ANNUAL REPORT

More life sciences computation solutions

2013

vlsci
LIFE SCIENCES COMPUTATION

VICTORIAN LIFE SCIENCES COMPUTATION INITIATIVE

Professor James McCluskey
Deputy Vice-Chancellor (Research)

THE UNIVERSITY OF MELBOURNE

02 May 2014

The Hon. Gordon Rich-Phillips MLC
Minister for Technology
Victorian Government
121 Exhibition Street
Melbourne 3000

Dear Minister

I am pleased to submit to you the Victorian Life Sciences Computation Initiative's 2013 Annual Report.

As we enter this final year of the first phase of this Initiative it is very pleasing to report that all the key performance indicators set for the enterprise have already been met. Our job now is to ensure that we can sustain and embed the facility and its highly skilled staff into the Australian research landscape and continue the fine work we see documented in this Report.

The University has already reaped rewards from its substantial contributions to the enterprise. Having promised to contribute at least $12.5m in cash in the first five years, through the period 2009-2014, this University will have made a cash contribution to VLSCI of $12.83m. Further, our counterparts at Monash and La Trobe Universities have also acknowledged the benefits flowing to their own institutions and have already committed to contribute cash to sustain the Initiative in the future.

This Report documents some of those benefits and outcomes. In the details we see international and national collaborations, employment opportunities, career and technical developments and a growing community engaging in this exciting field of computational biology. This is setting us up to be well-placed to play our part in this emerging industry, where it was reported, exactly one year ago in the *HealthcareITNews*, that the global bioinformatics market, valued at nearly $3.2 billion (US) in 2012, is forecast to grow to nearly $7.5 billion by 2017 (according to Wellesley, Massachusetts-based BCC Research).

It is particularly noteworthy for the University to see the level of engagement there is across the research community with the IBM Research Collaboratory for Life Sciences-Melbourne, with many high-profile and high-use projects relying on their expertise and in turn, passing on opportunities for training our students and for them to find careers beyond the academy. With the planned colocation of VLSCI within the Carlton Connect precinct, along with the IBM Research and Development Laboratory, it is expected that the relationship will deepen.

We thank you and the Victorian Government for making this opportunity available to Victorian researchers and their collaborators and for your ongoing interest in its progress.

Yours sincerely

James McCluskey

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Deputy Vice-Chancellor (Research)

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VICTORIAN LIFE SCIENCES COMPUTATION INITIATIVE (VLSCI)

The VLSCI is funded by the Victorian Government and contributing institutions, hosted by the University of Melbourne and includes the first IBM Research Collaboratory for Life Sciences. Switched on in 2010, this five year Initiative is bringing together supercomputer resources, computational biology expertise and an extensive skills development program to address the unique and growing demands for computational expertise in the life sciences today. It exists for all Victorian life science researchers and their collaborators and, as at March 2013, is the biggest supercomputer facility devoted to life sciences in the world.

ABOUT THE **VLSCI**

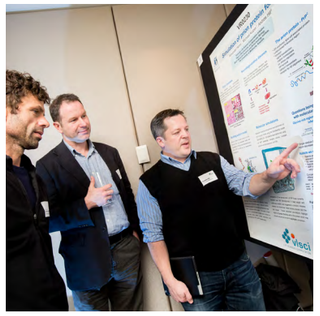
The Victorian Life Sciences Computation Initiative (VLSCI) combines collaborative research expertise with high end computing. The critical infrastructure and expertise offered by VLSCI has become essential to local life science research through its support and growth of the thriving specialities of Bioinformatics, Computational Biology and Computational Imaging.

WHAT DOES THE VLSCI DO?

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

- provides a world-class computational service that supports the transformation of life sciences research through high end computing
- provides a leading computing facility 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 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 specialist high-end facility focussed on the unique skills and services needed to remain competitive in life sciences computation.



WHY HAS THE VLSCI ACHIEVED 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 including hardware and software documentation and services to maximise user experience and ensure efficient access to computing resources appropriate to life sciences research.

The **Life Sciences Computation Centre (LSCC)** has built specialist teams to support researchers and drive capacity-building activities. Active across Australia, these expert teams have been spread across multiple research institutions to accelerate life science computation:

- The University of Melbourne - High Throughput Genomics
- Monash University - Computational Bio-imaging
- La Trobe University - Molecular Modelling

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 computation.

A specialist high-end facility focussed on the unique skills and services needed to remain competitive in life sciences computation.

INFRASTRUCTURE

- IBM Blue Gene/Q supercomputer - 4 racks
- High memory X86 systems for Genomics, Proteomics, Imaging applications
- Complemented by over 240 licensed software applications specific to life sciences
- Petascale computing

EXPERTISE

- Scientific and technical advice
- Scientific and technical collaboration
- IBM Research Collaboratory for Life Sciences
- Formal training and documentation
- Depth of life science project experience within team
- Skills development, community capacity building and educational resources

THE VLSCI SOLVES REAL **ISSUES FACED BY RESEARCHERS**

VLSCI provides the infrastructure, scale, expertise and scope to meet the biosciences industry's needs.

STEERING COMMITTEE
CHAIR'S REPORT

I am pleased to endorse this 2013 Annual Report of the Victorian Life Sciences Computation Initiative (VLSCI). I do so on behalf of the VLSCI Steering Committee, which includes senior nominees from Melbourne, Monash and La Trobe Universities, the Walter and Eliza Hall Institute (WEHI), Melbourne Health, the National Computational Infrastructure (NCI) and IBM, in addition to the Chair of the VLSCI Scientific Advisory Committee and the VLSCI Director, Professor Peter Taylor.

To fulfill its responsibility for reviewing all aspects of the operation of the VLSCI and for providing recommendations and strategic advice to the host institution, The University of Melbourne (The University), through the Deputy Vice-Chancellor (Research), the Committee met four times during the year, on 5 March, 21 May, 13 August and 10 December.

Much of the attention of the Committee during 2013 was focused on review of the VLSCI operations and its substantial achievements to date and especially on the important challenge of assuring the VLSCI's long-term sustainability beyond December 2014. This followed a major emphasis on sustainability planning during 2013 and involved commissioning and oversight of a substantial volume of high quality supporting documentation as a basis for strategic advice to The University.

The Steering Committee continued to be impressed by the overall progress and take-up of the VLSCI capabilities and was pleased to see the arrival and commissioning of the new IBM iDataplex x86 'Barcoo' system in July, marking the completion of all sub-stages of the VLSCI Stage 2 Peak Computing Facility (PCF) upgrade. The PCF continued to perform extremely well whilst 15% of the available Blue Gene/Q Service Units continued to be offered via the National Computational Merit Allocation Scheme (NCMAS) in order to contribute to meeting the national demand for access to high end computing facilities. The subscription-based project support model through institutional and project-based contributions to the Life Sciences Computation Centre (LSCC) generated substantial external funding and led to the introduction of a new 'Molecular Modelling' theme located at La Trobe University.

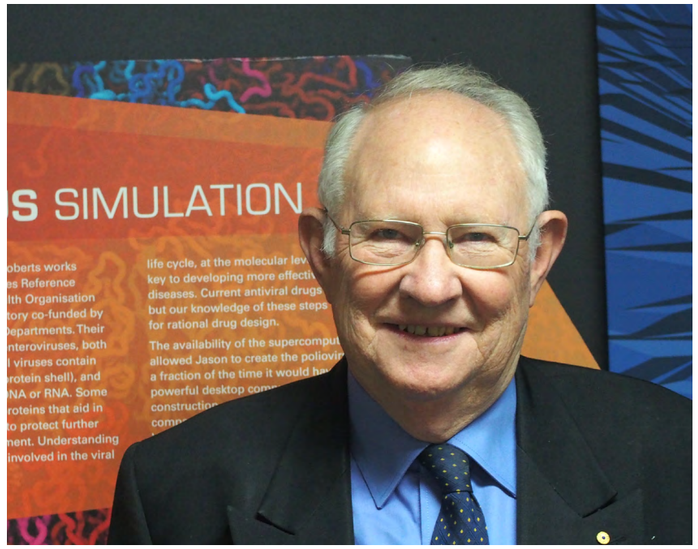
The Committee was pleased with the impact of VLSCI's outreach effort including the Director's August presentation to the Victorian Biotechnology Advisory Council and a public symposium held as part of The University's 'Festival of Ideas,' which combined a public event with a research showcase day on 3 October at which a number of 2013 users displayed their work. The calibre of media stories generated throughout the year was pleasing, including the filming by ABC TV of a significant story on the 'Environmental Modelling' research performed on VLSCI facilities for the '7.30 Report' (3 April), a front cover feature on The Age's '*Melbourne Magazine*' (April) of a polio virus model, with mention of VLSCI on the inside front cover and a story inside, and several opinion pieces by the Director in publications such as The Financial Review (7 January).

In support of its efforts to assist the VLSCI and The University to develop a robust strategy for achieving the long-term sustainability of this important initiative, on the advice of the Committee, The University engaged SPP (Strategic Planning Partners) to assist with development of an overarching 'Sustainability Plan,' which was submitted to the Victorian Government Department of State Development, Business and Innovation (DSDBI) on 30 April 2013.

