSTITUTE	VLSCI SERVICE UNITS	ALLOCATION TYPE
VR0290	**Start Up - Molecular modelling studies on bromodomain ligands as anticancer agents**	Chris Burns	WEHI	4000	Start-Up/ Discretionary
VR0292	**Start up - Formation of sugar radical cations in the gas phase**	Sandra Osburn	UoM	5000	Start-Up/ Discretionary
VR0294	**Start Up - Architectural building blocks of protein three-dimensional structures**	Arun Konagurthu	Monash	10000	Start-Up/ Discretionary
VR0296	**Electronic structural modelling and CPMD simulation for molecules**	Marawan Ahmed Feng Wang	Swinburne Swinburne	65000	RAS 8

PUBLICATION/PRESENTATION

Ahmed, M. Sadek, M.M., Abouzid, K.A., Wang, F., In Silico Design: Extended Molecular Dynamic Simulations of a New Series of Dually Acting Inhibitors against EGFR and HER2, Journal of Molecular Graphics and Modelling (44: 220–231). [2.022]

Ahmed, M., Bird, S., Wang, F., and Palombo, E.A., In silico investigation of lactone and thiolactone inhibitors in bacterial quorum sensing using molecular modeling, International Journal of Chemistry (5(4):9-16).

Wang, F., and Ahmed, M., Sitting above the Maze: Recent Model Discoveries in Molecular Science, Molecular Simulation (Invited Review) (DOI: 10.1080/08927022.2014.923570). [1.119]

Ahmed, M., Wang, F., Lavin, A., Le, C., Eltayebi, Y., Houghton, M., Tyrrell, L. and Barakat, L., Targeting the “Achilles heel” of the hepatitis B virus: A review of current treatments against covalently closed circular DNA (cccDNA), Drug Discovery Today. [5.964]

PROJECT ID	PROJECT TITLE	CHIEF INVESTIGATORS	INSTITUTE	VLSCI SERVICE UNITS	ALLOCATION TYPE
VR0299	**Computation of 13C NMR chemical shifts in cellulose**	Natalie Gilka Tony Bacic Mike Gidley	UoM UoM UQ	300000	RAS 8
	PUBLICATION/PRESENTATION				
	Gilka, N., Cellulose: Advances in Computational Modelling, February CoE Plant Cell Walls Meeting, Australia.*				
	Gilka, N., Computations: More General Aspects, TB Group Meeting, Australia.*				
VR0300	**Molecular simulation of the von Willebrand Factor - Factor VIII Binding Structure**	Tiffany Walsh	Deakin	801000	RAS 8
VR0301	**Antifouling and antimicrobial coatings**	George Yiapanis Irene Yarovsky	RMIT RMIT	500000 500000	RAS 8 RAS 9
	PUBLICATION/PRESENTATION				
	Yiapanis, G., Maclaughlin, S., Evans, E., and Yarovsky, I., Nanoscale Wetting and Fouling Resistance of Functionalized Surfaces: a Computational Approach, Langmuir. [4.384]				
	Ley, K., Christofferson, A., Winkler, D., Maclaughlin, S., Evans, E. and Yarovsky, I., Elucidating Mechanisms and Limitations of Anti-Fouling Surfaces, Molecular Modelling 2014: From biomolecules to materials, Australia.*				
	Ley, K., Christofferson, A., Winkler, D., Maclaughlin, S., Evans, E. and Yarovsky, I., Anti-fouling Effectiveness of PEG-modified surfaces: A Molecular Dynamics Study, 3rd Biennial Conference of the Combined Australian Materials Societies 2014, Australia.*				
	Ley, K., Yiapanis, G., Winkler, D., Maclaughlin, S., Evans, E., and Yarovsky, I., A computational study of protein adhesion on anti-fouling surfaces, International Conference on Nanoscience and Nanotechnology 2014, Australia.*				
	Ley, K., Christofferson, A., Winkler, D., Maclaughlin, S., and Yarovsky, I., Detailing Spontaneous Protein Adsorption on Responsive Surfaces, Nanotechnology & Medicines for Tomorrow, Melbourne, Australia.*				
VR0302	**Binding of ApoE4 to liposomes**	Matthew Perugini Matthew Downton	La Trobe IBM	900000 707000	RAS 8 RAS 9
VR0303	**Understanding how the ubiquitous glycolytic enzyme, GAPDH, aggregates**	Andre Samson	Monash	900000	RAS 8
	PUBLICATION/PRESENTATION				
	Samson, A.L., Knaupp, A.S., Kass, I., Kleifeld, O., Marijanovic, E.M., Hughes, V.A., Lupton, C.L., Buckle, A.M., Bottomley, S.P., and Medcalf, R.L., Oxidation of an exposed methionine instigates the aggregation of glyceraldehyde-3-phosphate dehydrogenase, Journal of Biological Chemistry. [4.600]				
VR0304	**DEPTH analysis of the world's breast and other cancers genomics and epigenomics data**	Enes Makalic John Hopper Daniel Schmidt Daniel Park Guoqi Qian Minh Bui	UoM UoM UoM UoM UoM UoM	5037000	RAS 8
VR0305	**Understanding the role of dynamics in engineering protein stability and function**	Ashley Buckle	Monash	4200000	RAS 8
VR0306	**Computing nano-bio interactions for nanomedicine**	Edmund Crampin	UoM	200000	RAS 8
VR0308	**Computational modelling of plant cellulose synthase-like (Csl) proteins**	Monika Doblin Tony Bacic Daniel Oehme	UoM UoM IBM	3000000	RAS 8
VR0309	**Interactions of coronary geometry and cellular dynamics as biomarkers for early lesion growth**	Steve Moore Tim David	IBM UC	225000	RAS 8
VR0310	**Simulations of intra-tumour mutation heterogeneity and evolution in colorectal cancer**	Oliver Sieber	WEHI	400000	RAS 8
	PUBLICATION/PRESENTATION				
	Mouradov, D., Sloggett, C., Jorissen, R.N., Love, C.G., Li, S., Burgess, A.W., Arango, D., Strausberg, R.L., Buchanan, D., Wormald, S., O'Connor, L., Wilding, J.L., Bicknell, D., Tomlinson, I.P.M., Bodmer, W.F., Mariadason, J.M., and Sieber, O.M., Colorectal cancer cell lines are representative models of the main molecular subtypes of primary cancer, Cancer Research. [9.284]				
	Mouradov, D., Colorectal cancer cell lines are representative models of the main molecular subtypes of primary cancer, 2014 AHMR Congress, Australia.*				
VR0311	**Developing an integrated transcriptome-proteome map for colorectal cancer**	Oliver Sieber	WEHI	1042000	RAS 8
VR0313	**Models to understand the role of cellular organisation in heart disease and cancer**	Edmund Crampin Vijay Rajagopal	UoM UoM	200000	RAS 8
VR0314	**Does the brain show disconnection in the earliest stages of multiple sclerosis**	Scott Kolbe	UoM	60000	RAS 8