A 'Business Case for Transitional Funding Support' was submitted to DSDBI on 10 October. Following a 'Request for Quotation' process, a 'Benefits Realisation Analysis' was conducted by ACIL Allen Consulting and submitted to DSDBI on 26 November.

In response to advice from these reports and with the support of the Steering Committee, VLSCI opened discussions with various parts of the Federal Government during the year, to increase awareness of the national value of the VLSCI and begin to make the case for ongoing support at the Federal level for this important piece of research infrastructure. The Committee was also satisfied with the positive interactions arising from Sustainability discussions as part of an initial campaign to engage with senior personnel within various stakeholder institutions. The initiation of an awareness-raising campaign highlighting the benefits of the VLSCI was also supported by the Committee.

After a busy year involving much external interaction and consultation, the Committee wishes to acknowledge the substantial advice and guidance provided by many senior figures from the VLSCI stakeholder organisations as well as the DSDBI officers responsible for VLSCI matters and their Independent Assessor, Dr Mike Sargent, AM FTSE.



The Steering Committee is satisfied with progress towards the long-term sustainability of the VLSCI and commends the VLSCI Director and staff for their achievement in transforming life sciences research in Victoria, as reported in this Annual Report. We share their assessment that the VLSCI has much to offer the national life sciences research community in years to come, and we strongly support them and their stakeholder organisations' efforts to ensure that the long-term vision for VLSCI as the national peak computing facility for the life sciences in Australia is achieved.

John W. Zillman AO FAA FTSE
Chair

FROM THE **DIRECTOR**

VLSCI Director Prof. Peter Taylor (l) with NCI Director and VLSCI Resource Allocation Scheme Committee (RAS Committee) Chair, Prof. Linsday Botten at the Research Showcase held in October. Image: Casamento Photography

It is my pleasure to commend to you my fourth VLSCI Annual Report. The data and stories contained herein document a complex operation which in four action-packed years has become an integral part of Australia's research infrastructure. Further, it offers a successful model for building Australia's capacity, skills and expertise in high-end and, more specifically, life sciences computation.

VLSCI commenced operations in 2010 as a Victorian Government Initiative designed to strengthen Victorian research capabilities and outcomes in the growing field of computational biology. Stakeholders, quite correctly, anticipated the exponential growth in data arising from the Human Genome Project and other technologies that make up the 'Biological Revolution', such as bio-imaging and molecular modelling. As predicted back in 2009, in January 2014 key industry player, Illumina, announced its new genomic sequencing system with the words, *Illumina Introduces the HiSeq X Ten Sequencing System - Breaks Barriers with World's First $1,000 Genome, Enabling 'Factory' Scale Sequencing for Population and Disease Studies*.

VLSCI has prepared the groundwork for the development of this new industry; nurturing networks, funding conference attendance, sponsoring conferences, running courses, hosting special interest groups and offering programs to inspire young students. The Life Sciences Computation Centre now has financial subscriptions from over 20 research groups who see the value in getting direct access to both their expertise and the computers. This model of engagement is one that has attracted attention across the bioinformatics community in Australia and overseas as a successful way to address the many issues experienced by this fledgling community. This significant high performance computation (HPC) facility demonstrates that Victoria's investment in this industry is serious and sustained. The concentration of resources helps to excite young people about a career in computational biology and it delivers results – including clinical implementation of new knowledge to which our people have contributed.

Having achieved all our stated objectives and delivered on all key performance indicators, those of us closely connected to the fast-paced developments occurring in computational biology feel that our work has only just begun.

After much reflection, research and planning in 2013, it became clear that a resource such as this should be supported and available nationally. In anticipation of this move, we had already made 15% of the IBM BlueGene/Q available nationally through National Computational Merit Allocation Scheme (NCMAS) (refer p.13). This Annual Report now documents the outcomes from researchers who took up this opportunity. One user commented: *We have not fully exploited VLSCI resources in the past but given the increasing load on National Computational Infrastructure (NCI), VLSCI will be very important in ensuring that we have adequate access to high performance computing facilities*.

Further to this end, the consultants conducting the Benefits Realisation Analysis Report (refer p.10) were asked to help us refine our Annual Reporting process to extract more accurate and useful data for existing stakeholders and to support our case for ongoing Victorian and national funding through national infrastructure funding schemes. Much of this data collected is included in this Annual Report and the rest is being shared with other Australian supercomputing centres and stakeholders to inform planning for future resource needs.

VLSCI is now a crucial part of research infrastructure and a centre for scientific and technical expertise servicing the important biosciences sector in Victoria. Were VLSCI to wind-up at the end of 2014, 90% of compute resources currently available to Victorian researchers would disappear, at a time when the high-risk, high-return biotechnology sector is once again starting to envision real returns from clinical genomics, precision medicine, environmental modelling and drug discovery – all of which rely on highly-skilled and well-equipped people to deliver results.

As one of our major users, Prof. Kerry Hourigan, Monash University, writes: *It takes considerable effort to build up such a facility and once this step has been taken, it needs only modest effort to keep it going.*

Professor Peter R. Taylor
Director

EXTERNAL EVALUATION REPORT
NOVEMBER 2013

As required in VLSCI's Grant agreement with the Victorian Government, an external evaluation was conducted during 2013. In researching their report, ACIL Allen Consultants interviewed staff, major users and stakeholders. The final report was submitted in November. Entitled *Evaluating the VLSCI: A Benefits Realisation Analysis,* it was overwhelmingly positive about developments to date and gave useful advice on strategies for tackling the challenges of the future to ensure VLSCI remains a strong and viable resource for Australian research and industry.

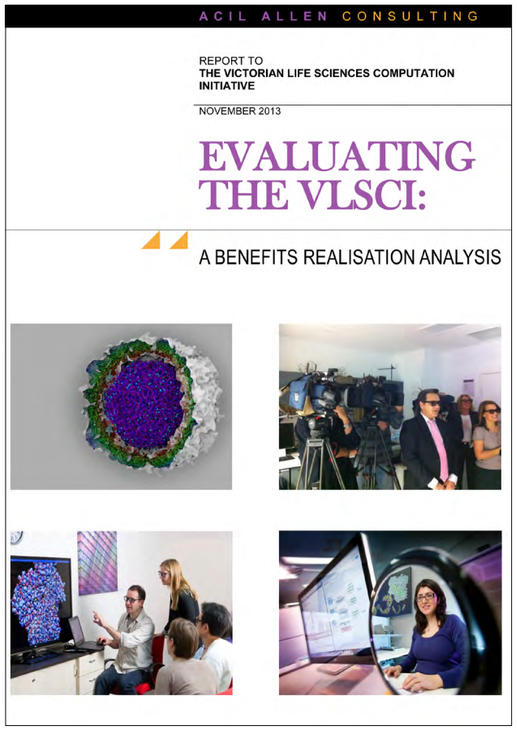
EXECUTIVE SUMMARY

…The ability to access supercomputers allows researchers to apply new, data intensive, technologies such as genomics in life sciences research. It also helps to accelerate the application of research results into changes in disease detection and diagnosis, developing new drugs for treatment of illnesses and drive changes in clinical practice. All of these things will have profound impacts on the health and wellbeing of populations in Australia and around the world.

The ten key findings of the Analysis were that VLSCI

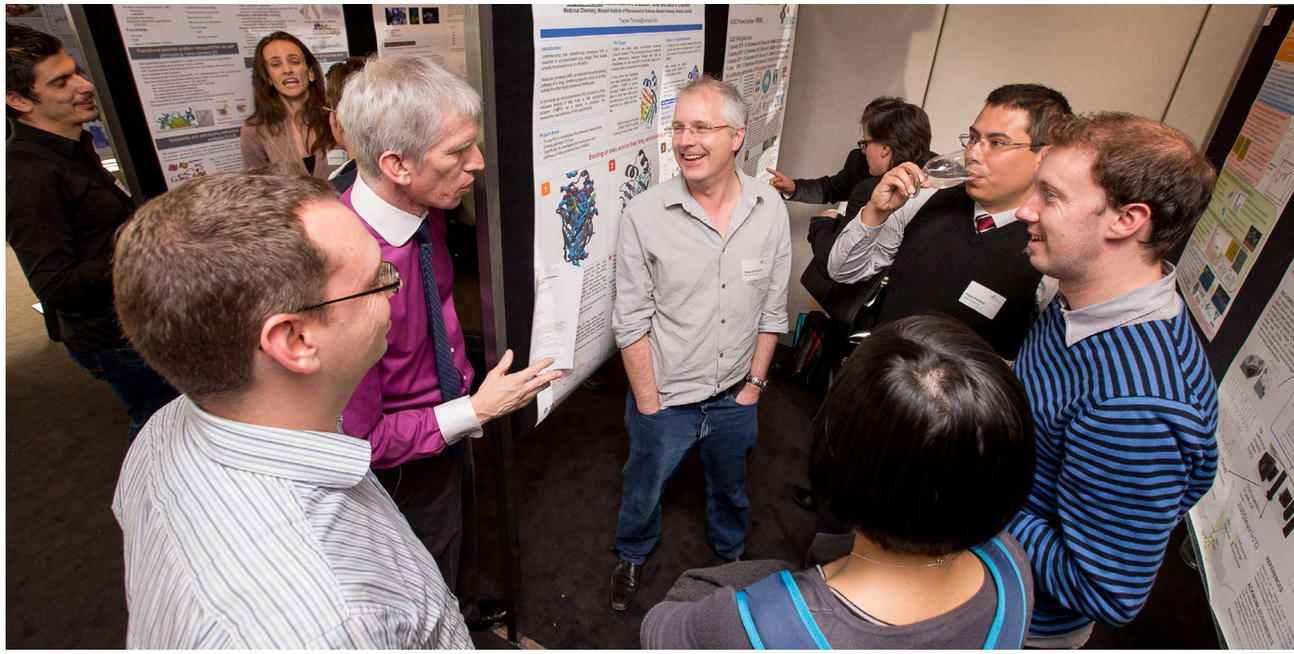
- is the world's top life sciences research supercomputer
- is a powerful mechanism for supporting life sciences research
- enables world class research by Victorian life sciences researchers
- supports Victoria's strong reputation in life sciences
- is highly effective at increasing collaboration
- is delivering benefits now
- will deliver more benefits in the future
- needs to transition to a more sustainable future
- should become more national in its approach
- governance arrangements need to evolve.

These findings have informed the Business Plan 2014 and continue to inform sustainability planning for the future. The full report may be requested from VLSCI Communications.



VLSCI remains a strong and viable resource for Australian research and industry.

The VLSCI possesses research focus and expertise specifically in applications of computation to life sciences.



TOXIN BINDING TO MEMBRANE PROTEINS: TOWARDS NOVEL TREATMENTS IN NEUROPATHOLOGY

Feedback from Dr Andrew Hung, Health Innovations Research Institute, RMIT University

As opposed to other HPC facilities, VLSCI possesses research focus and expertise specifically in applications of computation to life sciences, including computational structural biology (particularly important to this project). Thus in addition to HPC facilities, VLCSI also provides access to expertise, and intellectual and technical input into the project through seminars, meetings and support. VLSCI also facilitates collaboration in life sciences computation. It has provided a vital resource (both facilities and personnel) for the establishment and continuation of this project. We have made significant progress in understanding conotoxin interactions with neuronal receptors, which is leading towards development of viable drug therapies for brain diseases. A good example is our recent work on modified "dicarba" toxins. Towards this end, VLSCI has also enabled us to strengthen our cross-institute collaborations nationally and internationally. These collaborations will continue to yield research outputs leading, ultimately, to better health and treatment outcomes. VLSCI has also helped us establish further links with the existing computational biology community, and these will also ultimately benefit our research outcomes. VLSCI is an enormously vital resource and I would like to see it continue to develop as it has since its inception.

RESEARCH **ACTIVITY**

EMPLOYMENT

Chief Investigators allocated resources on VLSCI systems, reported on additional staff/students taken on as a result of their 2013 VLSCI project:

Undergraduate students *(predominantly UROP projects)* 37
PhD students 48
Post-graduate students 27
Other 4

GRANT INCOME

Chief Investigators allocated resources on VLSCI systems, reported on the importance of access to VLSCI facilities and their grant funding success:

Extremely important 39
Moderately important 10
Important 19
Somewhat important 5
Not very important 14
N/A 7

When asked about new funding applications which had been made as a result of work done on VLSCI systems, chief investigators reported that over $10m in predominantly Australian grants had been applied for, with $2.5m received and another $5.3m yet to be advised.

Chief investigators were asked to nominate what sources of grant income they accessed for work being carried out by them on VLSCI systems. This table summarises the data (note that the years 2016, 2017 and 2018 only contain secured funds to date):

INCOME YEAR	2013	2014	2015	2016	2017	2018
FUNDING SOURCE	$	$	$	$	$	$
ALL	**57,125,803**	**48,776,943**	**41,831,915**	**34,894,649**	**21,327,942**	**7,235,714**
International	5,821,628	5,657,291	1,725,000	1,695,000	1,695,000	
ARC	33,744,283	28,288,683	27,373,350	23,254,718	11,850,754	7,235,714
NHMRC	15,929,446	13,774,974	11,877,969	9,920,824	7,782,188	
Other, Vic.	361,397	215,280	125,714	12,857		
Other	1,269,049	840,715	729,882	11,250		

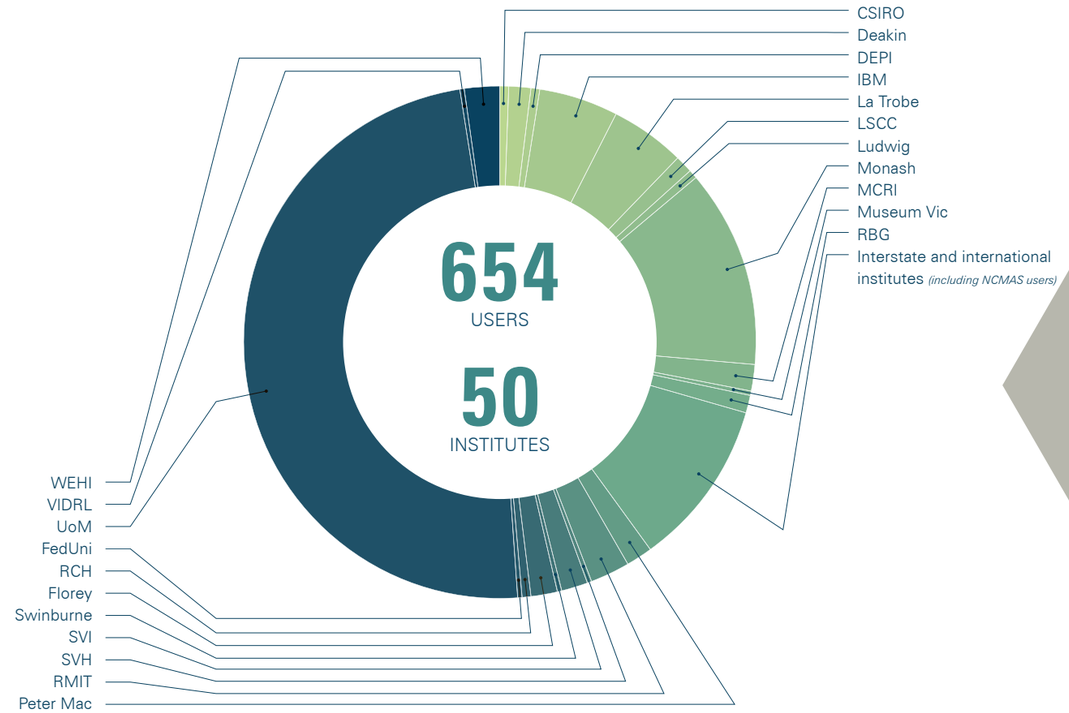
On a local scale, it has been an important factor in Monash University gaining the highest ERA 2012 ranking of a 5 in Biomedical Engineering and in Interdisciplinary Engineering... it has been of great benefit to a number of Australian Research Council grants for which high powered computing has been essential.

Kerry Hourigan, Monash University, Project: Prediction and Imaging of Vulnerable Plaque Evolution and Rupture

COLLABORATIONS, NON-VICTORIAN ACTIVITY

Chief Investigators allocated resources on VLSCI systems reported on the extent of their reliance upon collaborations to carry out projects. Of the 94 respondents, 64 reported they were working on projects with collaborators from other institutions, with 20 being Australian, 31 overseas and 9 with industry partners. Overseas collaborations extended to Japan, Egypt, France, UK, USA, New Zealand, Germany, the Netherlands, Sweden, Norway, Canada, UAE, Slovenia and Switzerland. As part of these collaborations, a total of 27 overseas users were accessing VLSCI systems in 2013, from Germany, China, USA, UK, Turkey, France, New Zealand, Denmark and Poland.

Interstate Australian users came from the Universities of Adelaide, Queensland, Sydney, Sunshine Coast, Western Australia, Wollongong and New South Wales, Curtin University and the Australian National University and are represented as National Computational Merit Allocation Scheme (NCMAS) users or as collaborators with Victorian researchers.



VLSCI is a wonderful facility to mention in the Research Environment sections of our grant applications. I firmly believe that this has assisted us in obtaining our grants by increasing the "scores" that we received for this aspect of our grant applications.