PROJECT ID	PROJECT TITLE	CHIEF INVESTIGATORS	INSTITUTE	VLSCI SERVICE UNITS	ALLOCATION TYPE
VR0316	**Molecular dynamic simulations of the apical membrane antigen 1 from Plasmodium falciparum**	Sheena McGowan	Monash	3000000	RAS 8
	PUBLICATION/PRESENTATION				
	Lim, S.S., Yang, W., Krishnarjuna, B., Kannan Sivaraman, K., Chandrashekaran, I. R., Kass, I., MacRaild, C.A., Devine, S.M., Debono, C.O., Anders, R.F., Scanlon, M.J., Scammells, P. J., Norton, R.S., and McGowan, S., Structure and dynamics of apical membrane antigen 1 from *Plasmodium falciparum* FVO, Biochemistry. [3.194]				
	McGowan, S., Structure and dynamics of apical membrane antigen 1 from *Plasmodium falciparum* FVO, VLSCI RAS Symposium, Melbourne, Australia.*				
VR0318	**Sampling activation pathways in ion channel function**	Toby Allen	RMIT	10000000	RAS 8
	PUBLICATION/PRESENTATION				
	Lev, B., Murail, S., Poitevin, F., Baaden, M., Delarue, M., and Allen, T.W., Solution of the allosteric signal transduction pathway for a pentameric ligand-gated ion channel, Biochemistry. [9.809]				
	Lev, B., Murail, S., Poitevin, F., Baaden, M., Delarue, M., and Allen, T.W., Activation pathways for ligand-gated channels, 2015 Snowmass Free energy Meeting, CO, USA.*				
	Allen, T.W., Membrane and Ion channel Mechanisms, Australian National University, RSB, Australia.*				
	Allen, T.W., Solving the gating mechanisms for a pentameric ligand-gated ion channel, Institut Pasteur, France.*				
VR0319	**Computational model of the plant cell wall**	Tony Bacic Mike Gidley Daniel Oehme	UoM UQ IBM	6000000	RAS 8
	PUBLICATION/PRESENTATION				
	Oehme, D.P., Downton, M., Doblin, M.S., Wagner, J., Gidley, M., and Bacic, A., Elementary Cellulose Microfibrils: Structure, Dynamics and Interactions, 5th International Conference on Plant Cell Wall Biology, Australia.*				
VR0323	**Dalton development**	Peter Taylor	VLSCI	40000	Start-Up/ Discretionary
VR0324	**Start Up - Direct numerical simulation of transitional and turbulent flow in arterial geometries**	Jagmohan Singh Murray Rudman	Monash Monash	5000	Start-Up/ Discretionary
VR0325	**Start Up - Malaria genetics and epidemiology**	Thomas Rask	UoM	24479.5	Start-Up/ Discretionary
VR0326	**Start Up - Assembly of HIV-1 Gag and GagPol precursor proteins during virion formation**	Katharina Kopp	CSIRO	28555	Start-Up/ Discretionary
VR0329	**A quantum mechanical description of irradiation damage in DNA**	Amanda Barnard Manolo Per	CSIRO CSIRO	20000	Start-Up/ Discretionary
VR0335	**Start Up - Evaluation of LC-MS metabolomics tools**	Sean O'Callaghan	UoM	11250	Start-Up/ Discretionary
VR0339	**Startup - HealthHack 2014**	Bernie Pope Philippa Griffin	VLSCI UoM	5000	Start-Up/ Discretionary
VR0345	**Startup - Analysis of mass spectrometry data, metabolomics and high performance computing**	Andrew Isaac Bernie Pope	VLSCI VLSCI	6250	Start-Up/ Discretionary
VR0346	**Startup - Quantitative analysis of large confocal data sets**	Verena Wimmer	Florey	6250	Start-Up/ Discretionary
NCE31	**Electromagnetic structure of matter**	Derek Leinweber James Zanotti Waseem Kamleh	UoA UoA UoA	1000000	NCMAS
	PUBLICATION/PRESENTATION				
	Zanotti, J., Nucleon Structure from Lattice QCD, International Workshop on Frontiers of QCD, India.*				

PROJECT ID	PROJECT TITLE	CHIEF INVESTIGATORS	INSTITUTE	VLSCI SERVICE UNITS	ALLOCATION TYPE
NCE87	**Theoretical investigation of surfaces and interfaces for industrial and biomedical applications**	Irene Yarovsky Nevena Todorova	RMIT RMIT	600000	NCMAS
	PUBLICATION/PRESENTATION				
	Todorova, N. Ciapini, C., Mager, M., Simona, B., Patel, I.I., Stevens, M.M., and Yarovsky, I., Surface presentation of functional peptides determines cell internalization efficiency of TAT modified nanoparticles, Nano Letters. [12.940]				
	Andresen, H. Mager, M., Grießner, M., Charchar, P., Todorova, N., Bell, N., Theocharidis, G., Bertazzo, S., Yarovsky, I., and Stevens, M.M., Epitope-tagged gold nanoparticles in immune complex forming systems: on feasibility, mechanism and limitations of single-step immunoassays, Chemistry of Materials. [8.535]				
	Ren, J., Satoh, K., Goh, T., Blencowe, A., Nagai, K., Ishitake, K., Christofferson, A., Yiapanis, G., Yarovsky, I., Kamigaito, M., and Qiao, G., Stereospecific cyclic poly(methylmethacrylate) and its topology-guided hierarchically-controlled supramolecular assemblies, Angewandte Chemie International Edition. [11.336]				
	Yiapanis, G., Maclaughlin, S., Evans, E., and Yarovsky, I., Nanoscale wetting and fouling resistance of functionalized surfaces: a computational approach, Langmuir. [4.384]				
	Leung, A., Prime, E., Tran, D., Fu, Q., Christofferson,A., Yiapanis, G., Yarovsky, I., Qiao, G.G., and Solomon, D.H., Dynamic performance of duolayers at the air/water interface - Part A: Experimental analysis, Journal of Physical Chemistry B. [3.377]				
NCf91	**Free energy simulations of ion channels and transporters**	Serdar Kuyucak	SydneyUni	1000000	NCMAS
	PUBLICATION/PRESENTATION				
	Heinzelmann, G., and Kuyucak, S., Molecular dynamics simulations elucidate the mechanism of proton transport in the glutamate transporter EAAT3, Biophysical Journal. [3.832]				
	Heinzelmann, G., and Kuyucak, S., Molecular dynamics simulations of the mammalian glutamate transporter EAAT3, PLOS One. [3.534]				
NCdq3	**Understanding the structural basis of pathogenic modulation of the immune response**	Mark Agostino	Curtin	200000	NCMAS
	PUBLICATION/PRESENTATION				
	Agostino, M., Mancera, R.L., Ramsland, P.A., and Fernández-Recio, J., Optimization of protein-protein docking for predicting Fc- protein binding modes, XII Symposium on Bioinformatics 2014, Spain.*				
	Agostino, M., Mancera, R.L., Ramsland, P.A., and Fernández-Recio, J., Prediction of immunoglobulin-protein interactions involved in immune response evasion by microorganisms, Lorne Proteins 2014, Australia.*				
NCw47	**Direct numerical simulations and large eddy simulations of turbulent combustion**	Evatt Hawkes	UNSW	1000000	NCMAS
	PUBLICATION/PRESENTATION				
	Karami, S., Hawkes, E.R., and Talei, M., Edge flame dynamics in a turbulent lifted jet flame, Studying Turbulence Using Numerical Simulation Databases - XV: Proceedings of the 2014 Summer Program, USA.*				
	Karami, S., Hawkes, E.R., and Talei, M., Direct numerical simulation of a turbulent lifted flame: stabilisation mechanism, 19th Australasian Fluid Mechanics Conference, Australia.*				
	Karami, S., Hawkes, E.R., and Talei, M., The structure of a turbulent lifted flame, The Third International Education Forum on Environmental and Energy Science, Australia.*				
	Karami, S., Hawkes, E.R., and Talei, M., Mechanisms of flame stabilisation at low lifted height in a turbulent lifted slot-jet flame, Journal of Fluid Mechanics. [2.294]				
NCEW9	**Clinical microbiology in the genomic era**	Mitchell Stanton-Cook Nouri Ben Zakour Scott Beatson	ANU UQ UQ	600000	NCMAS
NCM72	**From molecules to cells: Understanding the structural and dynamic properties of cellular components at an atomic level**	Alan Mark Alpeshkumar Malde	UQ UQ	400000	NCMAS
	PUBLICATION/PRESENTATION				
	Caron, B., Mark, A. E. and Poger, D., Some Like It Hot: The Effect of Sterols and Hopanoids on Lipid Ordering at High Temperature, The Journal of Physical Chemistry Letters (DOI: 10.1021/jz5020778). [6.687]				
	O'Mara, M.L., and Mark, A.E., Structural characterization of two metastable ATP-bound states of P-glycoprotein, (PLoS ONE. E91916). [3.534]				
	Koziara, K.B., Stroet, M., Malde, K.A., and Mark, A.E., Testing and validation of the Automated Topology Builder (ATB) version 2.0: Prediction of hydration free enthalpies, Journal of Computer Aided Molecular Design (28, 221-33). [2.782]				
	Brooks, A.J., Dai, W., O'Mara, M.L., Abankwa, D., Chhabra, Y., Pelekanos, R.A., Gardon, O., Tunny, K.A., Blucher, K.M., Morton, C.J., Parker, M.W., Sierecki, E., Gambin, Y., Gomez, G.A., Alexandrov, K., Wilson, I.A., Doxastakis, M., Mark, A.E. and Waters, M.J., A new cytokine receptor activation paradigm: activation of JAK2 by the Growth Hormone Receptor, Science (344, 1249783). [31.477]				
	Poger, D., and Mark, A.E., The activation of the epidermal growth factor receptor: a series of twists and turns, Biochemistry. [3.194]				