David Grayden, University of Melbourne, Project: Computational Neuroscience: Modelling the brain at microscopic, mesoscopic and macroscopic levels

OUR **PEOPLE**

DIRECTORATE

Prof. Peter R. Taylor *Director*
Ms Karin Diamond *Business Manager*
Ms Monalisa D'souza *Executive Officer (to Feb. 2013)*
Ms Fiona Kerr *Executive Officer (from Apr. 2013)*
Ms Claudia Curcio *Reception/Administration Assistant*

OUTREACH & COMMUNICATIONS

Ms Helen Gardiner *Communications and Development Manager*
Dr Christina Hall *Communications Officer*

PCF

Dr Vera Hansper *PCF Manager*
Mr Bob Danani *HPC Specialist*
Dr Andrew Isaac *Specialist Programmer*
Mr James Kelly *HPC Specialist IBM (to Nov 2013)*
Dr Jeff Tan *HPC Specialist IBM (from Aug 2013)*
Dr Michael Kuiper *Computational Molecular Scientist*
Mr Mark Nelson *HPC Specialist IBM (to Sept. 2013)*
Mr Matthew Wallis *HPC Specialist IBM (from Sept. 2013)*
Mr Brett Pemberton *Systems Administrator (to Oct. 2013)*
Dr Matthew Hodges *Systems Administrator (from Nov. 2013)*
Dr Bernard Pope *Specialist Programmer*
Mr Chris Samuel *Senior Systems Administrator*
Mr Carl Thomas *Storage and Infrastructure Administrator*
Ms Jin Zhang *Systems Administrator*

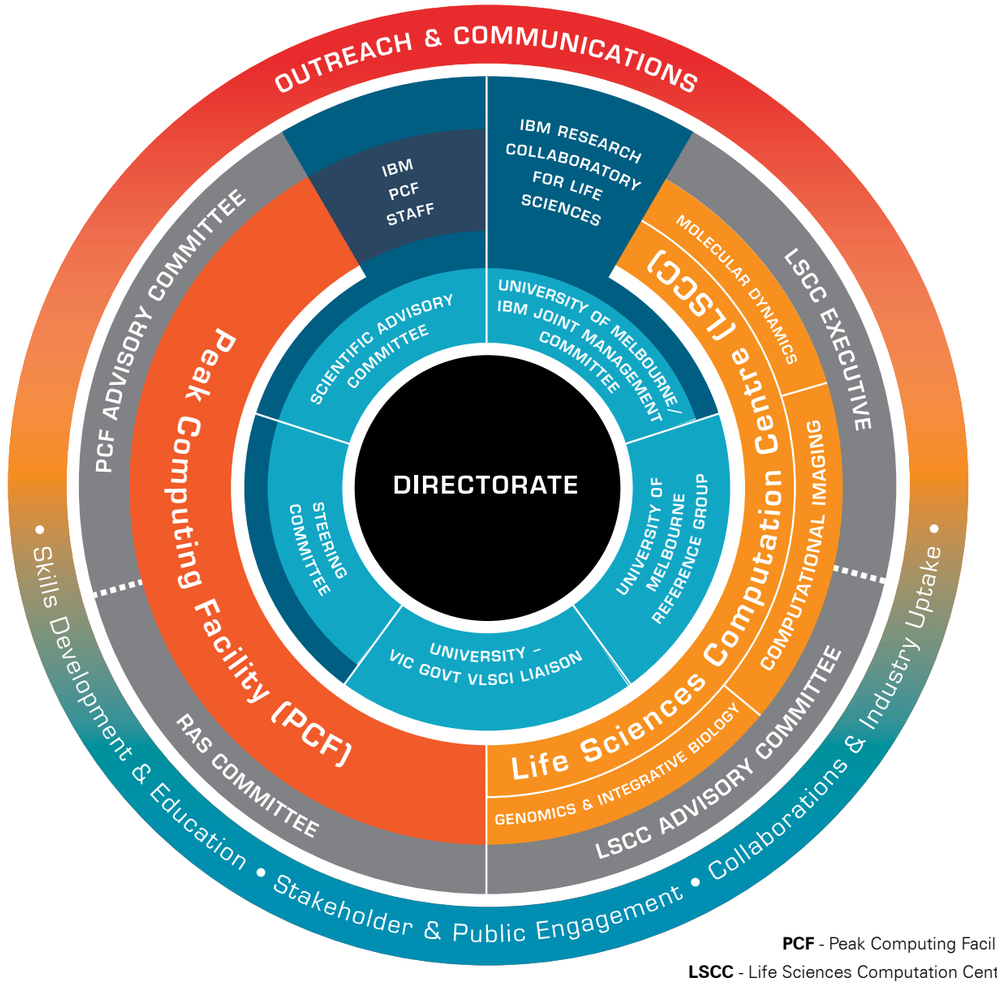
LSCC

(all from Central precinct unless otherwise noted)
A/Prof. Andrew Lonie *Head of LSCC*
Ms Charlotte Anderson *Bioinformatician/ Research Assist (from Feb. 2013)*
Dr David Barnes *Senior Research Fellow (South Eastern precinct)*
Dr Dieter Bulach *Senior Research Scientist (South Eastern precinct)*
Ms Jessica Chung *Bioinformatician/Research Assist (from Feb. 2013)*
Dr Ira Cooke *Research Scientist (Northern precinct)*
Ms Harriet Dashnow *Research Scientist (from Dec. 2013)*
Dr Enis Afgan *Research Scientist*
Dr Nathan Hall *Senior Research Scientist (Northern precinct)*
Dr Nuwan Goonasekera *Software Engineer*
Mr Simon Gladman *Research Scientist (South Eastern precinct)*
Dr Chol-hee Jung *Research Scientist*
Mr Yousef Kowsar *Scientific Software Developer (from May 2013)*
Dr Khalid Mahmood *Research Scientist*
Ms Liz Milla *Systems Administrator/ Scientific Developer (to Dec. 2013)*
Dr Juan Nunez-Iglesias *Research Scientist (South Eastern precinct)*
Dr Amanda Ng *Computational Biomedical Imaging Scientist (South Eastern precinct)*
Dr David Powell *Research Scientist (South Eastern precinct)*
Dr Gayle Philip *Research Scientist*
Dr Torsten Seemann *Senior Research Scientist (South Eastern precinct)*
Dr Clare Sloggett *Research Scientist*
Dr Michael Thomas *Molecular Modelling Scientist (Northern precinct)*

IBM

Dr John Wagner *IBM Manager*
Dr Matthias Reumann *IBM Researcher (to Feb. 2013)*
Dr Daniel Oehme *IBM Postdoctoral Researcher (from Feb. 2013)*
Dr Stephen Moore *IBM Researcher*
Dr Matthew Downtown *IBM Researcher*

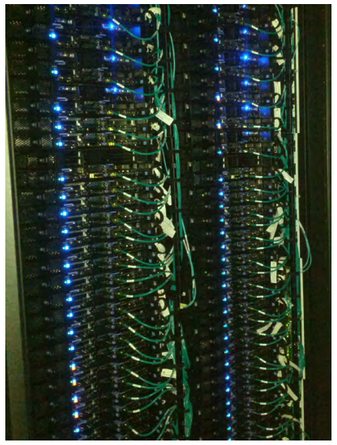
ORGANISATIONAL DIAGRAM



PCF - Peak Computing Facility
LSCC - Life Sciences Computation Centre
RAS COMMITTEE - Resource Allocation Scheme Committee

SUPERCOMPUTER SYSTEMS

Since July 2012, operating at the petascale



2013 HIGHLIGHTS

- New IBM x86 system “Barcoo” installed in July 2013, doubling capacity available to users and adding high-memory nodes for big genomics jobs.
- All x86 systems were upgraded to run the most recent version of RedHat, and to adopt the same scheduler, called SLURM, as is used on the BlueGene/Q.
- Resource allocation applications for 2013 saw a record number of applications for access to resources: 70 in round 6 and 21 in round 7.
- With 15% of the BlueGene/Q system made available at the national level through the National Computation Merit Allocation Scheme, a total of 11 applications successfully applied for resources.
- As at November 2013, ranking No. 48 in Top 500, No. 30 in Top Green 500 and equal No. 7 in Graph 500.
- Refer pages 64-85 for all projects running on VLSCI systems in 2013.

The VLSCI Peak Computing Facility (PCF) represents a significant investment in High Performance Computing, providing computer processing infrastructure and computational expertise to Victorian Life Sciences researchers and their collaborators. It is a world class petascale facility with four systems built on two architectures (BlueGene/Q and x86). Each system offers varying memory and data-handling capacities to suit the large memory computational resources required from genomics through to high capacity processing of computational imaging data.

SOFTWARE

From ‘ACG’ to ‘Zlib’ over 220 licensed software applications specific to life sciences are installed on VLSCI’s systems.

EXPERTISE

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

PCF HARDWARE – TECHNICAL DATA

Hosted at The University of Melbourne and accessible only through a remote network.

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.

As at 31 December 2013, VLSCI’s Avoca is ranked 48 in the global Top 500 list of the most powerful computer systems. The list is updated twice a year, in June and November, and is avidly followed by high performance computer enthusiasts. The peak performance was measured using the LINPACK Benchmark – regarded as the industry benchmark for high performance computing. As at 31 December 2013 VLSCI’s Avoca was the fastest computer on the TOP500 list dedicated to life sciences computation.

At Supercomputing 2013, held in Denver Colorado, USA in November, Avoca was also ranked equal 7th in the Graph 500, a relatively new benchmark which has been established to more accurately test data intensive applications such as those used in the life sciences.

SGI ALTIX XE CLUSTER - BRUCE

- Peak performance of 11.6 teraFLOPS.
- 1088 Intel Nehalem compute cores (8 per node) running at 2.66GHz.
- 110 nodes with 24GB RAM per node.
- 20 nodes with 48GB RAM per node.
- 6 nodes with 144GB RAM per node.
- Connected to a high speed, low latency QDR Voltair Fabric InfiniBand network for inter-process communications.
- Connected to a 100TB Panasas file system.
- The system 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 (NEW IN JULY 2013)

- 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.

STORAGE INFRASTRUCTURE:

- 100TB Panasas Parallel Data Store (attached to Bruce).
- 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).

THE PEAK COMPUTING FACILITY
SERVICES

SYSTEMS SUPPORT SERVICES

VLSCI uses a help request ticketing system to ensure user requests are dealt with promptly and efficiently.

This chart shows that 1292 help request tickets were dealt with by the PCF staff in 2013. This compares with 912 in 2012 and generally reflects increased demand by new users to the systems and with users making adjustments to the new job scheduler, SLURM.

REPORTING

VLSCI users are required to submit quarterly usage reports to their online account and indicate the amount of 'in-kind' contributions people have made to the Initiative through activity being generated through access to the facility. By this measure, in 2013 there was a substantial increase in researcher interactions and contributions continue to be over budget for the Initiative. For more information, refer to the Financial Reports from pages 96-97. In-kind contributions are fully accounted for in the *Financial Supplement to 2013 Annual Report* 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:

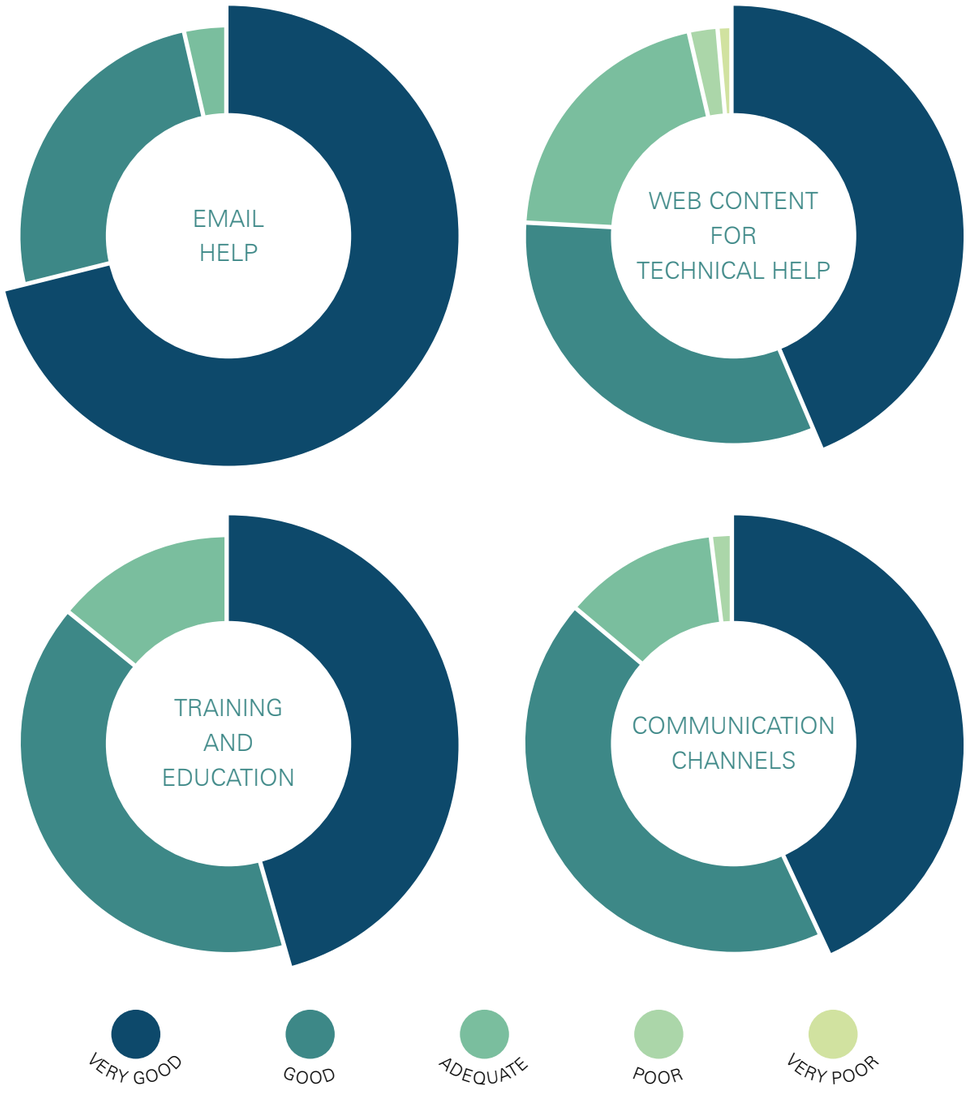
MACHINE	NAME	2011 (%)	2012 (%)	2013 (%)
SGI x86	Bruce	76.0	85.5	91
iDataplex x86	Barcoo*			82
iDataplex x86	Merri	73.5	86.0	88
BlueGene/Q	Avoca		98.0	96
BlueGene/P	Tambo**	97.5	96.0	

** Barcoo came online in late July 2013*

*** Tambo was decommissioned in mid 2012*

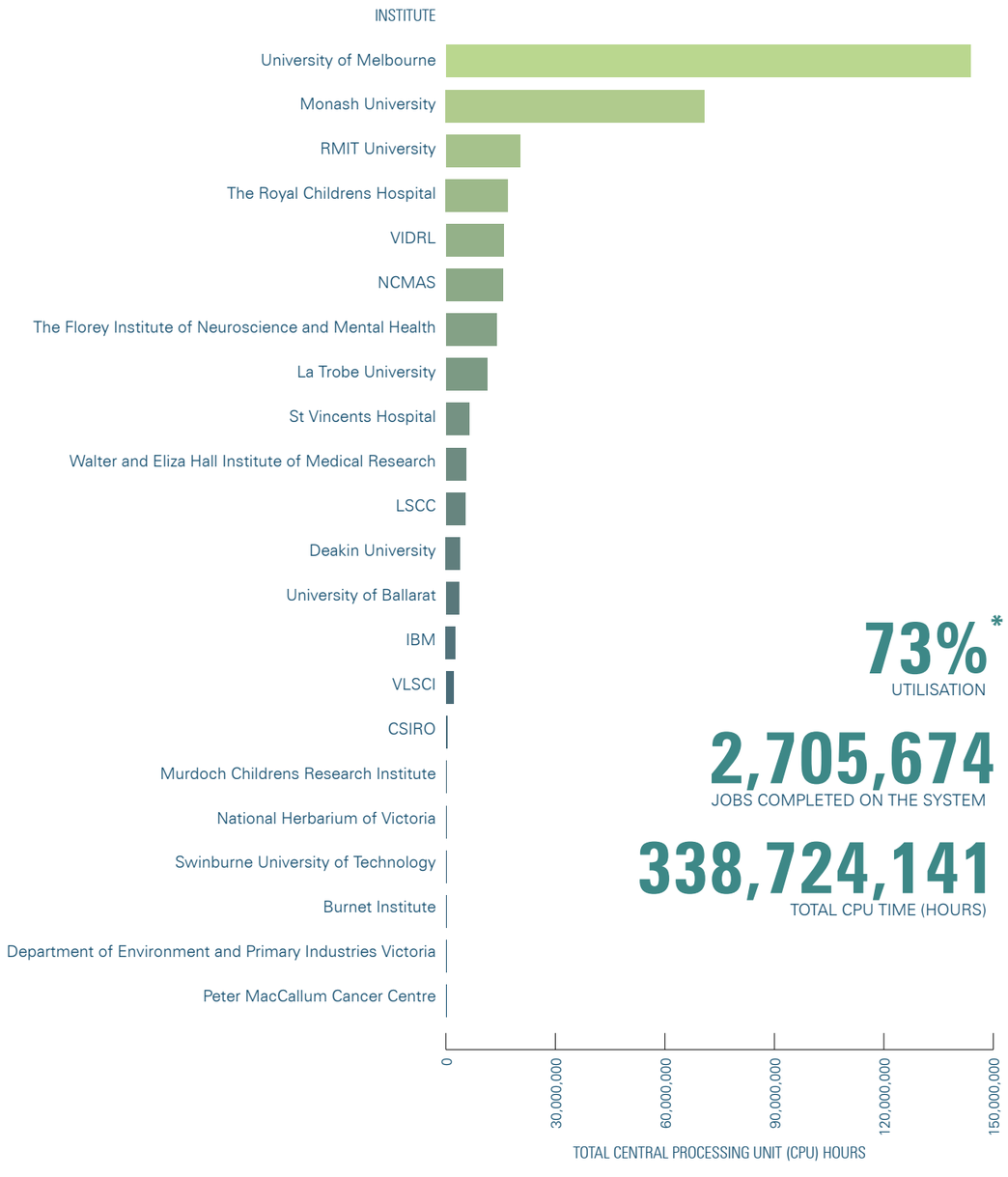
ANNUAL REPORTING AND SATISFACTION SURVEY

ACIL Allen Consulting recommended an overhaul of the annual reporting process for users and a more detailed questionnaire was produced for the 2013 reporting year. The information collected informs much of this Report. Among the 94 respondents, overall user satisfaction remains very high and staffing levels committed to this important Initiative remain a key reason for this.