PROJECT ID	PROJECT TITLE	CHIEF INVESTIGATORS	INSTITUTE	VLSCI SERVICE UNITS	ALLOCATION TYPE
NCV15	**Molecular simulations of enzymatic catalysis**	Haibo Yu	UoW	400000	NCMAS
	PUBLICATION/PRESENTATION				
	Nguyen, P.T., Yu, H., and Keller, P.A., Identification of chikungunya virus nsP2 protease inhibitors using structure-base approaches, Journal of Molecular Graphics & Modelling [2.022]				
	Griffiths, T.M., and Yu, H., Oxygen Binding Sites in Obelin: A computational study into the formation of active photoproteins, Luminescence. [1.675]				
NCg15	**Simulation studies of biological and synthetic channels**	Ben Corry	ANU	500000	NCMAS
	PUBLICATION/PRESENTATION				
	Martin, L.J., Corry, B., Locating the route of entry and binding sites of benzocaine and phenytoin in a bacterial voltage gated sodium channel, PLoS Computational Biology. [4.829]				
	Thomas, M., Corry, B., and Hilder, T., What have we learnt about the mechanisms of rapid water transport, ion rejection and selectivity in nanopores from molecular simulation?, Small. [7.514]				
	Thomas, M., and Corry, B., Thermostat choice significantly influences water flow rates in molecular dynamics studies of carbon nanotubes, Microfluidics and Nanofluidics. [2.665]				
	Smith, N.E., Vrielink, A., Attwood, P.V., and Corry, B., Binding and channelling of alternative substrates in the enzyme DmpFG: A molecular dynamics study, Biophysical Journal. [3.832]				
	Smith, N.E., Swaminathan Iyer, K., and Corry, B., The confined space inside carbon nanotubes can dictate the stereo- and regioselectivity of Diels-Alder Reactions, Physical Chemistry Chemical Physics. [4.198]				
NCEZ1	**Simulations of bio-active assemblies for improved discovery of novel drugs**	Johannes Zuegg	UQ	200000	NCMAS
NCEZ8	**Shear induced platelet aggregation characterising shear forces in in-vitro geometries**	Kris Ryan	Monash	500000	NCMAS
	PUBLICATION/PRESENTATION				
	Yang, W., Kass, I., Buckle, A.M., and McGowan, S., Structural analysis of *Plasmodium falciparum* aminopeptidase PfA-M1, Lorne Conference on Protein Structure and Function, Australia.*				
NCEU8	**Characterising the M1 and M17 malarial aminopeptidases for design of new antimalarial agents**	Sheena McGowan	Monash	500000	NCMAS
NCN67	**Advanced modelling of biological fluid flows**	Kerry Hourigan	Monash	1000000	NCMAS
NCq75	**Toxin binding to membrane proteins - New tools for molecular neuroscience**	Andrew Hung	RMIT	500000	NCMAS
	PUBLICATION/PRESENTATION				
	Chhabra, S., Belgi, A., Bartels, P., Robinson, S.D., Kompella, S.N., Hung, A., Adams, D.J. *et al*., Dicarba analogues of α-conotoxin RgIA. Structure, stability and activity at potential pain targets, Journal of Medicinal Chemistry. [5.48]				
	Kompella, S.N., Hung, A., Adams, D.J. *et al*., Alanine scan of α-conotoxin RegIIA reveals a selective α3β4 nicotinic acetylcholine receptor antagonist, Journal of Biological Chemistry. [4.600]				
	Kompella, S.N., Hung, A., Adams, D.J., *et al*., Species difference in α-conotoxin RegIIA inhibition of nAChRs: molecular basis for differential sensitivity, Australian Physiological Society Meeting, Australia.*				
	Suresh, A., Hung, A., and Adams, D.J., Computational identification of structural and interaction properties of GID α-conotoxins at the α7 and α4β2 nicotinic receptor, Wellcome Trust Nicotinic Receptors Conference, United Kingdom.*				
NCEX0	**Understanding the role of protein dynamics in E3 ligase function**	Itamar Kass Natalie Borg	Monash Monash	400000	NCMAS
NCG23	**Molecular interactions**	Meredith Jordan	SydneyUni	200000	NCMAS

10.

Governance

Funded by the Victorian Government and hosted at the University of Melbourne for other contributing stakeholders, governance of VLSCI was managed under the following groups and committees until the end of 2014.

University Reference Group

The University of Melbourne (UoM) formed the VLSCI Steering Group in August 2008 to direct the development of the VLSCI. With the appointment of the VLSCI Steering Committee the group was transformed into a University Reference Group to provide advice to the University on recommendations of the Steering Committee. The group has reviewed the University's responsibilities in the Grant Agreement particularly for the financial model and risk management plan. This Group met a total of twice in 2014, in January and October.

Prof. Liz Sonenberg *Pro Vice-Chancellor (Research Collaboration), UoM (Chair)*
Prof. James McCluskey *Deputy Vice-Chancellor (Research), UoM*
Prof. Peter R. Taylor *Director*
Prof. John Zillman *Chair, VLSCI Steering Committee*
Mr John Bruzzaniti *Director, Major Projects, UoM*
Ms Karin Diamond *Business Manager (Observer)*
A/Prof. Andrew Lonie *Head, LSCC (Observer)*
Ms Fiona Kerr *Executive Officer (Secretary)*

Victorian Life Sciences Computation Initiative Sustainability Planning Seniors Group (arising out of the VLSCI Liaison Group)

Representatives of The University of Melbourne and the (then) Department of State Development, Business and Innovation (DSDBI) continued to liaise regularly to review the implementation of the approved Business Plan. Three meetings were held in 2014, in January, March and June.