SYSTEM **USAGE**

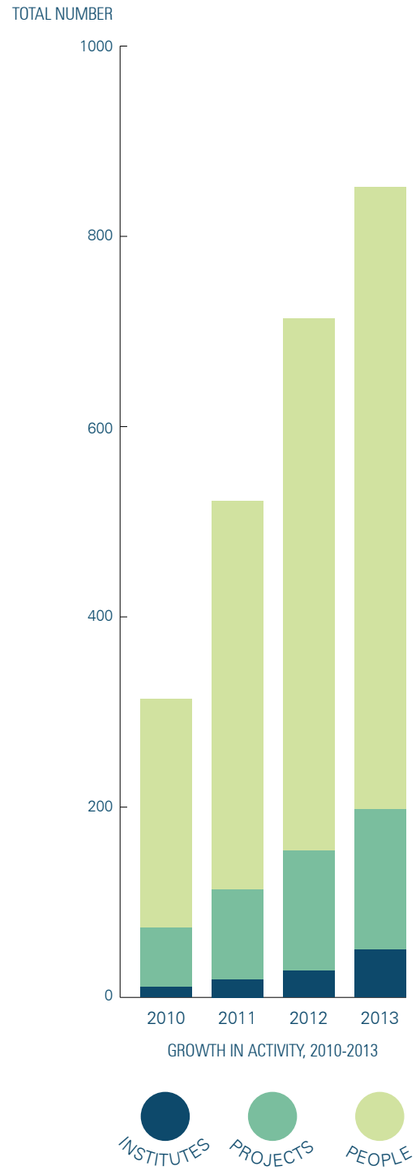
The distribution of usage between Institutes for the period 1 January to 31 December 2013.



73%*
UTILISATION

2,705,674
JOBS COMPLETED ON THE SYSTEM

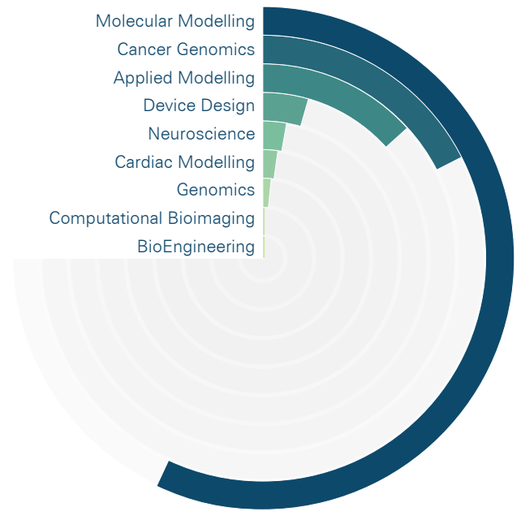
338,724,141
TOTAL CPU TIME (HOURS)



COMPUTER RESOURCES

Allocated by discipline

The Resource Allocation Scheme Committee (RAS Committee) is a peer review committee awarding compute resources based upon merit. The research fields of projects running on VLSCI systems over 2013 may be categorised into the following broad discipline areas: Molecular Modelling & Dynamics, Cardiac Modelling, Device Design, Neuroscience, Cancer Genetics, Applied Modelling, Genomics, Computational BioImaging and BioEngineering. Resources were allocated to projects by discipline in 2013 approximately as follows:



**Utilisation is derived by dividing actual usage by the amount of resources (CPU hours) allocated. This figure is an average of the two systems. The x86 systems' utilisation figure is 97% and reflects the software suitability and high adoption of these systems by bioinformatics projects in particular. The BG/Q utilisation figure is 72% and this reflects the greater complexity of the work designed to use such tremendous capacity, where there is more time needed to design and refine each project to maximise the usage and to ensure large parallel jobs can be run efficiently. Refer to the IBM Collaboratory report on pages 30 to see some of the larger projects being created to take advantage of this capacity.*

Dr Vera Hansper
PCF Manager

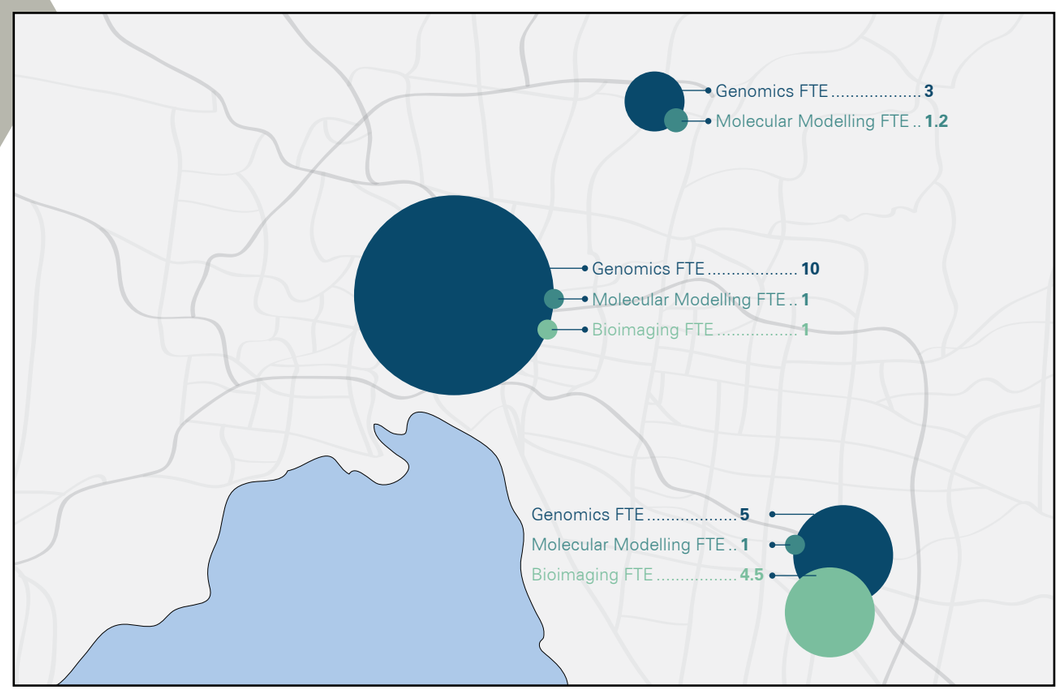
LIFE SCIENCES
COMPUTATION CENTRE

2013 was a successful and transformative year for the LSCC.

2013 was a successful and transformative year for the LSCC with staff engaging with researchers from a wide range of research institutes in subscription-based collaborations, having spent the previous two years building a significant profile in bioinformatics experience and expertise, and demonstrating utility to the Victorian community. The LSCC is now well established as:

- a 'shop-front' for researchers looking for expertise and advice on data analysis, experimental planning and grant preparation
- a hub for collaborative supervision and training of students in cross-disciplinary computational biology research
- a professional and supportive environment for in-house bioinformaticians and computational biologists with the potential for career progression at a time when this profession is still being established.

Staffing reached capacity in 2013, with 27 full-time equivalent experts now located across Melbourne's Central, Northern and South-eastern research precincts, across the research 'themes':



LSCC SUBSCRIPTIONS

The LSCC started 2013 with two institutional subscribers: the Cancer Council Victoria and the Eastern Hill medical precinct (through the Department of Medicine, St Vincent's Hospital). Another 40 projects were supported with LSCC resources, and over the year, ten of those opted to formally subscribe to the service. At the start of 2014, 20 institutes were signed up for a range of project-based and institutional subscriptions, with staff allocated accordingly:

SUBSCRIBER	PROJECT(S)	INST/ PROJECT	LSCC THEME	FTE
Cancer Council Victoria	Genetic and epigenetic risk factors in breast, colorectal, prostate cancer	Inst	Genomics	2
Eastern Hill Precinct - SVI, SVH, CERA	EMPathy project, genetic risk factors in eye disease	Inst	Genomics	1
La Trobe Institute of Molecular Sciences	Various basic and applied genomics research projects	Inst	Genomics	1
La Trobe Institute of Molecular Sciences	Various projects + capacity building	Inst	Molecular Modelling	1
MCRI / ANU	Genetic basis of monogamy	Project	Genomics	0.4
Monash Health Translation Precinct	Various biomedical genomics research projects	Inst	Genomics	1
Monash University - Biomedical Sciences: Biochemistry	Novel RNAseq method development	Project	Genomics	0.8
Monash University - Central Clinical School / Alfred Hospital	Various biomedical genomics research projects	Inst	Genomics	1
Monash University - Psychology	IMAGE-HD: neuroimaging in Huntington's Disease	Project	Computational Bioimaging	2
NeCTAR Endocrine Virtual Laboratory	Genomics workflows and variant registries for endocrine disease	Project	Genomics	1
NeCTAR Genomics Virtual Laboratory	Infrastructure for genomics in Australia	Project	Genomics	3
Peter Mac - International Cancer Genomics Consortium	Tumourigenesis and drug resistance in ovarian cancer	Project	Genomics	0.8
Royal Melbourne Hospital - Surgery	Understanding metastasis in prostate cancer	Project	Genomics	1
University of Melbourne - Centre for Translational Pathology	Clinical genomic tests for ovarian cancer	Project	Genomics	0.6
University of Melbourne - Dental School	The Oral Health CRC: understanding microbial populations in dental disease	Inst	Genomics	1
University of Melbourne - Genetic Epidemiology	Genetic risk factors in breast cancer	Project	Genomics	0.5
University of Melbourne - Microbiology and Immunology	Various genomics research projects	Inst	Genomics	1
University of Melbourne - School of Population Health	Genetic risk factors in breast cancer	Project	Genomics	0.5
General consulting	Infrastructure and capacity building	N/A	Genomics	3
General consulting	Infrastructure and capacity building	N/A	Computational Bioimaging	2
General consulting	Various projects + capacity building	N/A	Molecular Modelling	1

In 2013, subscriptions accounted for $645,000 of income to the LSCC and projected subscription income for 2014 is over $1million. Subscribers acknowledge the benefits of getting direct access to the LSCC's resource allocation on VLSCI systems and the capacity-building work of embedded LSCC staff who deliver formal and informal skills development and training. In turn, these subscriptions enable the LSCC to expand, develop tools, build resources and expertise and offer further career development for staff.

OTHER LSCC **2013 HIGHLIGHTS**

The LSCC is now effectively operating 'at capacity' in terms of staffing and budget and the staff have highly complementary skills and expertise to offer the research community. The Monash-based Victorian Bioinformatics Consortium (VBC) is fully engaged in supporting LSCC subscriptions and projects – effectively acting as the Monash node of the LSCC Genomics theme and staff interact extremely effectively across nodes – as was originally envisaged when the LSCC was established. The Genomics theme has established a series of expertise groups that have been highly successful in advising on research project planning and analysis approaches to multiple researchers and students; and community engagement and support is strong.

The LSCC Computational Bioimaging theme has built a very successful embedded support and collaboration model with the Department of Psychology at Monash University, plus further capacity building and training carried out through the theme based at Monash Biomedical Imaging and MASSIVE. A number of leading-edge tools and workflows have been built, tested and shared with the research community across Melbourne. Highlight events in 2013 were the launch of the International Neuroinformatics Coordinating Facility Victorian node and the Google Summer of Code project (refer p.41/42 for details).

A NEW THEME – MOLECULAR MODELLING AND DYNAMICS

Following analysis of the numbers and types of projects running on VLSCI systems (refer Computer Resources allocated by Discipline on p. 21), the decision was taken to expand the genomics theme to incorporate integrated biology (proteomics) and then create a new theme in Molecular Modelling and Dynamics. With Theme Leader A/Prof. Brian Smith, Principal Research Fellow, Deputy Head of School, Faculty of Science, Technology and Engineering, School of Molecular Sciences Department of Chemistry, La Trobe Institute for Molecular Science, this group has already developed a regular meeting program, established on-line training materials for students and researchers and is focused on adding value to existing VLSCI users through direct support and conference sponsorships.

In 2013 the Outreach program assisted with the growth of this community of researchers in this field in many ways. After an approach by RMIT Vice-Chancellor's Senior Research Fellow, A/Prof. Toby Allen, the Outreach program supported the 4th Workshop on Computational Modelling of Proteins and Membranes in July and the November

Adding value to existing VLSCI users through direct support and conference sponsorships.

Australian Society for Biophysics meeting. A biophysicist, A/Prof. Allen was attracted back to work in Australia after ten years working at UC Davis, USA and he maintains a number of important international collaborations.

A/Prof. Smith also welcomed new staff member Dr Michael Thomas and together they worked with Dr Michael Kuiper, VLSCI's Molecular Scientist, to develop useful methods for drug docking and large job management on a high capacity computational resource, and shared it with the research community through GITHUB. Additional methods include those for visualisation and animation. Concurrently, the resources were introduced to MM students and researchers in the MM capacity-building seminars and conferences supported by the Outreach program.

EXAMINATION OF THE SPECIFIC MECHANISMS OF VACCINE-DERIVED POLIOVIRUS ANTIVIRAL DRUG INTERACTIONS

The exciting polio virus modeling work carried out on the BG/Q by Jason Roberts at VIDRL, with support from Dr Michael Kuiper, continued to deliver results in 2013 with significant progress made in the reconstruction of non-polio enteroviruses. Three genogroups of EV-A71 were reconstructed, coincident with an outbreak of the virus in Australia that was associated with a number of deaths and paralysis cases in children during 2013. Further work on these viruses continues in collaboration with other research groups. Sequence data representing the full capsid of variants of the newly described virus EV-C96 and the novel virus EV-A120 discovered by VIDRL were obtained and preliminary models constructed, with a number of manuscripts prepared for publication at year end. The research continued to attract collaborators throughout the WHO Reference Laboratory network worldwide.

Dr Robert Kuhn, Associate Director of the UCSC Genome Browser presented a workshop to LSCC staff and associates in August. He is photographed here at far right with (from l:r:) Charlotte Anderson, LSCC, Clare Sloggett, LSCC, Maria Doyle, PeterMac. Image:VLSCI

MAJOR BENEFITS TO THE RESEARCH COMMUNITY TO DATE BY THE LSCC

Advocacy for local and national funding and infrastructure: The LSCC has strategically identified and applied for external funding and resource opportunities on behalf of collaborators, including programs such as National Collaborative Research Infrastructure (NCRIS), National eResearch Collaboration Tools and Resources (NeCTAR); the Research Data Storage Initiative, VLSCI and NCI compute infrastructure. An example is the significant funding of LSCC staff from the national Genomics Virtual Laboratory (GVL) program, with LSCC staff developing the GVL training materials and now training collaborators in its use.

Leveraging common platforms, tools, pipelines, training: Bioinformatics units/centres typically spend considerable time establishing and maintaining analysis platforms, best-practice workflows and training materials that are then used by staff across multiple projects. The LSCC focusses this effort through economies of scale so that a broad set of best-practice 'industrial scale' reproducible genomic analyses are then made available to all staff and collaborators.

Community building and training: The LSCC has also solidly established itself as a centre for capacity and community building in bioinformatics and computational biology, hosting regular meetings with representation across the Victorian bioinformatics community and developing infrastructure (such as the GVL), resources and training programs to enable researchers at all levels to employ best practice for a range of life science computation applications.

LSCC CAPACITY BUILDING
PROJECTS

PROJECT TITLE	RESEARCHER	INSTITUTE
Interaction of PRMT5 with short hairpin RNA in Erythroid leukemia	A/Prof. David Curtis	Alfred
Immune profile of schizophrenic patients with drug sensitivities	Dr Kathlyn Ronaldson	Alfred
Why is Vancomycin Resistance becoming more common in Australia	Prof. Paul Johnson	Austin
Genetic and epigenetic effects of L-sulforaphane	Dr Tom Karagiannis	Baker IDI
Sequence analysis of exosomal RNA	A /Prof. Andrew Hill	Bio21
Genetic and epigenetic risk factors in breast, colorectal, prostate cancer	Prof. Graham Giles	Cancer Council
Targeted sequencing of a myopia linked gene region to identify disease associated changes	A/Prof. Paul Baird	CERA
Identification of genetic variants associated with myopia and ocular biometrics	Dr Maria Schache	CERA
The role of genetics and epigenetics in the development of Multiple Sclerosis	Dr Judith Field	Florey
Towards healthier ageing	A/Prof. Cassandra Szoeke	Florey
Stress transcriptomics: development of tests to reduce the incidence of summer mortality in abalone	Dr Jan Strugnell	La Trobe
Pipeline for polymorphism mapping in parasitic nematodes	Dr Grant Warwick	La Trobe
Genomics and Proteomics of the Apple scab fungus	Dr Kim Plummer	La Trobe
Global Ants DB: An international database of ant species abundances and morphological traits	Dr Heloise Gibb	La Trobe
Pipeline for polymorphism mapping in parasitic nematodes	Dr Warwick Grant	La Trobe
Population Genomics using RAD-Seq	Dr Nick Murphy	La Trobe
Dictostelium Genomics Project	Prof. Paul Fisher	La Trobe
Differential Expression of Membrane Proteins under Heat-Shock	Prof. Nick Hoogenraad	La Trobe
Cephalopod Toxin Proteomics	Dr Jan Strugnell	La Trobe
Differential Expression in the study of Myopia	Prof. Sheila Crewther	La Trobe
High throughput genomic activities within the Life Sciences Computation Centre (LSCC)	A/Prof. Andrew Lonie	LSCC
Unravelling the genetics of common epilepsies	Dr Michael Hildebrand	MBC
Genome wide DNA methylation profiling of Childhood B- Cell Acute Lymphoblastic Leukaemia	Dr Nicholas Wong	MCRI
Function of gingipain genes in peridontal disease	A/Prof. Stuart Dashper	MelbDental
Integrated analysis of high content screening outputs to identify regulators of bladder cancer	Dr Elizabeth Williams	MHTP
Assembly and annotation of all bacterial genomes in the NCBI Sequence Read Archive	Dr Torsten Seemann	Monash
Targeting macrophage subtypes as a strategy for chronic inflammatory lung disease therapy	Dr Margaret Hibbs	Monash
Registration of CT and MRI images for advanced segmentation and visualisation of anatomy	Dr Colin McHenry	Monash
Measurement and prediction of vulnerable plaque formation and rupture	Dr Pauline Assemat	Monash
Understanding antibiotic resistance in Acinetobacter baumannii	Dr John Boyce	Monash
Comparative genomics to decode Lipopolysaccharide diversity in Leptospira	Dr Gerald Murray	Monash
Investigation of mobile elements in Clostridium difficile	A/Prof. Dena Lyras	Monash
Human haplotype sequencing of sorted chromosomes	Dr Nick Murphy	Monash
Evolution of Dichelobacter nodosus and the spread of Ovine Footrot through Europe	Prof. Julian Rood	Monash