Mr Grantly Mailes *Deputy Secretary, DSDBI*
Ms Amelia King *Senior Policy Officer, CRC Bid Support Program Manager, Technology Policy, Innovation & Technology, DSDBI*
Mr Matthew Dummett *Director, Science & Technology Policy, DSDBI*
Prof. James McCluskey *Deputy Vice-Chancellor (Research), UoM*
Prof. Liz Sonenberg *Pro Vice-Chancellor (Research Collaboration & Infrastructure), UoM*
Prof. Peter R. Taylor *Director*
Ms Karin Diamond *Business Manager*

Dr Mike Sargent (VLSCI's Independent Advisor) attended the January and March meetings by invitation. Ms Jane Gardam (Manager, Science and Technology Policy, DSDBI) attended the January meeting; Ms Leonie Walsh (Victoria's Lead Scientist) attended both the January and June meetings; Phillip Marley (Manager, Biotechnology Research and Technology, DSDBI) attended the March and June meetings; Mr Cameron Boardman (Executive Director, Innovation Industry and Technology Programs, DSDBI) attended the June meeting.

Scientific Advisory Committee

The Scientific Advisory Committee advises the Director on the appropriate use of the LSCC and the PCF. It also considers opportunities to initiate new research areas and collaborations to take advantage of the capabilities of the LSCC and the PCF. The Committee met twice in 2014, in March and September.

Prof. Tony Bacic *Director, Bio21 Institute (Chair)*
Prof. Mark Ellisman *Director, National Center for Microscopy & Imaging Research Chemistry, University of California, San Diego*
Prof. John Hopper *Director (Research), Melbourne School of Population Health, UoM*
Prof. Mark Ragan *Head, Genomics and Computation Biology Division, Institute for Molecular Bioscience, UQ*
Prof. Terry Speed *Laboratory Head, Bioinformatics, WEHI*
Prof. James Whisstock *ARC Federation Fellow, Honorary NHMRC Research Fellow, Department of Biochemistry & Molecular Biology, Monash University*
Prof. Marc Wilkins *Director, Ramaciotti Centre for Gene Function Analysis, UNSW*
Dr John A. Taylor *Leader, Computational & Simulation Sciences, CSIRO*
Dr Ajay Royyuru *Director, Computational Biology Center, IBM Thomas J. Watson Research Center, New York State, USA*
Prof. Peter R. Taylor *Director, VLSCI*
Prof. Justin Zobel* *Program Leader & Principal Research Fellow, NICTA, Head, Department of Computing & Information Systems, UoM (Observer)*
Prof. Brian Smith* *Theme leader, Molecular Modelling, LSCC (Observer)*
Prof. Gary Egan* *Theme leader, Computational Imaging, LSCC, Director, Monash Biomedical Imaging, Monash University (Observer)*
Ms Fiona Kerr *Executive Officer (Secretary)*

*Professors Zobel, Smith and Egan are invited to attend this meeting as observers in their role as LSCC theme leaders.

A./Prof. Andrew Lonie (LSCC Head), Dr Vera Hansper (PCF Manager) and Dr John Wagner (Manager, IBM Research Collaboratory for Life Sciences – Melbourne) attended the March and September meetings. Ms Helen Gardiner (Communications Manager) also attended the September meeting.

Steering Committee

The role of the Steering Committee is to provide advice to the University on the overall Initiative and especially with strategies, policies and performance of the VLSCI. The Committee met four times in 2014, in February, July, September and December.

Prof. John Zillman AO *Chair*
Prof. Paul Bonnington *Director, eResearch Centre, Monash University*
Prof. Trevor Kilpatrick *Director, Melbourne Neuroscience Institute, UoM*
Dr Mark Kosten *Director, eResearch, La Trobe University (retired July 2014)*
Prof. David Bowtell *Head, Cancer Genomics & Genetics, Peter MacCallum Cancer Institute*
Dr Ajay Royyuru *Director, Computational Biology Center, IBM Thomas J. Watson Research Center, New York State, USA*
Prof. Tony Bacic *Chair, VLSCI Scientific Advisory Committee*
Prof. Brian Smith *Faculty of Science, Technology and Engineering, Deputy Head, La Trobe Institute for Molecular Science, La Trobe University (from September 2014)*
Prof. Ian Smith *Pro Vice Chancellor, Research & Research Infrastructure, Monash University*
Prof. Robin Stanton *Deputy Chair, NCI Board*
Prof. Peter R. Taylor *Director*
Prof. Ingrid Winship *Executive Director of Research, Melbourne Health, Chair, Adult Clinical Genetics, Melbourne Health*
Prof. Justin Zobel *Program Leader & Principal Research Fellow, NICTA, Head, Department of Computing & Information Systems, UoM*
Ms Fiona Kerr *Executive Officer (Secretary)*
Prof. Liz Sonenberg *Pro Vice-Chancellor (Research Collaboration & Infrastructure), UoM (Observer)*
Ms Amelia King *Senior Policy Officer, CRC Bid Support Program Manager, Technology Policy, Innovation & Technology, DSDBI (Observer)*

Prof. James Whisstock (ARC Federation Fellow, Honorary NHMRC Principal Research Fellow, Department of Biochemistry & Molecular Biology, Monash University) attended the July meeting as an alternate for Prof. Ian Smith. Dr John Wastell (Head of Information Technology Services, WEHI) attended the September meeting as an alternate for Prof. O'Connor. Prof. Patricia Desmond (Director, Department of Radiology, The Royal Melbourne Hospital) attended the December meeting as an alternate for Prof. Winship.

Ms Karin Diamond (Business Manager), Ms Helen Gardiner (Communications Manager), Dr Vera Hansper (PCF Manager) and A/Prof. Andrew Lonie (LSCC Head) attended the February, July and September meetings. Dr Matthew Downton (IBM Research Staff Member) attended the February meeting as a representative of IBM. Dr John Wagner (Manager, IBM Research Collaboratory for Life Sciences – Melbourne) attended the July and September meetings.

PCF Resource Allocation Scheme Committee

On a request from The University, the Steering Committee accepted the responsibility for control over the establishment of the Resource Allocation Scheme Committee (RAS Committee) and responsibility for the appointment of its members. Applications to the Resource Allocation Scheme are reviewed by the RAS Committee that determines the resource grants for each application. This Committee also advises the PCF Manager on the appropriateness of Start Up Applications that may be received at any time of the year and this would normally be conducted out-of-session rather than through a formal meeting. This Committee met once in 2014 in December.

Prof. Lindsay Botten *National Computational Infrastructure (NCI), Australian National University (Chair)*

Prof. David Abramson *Director, Research Computing Centre, UQ*

Prof. Debra Bernhardt *Group Leader, Australian Institute for Bioengineering & Nanotechnology, UQ*

Prof. Ben Cocks *Research Director, Biosciences, Victorian Department of Primary Industries*

Dr Vera Hansper *PCF Manager (Secretary)*

Prof. Richard Huggins *Department of Mathematics & Statistics, UoM*

Prof. Rao Kotagiri *Department of Computing & Information Systems, UoM*

Prof. Brian Smith *Faculty of Science, Technology & Engineering, Deputy Head, La Trobe Institute for Molecular Science, La Trobe University*

Prof. Salvy Russo *Deputy Head (Research), School of Applied Sciences, RMIT University*

Dr Jing-Jia Luo *Centre for Australian Weather & Climate Research, Bureau of Meteorology*

A/Prof. Ashley Buckle *NHMRC Senior Research Fellow, Department of Biochemistry & Molecular Biology, Monash University*

Prof. Tiffany Walsh *Institute for Frontier Materials, Deakin University*

Prof. David Balding (Department of Mathematics and Statistics, UoM) attended the December meeting as an alternate for Prof. Huggins.

Ms Helen Gardiner (Communications Manger), Dr Andrew Isaac (VLSCI PCF Specialist Programmer) and Ms Fiona Kerr (VLSCI Executive Officer) attended the meeting held in December.

PCF Advisory Committee

The PCF Advisory Committee comprises active users on the machines in the PCF. They provide valuable feedback about the user experience and advice to the PCF Manager on the operations and performance of the PCF. Whilst the Committee did not formally meet in 2014 members provided out-of-session advice and consultation on specific issues as they arose.

Dr Vera Hansper *PCF Manager (Chair)*

Dr Mike Kuiper *Molecular Modelling Scientist, VLSCI*

Mr Jason Roberts *Senior Medical Scientist, National Enterovirus Reference Laboratory, WHO Poliomyelitis Regional Reference Laboratory, Victorian Infectious Diseases Reference Laboratory*

Ms Denise Wootten *Faculty of Pharmacy & Pharmaceutical Sciences, Monash University*

Ms Melissa Buskes *Department of Chemistry, La Trobe University*

Mr Colin Hales *Department of Electrical & Electronic Engineering, UoM*

Mr Evan Thomas *Computational neuroscientist, Florey Neuroscience and Mental Health Institute*

Sustainability Subgroup

The Sustainability Subgroup comprises nominated representatives of the VLSCI Steering Committee. The Committee is convened at the request of the Steering Committee to consider specific matters that may require further examination or consideration. The Committee did not convene in 2014.

Prof. John Zillman *Chair, VLSCI Steering Committee*

Prof. Peter R. Taylor *Director (Chair)*

Dr Mark Kosten *Director, eResearch, La Trobe University (retired July 2014)*

Prof. Trevor Kilpatrick *Director, Melbourne Neuroscience Institute, UoM*

Prof. Paul Bonnington *Director, eResearch Centre, Monash University*

Ms Fiona Kerr *Executive Officer (Secretary)*

LSCC Executive Committee

The LSCC Executive is comprised of the LSCC Head, the VLSCI Director and the current LSCC Theme Leaders. Note that this guarantees representation for each hub institution, as each hub is host to at least one Theme Leader. The role of the Executive is to provide strategic research management of the LSCC. The Committee did not convene in 2014.

Prof. Peter R. Taylor *Director (Chair)*
A/Prof. Andrew Lonie *Head, LSCC*
Prof. Justin Zobel *Program Leader & Principal Research Fellow, NICTA, Head, Department of Computing & Information Systems, UoM*
Prof. Gary Egan *Director, Monash Biomedical Imaging (MBI), Monash University*
Prof. Brian Smith *Faculty of Science, Technology & Engineering, Deputy Head, La Trobe Institute for Molecular Science, La Trobe University*
Ms Fiona Kerr *Executive Officer (Secretary)*

LSCC Advisory Committee

The LSCC Advisory Committee (LAC) is a superset of the LSCC Executive with the addition of one member of the VLSCI SAC and one member of the VLSCI Steering Committee. Project and (human) resource requests are considered by the LAC bi-annually and it also decides on LSCC resource allocations to projects (and thus determination of LSCC Approved Activities). In this way the LAC provides budget oversight. The LAC operates as a resource allocation committee, advising the Director what projects should be supported, for how long, and with what LSCC resources. The Committee met once in 2014 in February.

A/Prof. Andrew Lonie *Head, LSCC (Chair)*
Prof. Peter R. Taylor *Director*
Prof. Gary Egan *Director, Monash Biomedical Imaging (MBI), Monash University*
Prof. Brian Smith *Faculty of Science, Technology & Engineering, Deputy Head, La Trobe Institute for Molecular Science, La Trobe University*
Prof. Terry Speed *Laboratory Head, Bioinformatics, WEHI*
Prof. Trevor Kilpatrick *Director, Melbourne Neuroscience Institute, UoM*
Prof. Justin Zobel *Program Leader and Principal Research Fellow, NICTA, Head, Department of Computing & Information Systems, UoM*
Ms Fiona Kerr *Executive Officer (Secretary)*

RAS Committee Member, Prof. Brian Smith, La Trobe University, listening to a speaker at the RAS Presentation Day.

11.

Financials

Preamble

This is the final year of reporting under this Grant Agreement (to end 2014) (The Grant). VLSCI's initial funding has been sourced from the now Department of Economic Development, Jobs, Transport and Resources (ECODEV) under a $50 million grant from the Victorian Government and direct cash investment from The University of Melbourne (The University).

The University administers the Initiative's funds in accordance with the terms and conditions of the Grant. Interest received on the Grant funds has been generated through investment of those funds.

Account Structure

VLSCI Cash Funds

Grant funds from ECODEV reside in a separate project account - that account earning interest at Reserve Bank Rate less 40 basis points. Expenditure from the Grant is in accordance with the approved categories of expenditure, namely the Peak Computing Facility (PCF), Life Sciences Computation Centre (LSCC), Communications, Skills & Outreach Program and the Directorate.

Cash funding provided by The University ($12.82 million) is made up of a combination of direct funding from Melbourne Research and central Infrastructure Funding. In 2014 income was received from project subscription fees for LSCC services and this amounted to more than $2 million. Growth in LSCC project subscriptions has been substantial and further growth is anticipated in coming years. These funds were applied to activities of the LSCC and VLSCI and will contribute to ongoing operations in the 2015 and 2016 years. University funds reside in a separate project account.

Expenditure from this project account consists of salaries and expenditure categories not covered by the Grant funds.

All expenditure from both project accounts is made in accordance with the University's approved Financial Policies and Procedures.

In-Kind Contributions

In-Kind Contributions are accounted for by reference to the In-Kind Accounting Contribution Framework, which has been approved at a number of levels - The University's Financial Operations Department, Internal Audit and External Auditors (Oakton). The Framework is provided in a number of documents - including the preliminary 2009 Annual Report and the 2011 Business Plan - Revised.

2014 Financial Results

2014 Audit

The 2014 accounts have been reviewed by The University's Internal Audit Department and Oakton. Oakton's Audit Statement confirms the accuracy of both the accounts and the in-kind contributions and this statement, including the detailed accounts, and is published as part of the Financial Supplement to the Annual Report 2014.

Income

Income to the Initiative in the 2014 year consisted of interest earned from Grant funds and direct income support from the University. As noted above, approximately $2 million of income was earned by the LSCC as subscription income. Income to the Grant was in line with budget expectations. The University Contribution account met budget.

In-Kind Contributions

The framework for accounting for in-kind contributions was devised to capture the activities of individuals who contribute their time and the resources of their representative institutions to the VLSCI. Once again, it is pleasing to report that in-kind contributions for the 2014 year were 34% over budget for Victorian institutions. 2014 was the second year in which contributions were received from non-Victorian institutions accessing the systems and those contributions amounted to 14% of contributions from all sources.

The most significant contribution of $11.9 million in 2014 was that of individual staff working on LSCC and PCF projects. Data on the contributions of individual staff and students has been captured, specifically detailing the fraction of time spent on their project at individual salary and stipend levels. Conservative salary on-costs and overheads (to incorporate institutional resources) have then been added. A detailed report showing contributions to the LSCC & PCF is available as part of the Financial Supplement to the Annual Report 2014. This report shows activity by quarter, detailing the project, institution, details of individual staff members and students, salary level and percentage of time spent on projects. Contributions to VLSCI activities from individuals providing their time and expertise to Outreach and Directorate endeavours remain substantial, at in excess of $300,000.

Initiative Expenditure

Grant expenditure was made in accordance with the approved categories of expenditure, as agreed in the current Business Plan, and always in accordance with the University's policies and procedures. Overall expenditure was 1% under budget.

Expenditure from University Funds was 28% under budget. Electrical costs continue to be lower than anticipated and savings were vigorously sought throughout the year.

Summary

2014 was the last year of the initial Grant that saw the continuation of major expenditure related to high performance computing capital equipment, substantial growth in LSCC income and continued significant Outreach and Communications activity as well as modest expenditure to maintain the activities of the Directorate. The finances of the Initiative were managed pursuant to the agreements, policies, procedures and budgets referenced above. Once again, the overall result was sound and pleasing.

GRANT ACCOUNT STATEMENT

Grant Account Statement of Income & Expenditure for the period - 1 January 2014 to 31 December 2014

CARRY FORWARD CASH BALANCE	**14,731,742.93**
INCOME	
Interest Income Earned	262,626.27
TOTAL INCOME	**262,626.27**
SALARY EXPENDITURE	
LSCC Staff & Overheads	1,373,624.88
Salary Support - Victorian Universities & Institutes	1,330,191.41
Salary Expenditure	**2,703,816.29**
NON SALARY EXPENDITURE	
Consumable Goods and Services	97,086.16
Entertainment & FBT	943.85
Expensed Assets	15,390.58
Expert Services	344,142.93
IBM Fitout Supply - Scheduled Payments	2,314,813.00
Infrastructure Related Assets	300,000.91
Printing, Photography / Reprints, Phoroxopyinf	3,131.43
Student Support - Scholarships	151,283.49
Travel, Conf & Entertainment	145,722.92
Other (Non-Salary) Expenditure	**3,372,515.27**
TOTAL EXPENDITURE - SALARIES, MAJOR PCF & OTHER	**6,076,331.56**
TOTAL AVAILABLE (CASH)	**8,918,037.64**

UNIVERSITY CONTRIBUTION
ACCOUNT STATEMENT

University Contribution Statement of Income & Expenditure for the period - 1 January 2014 to 31 December 2014

CARRY FORWARD CASH BALANCE	**2,931,768.58**
INCOME	
Member Contributions	300,000.00
Other Grant Income	2,047,707.68
TOTAL INCOME	**2,347,707.68**
SALARY EXPENDITURE	
Directorate Salaries & Overheads	592,976.79
Outreach Salaries & Overheads	253,738.32
PCF Salaries & Overheads	965,400.59
Accounting System Payroll Transactions	6,334.53
Salary Expenditure	**1,818,450.23**
NON SALARY EXPENDITURE	
Consumable Goods and Services	25,149.87
Expensed Assets	125,877.89
Expert Services	53,513.58
Finance Related Costs	679.39
Infrastructure Related Costs	166,617.17
Student Support	32,428.66
Student Support (Grant Transfer for 2014 Interns)	-154,839.00
Travel, Conf & Entertainment	43,199.95
Other (Non-Salary) Expenditure	**292,627.51**
TOTAL EXPENDITURE	**2,111,077.74**
TOTAL AVAILABLE (CASH)	**3,168,398.52**

GLOSSARY

AGRF ..... Australian Genome Research Facility Ltd
ANDS ..... Australian National Data Service
ARC ..... Australian Research Council
Baker IDI ..... Baker IDI Heart and Diabetes Institute
Bio21 ..... Bio21 Institute
Burnet ..... Burnet Institute
CCS ..... Monash University's Central Clinical School
CCV ..... Cancer Council Victoria
CEC ..... Cancer Council Victoria's Cancer Epidemiology Centre
CERA ..... Centre for Eye Research Australia
Curtin ..... Curtin University
Deakin ..... Deakin University
DEPI ..... Department of Environment & Primary Industries Victoria
EMBL ..... European Molecular Biology Laboratory
Eng UoM ..... Melbourne School of Engineering, University of Melbourne
FedUni ..... Federation University
Florey ..... Florey Institute of Neuroscience and Mental Health
IBM ..... IBM Research Collaboratory for Life Sciences - Melbourne
KAUST ..... King Abdullah University of Science and Technology, Saudi Arabia
La Trobe ..... La Trobe University
LSCC ..... Life Sciences Computation Centre – VLSCI
Ludwig ..... Ludwig Institute for Cancer Research
Max Planck ..... Max Planck Institute of Biochemistry
MBC ..... Melbourne Brain Centre
MCRI ..... Murdoch Children's Research Institute
MDS ..... Melbourne Dental School, University of Melbourne
MHTP ..... Monash Health Translation Precinct Medical Genomics Facility
MIMR ..... Monash Institute of Medical Research
MIPS ..... Monash Institute of Pharmaceutical Sciences
Monash ..... Monash University
Museum Vic ..... Museum Victoria
NCI ..... National Computational Infrastructure
NCMAS ..... National Computational Merit Allocation Scheme
NeCTAR ..... National eResearch Collaboration Tools and Resources
NHMRC ..... National Health and Medical Research Council
NICTA ..... Information and Communications Technology Research Centre of Excellence
Oxford ..... Oxford University, Britain
PCF ..... Peak Computing Facility - VLSCI
PDI ..... Peter Doherty Institute for Infection and Immunity
Peter Mac ..... Peter MacCallum Cancer Centre
RAS ..... Resource Allocation Scheme
RBG ..... Royal Botanic Gardens
RCH ..... The Royal Children's Hospital
RMH ..... Royal Melbourne Hospital
RMIT ..... RMIT University
RWH ..... Royal Women's Hospital
Sanger ..... Sanger Institute
SVH ..... St Vincent's Hospital
SVI ..... St Vincent's Institute
Swinburne ..... Swinburne University of Technology
SydneyUni ..... The University of Sydney
UC ..... University of Canterbury
UNSW ..... University of New South Wales
UoA ..... The University of Adelaide
UoM ..... The University of Melbourne
UoN ..... University of Newcastle
UoSC ..... University of the Sunshine Coast
UoW ..... University of Wollongong
UROP ..... Undergraduate Research Opportunities Program (Biomedical Research Victoria)
UQ ..... The University of Queensland
UWA ..... The University of Western Australia
VABC ..... Victorian AgriBiosciences Centre
VBC ..... Victorian Bioinformatics Consortium
VCB ..... Victorian Cancer Biobank
VIDRL ..... Victorian Infectious Diseases Reference Laboratory
VLSCI ..... Victorian Life Sciences Computation Initiative
WEHI ..... Walter & Eliza Hall Institute of Medical Research

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Publication Details

COORDINATION ..... VLSCI Communications

PUBLISHED BY ..... VLSCI Directorate

DESIGN ..... Chocolate Designs

PO Box 2577

Fitzroy Victoria 3065

TELEPHONE ..... + 61 419 591 819

WEB ..... www.chocolatedesigns.com.au

Technical Information

Cover printed on 300gsm Sovereign A2 – Gloss.

Sovereign A2 – Gloss is proudly made FSC certified by Hankuk paper who also carry the ISO 14001 EMS accreditation. Manufactured with elemental chlorine free pulps. Full 'cradle to grave' LCA completed according to international standards.

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