PROJECT TITLE	RESEARCHER	INSTITUTE
The transcriptional profile of an in vivo mouse infection of Clostridium perfringens	Prof. Paul Hertzog	Monash
Identifying antibodies to Schistosoma infection in Chinese water buffalo	Dr Michael de Veer	Monash
Mini-pig pedigrees as a model for human mitochondrial disease	Prof. Justin St John	Monash
Transcriptome of the spiny mouse, a model for human embryo development	Dr Hayley Dickinson	Monash
Neuroimaging in Huntingtons Disease	Prof. Nellie Georgiou-Karastianis	Monash
Molecular Epidemiology of Vibrio cholerae associated with the cholera outbreak in Papua New Guinea	Dr Andrew Greenhill	Monash
Imaging the process of life	Prof. Christophe Marcelle	Monash
3'-Seq: a novel method for quantitative analysis of gene expression in eukaryotic transcriptomes	Dr Traude Beilharz	Monash
Using NGS to resolve deep phylogenetic relationships within terrestrial molluscs and brittlestars	Dr Adnan Moussalli	MuseumVic
High throughput genomic activities including International Cancer Genomics Consortium projects such as Tumourigenesis and drug resistance in ovarian cancer	Prof. David Bowtell	Peter Mac
High throughput genomic activities	A/Prof. Ian Campbell	Peter Mac
Deciphering the functionality of genetic data through integrative bioinformatics approaches	Dr Kaylene Simpson	Peter Mac
Identification of breast cancer predisposing genes using genome sequencing	Dr Maria Doyle	Peter Mac
VCCC Human DNA Variation Repository	Dr Andrew Fellowes	Peter Mac
Characterising the activation and mobilization of transposable elements in intestinal cancer	Dr Robert Ramsay	Peter Mac
Determining the molecular profile of lethal prostate cancer	Dr Geoff MacIntyre	RMH
A description of the intestinal bacterial community of the premature infant	Dr Leah Hickey	RWH
Genomic and Transcriptomic Characterization of Micropapillary Adenocarcinoma	Dr Gavin Wright	SVH
Transcriptome analysis of lymphatic malformation endothelial cells	Dr Caroline Taylor	SVH
Novel biomarkers of endothelial disruption, platelet activation and myocardial ischemia in CVD	Dr Christopher Judkins	SVH
Bioinformatics for EMP-associated gene expression and EMPathy Target Discovery data integration	A /Prof. Erik Thompson	SVI
The mechanism of accelerated type 1 diabetes in non-obese diabetic mice deficient in granzymeA	Dr Helen Thomas	SVI
High throughput genomic activities	Prof. Justin Zobel	UoM
High throughput genomic activities	Prof. Melissa Southey	UoM
High throughput genomic activities	Prof. John Hopper	UoM
Pathogen Genomics and Genetics Program	Prof. Robin Gasser	UoM
Targeted sequencing of ESR1 and other hormone metabolism genes and risk of breast cancer	Prof. John Hopper	UoM
Transcriptome profiling of glioma stem cells: subtype analysis and molecular target discovery	Dr Theo Mantamadiotis	UoM
Cancer Predisposition Genes Identification	Dr Daniel Park	UoM
Using RNAseq to understand how Staphylococcus aureus Responds and Adapts to Antibiotics	A /Prof. Tim Stinear	UoM
Understanding how bacteria cause persistent infection	A/Prof. Ben Howden	UoM
Developing algorithms for biomarker identification in human cancer tissue sections	Dr Anne Thompson	VCB

LSCC USER FEEDBACK

As for 2012, in 2013 recipients of LSCC resources were asked to provide feedback on their interactions with the LSCC*. Responses were overwhelmingly positive and some highlights are listed here.

INTEGRATED GENOMICS FOR LETHAL PROSTATE CANCER

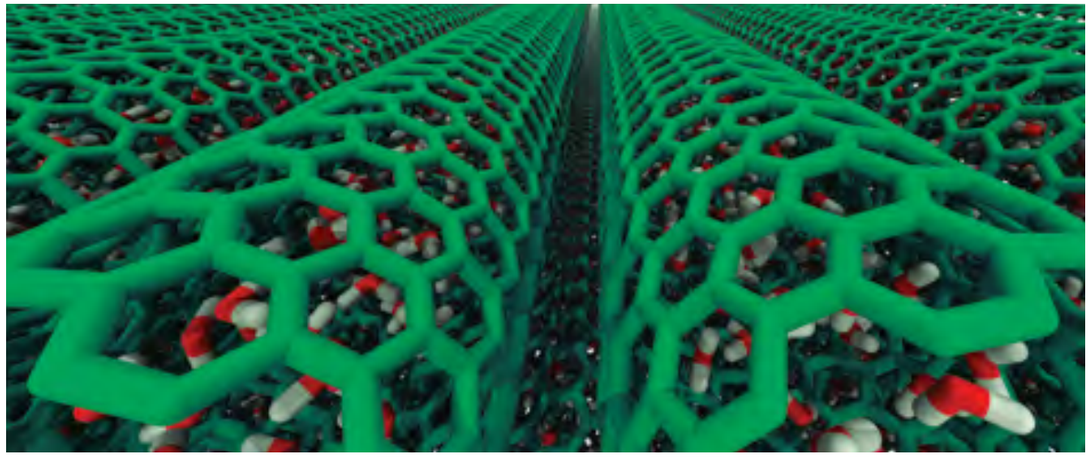
Institution Royal Melbourne Hospital/UoM Department of Surgery/ NICTA/ Australian Prostate Cancer Research Centre, Epworth Hospital
Collaborator Dr Geoff McIntyre, NICTA
LSCC staff Dr Clare Sloggett

Chris Hovens and his team at Australian Prostate Cancer Research Centre Epworth had carried out whole genome sequencing and RNA sequencing for a range of samples but had no bioinformatics capability to process the data. They engaged Dr Geoff Macintyre to oversee the analysis of these samples. While NICTA had the expertise to perform the analysis, they did not have the computational resources and lacked the staff to carry out the coding required. LSCC was brought onto the project to provide not only computational resources to carry out this analysis, but to provide expertise in pipelining and coding to generate a fully functional whole genome sequencing analysis pipeline and a RNA-SEQ analysis pipeline.

The project has yielded the following outcomes:

- a fully featured whole genome sequencing analysis pipeline that provides high-quality somatic mutation calling for cancer samples
- a fully featured RNA-SEQ analysis pipeline that incorporates state of the art software for performing differential expression analysis
- a high impact publication looking into subclonal origin of lethal prostate cancer (in preparation)
- a high impact publication looking into hormone driven structural rearrangements in cancer (in preparation)
- an ongoing collaboration with researchers from the Cancer Genome
- Project at the Wellcome Trust Sanger Centre, Cambridge UK
- a successful NHMRC grant application for studying lethal prostate cancer (NHMRC APP1047581, AUD$689,673 2013-2015).

The LSCC subscription provided critical resources for this project that otherwise would have been sought overseas. The sheer scale in terms of size and processing power required to analyse these genomics data meant that a high-performance computing facility was required, along with the expertise to utilise it. By engaging Dr Clare Sloggett in the LSCC we were given access to someone who could provide that expertise and carry out rapid and high quality development of analysis pipelines. The capability now developed as a result of this project allows us to perform sophisticated genomic analyses comparable to top research institutes around the world. Without the subscription, this project would not have been possible to carry out locally.



TOP: Lorne conference, summer 2013/14, Image: VLSCI. BOTTOM: UoM MSc Computer Science student Mahtab Mirmomeni worked with LSCC staff to develop the GVL tutorials. Image: Casamento photography.

BIOINFORMATICS SUPPORT FOR THE PRECINCT

Institution/s Eastern Hill Academic Centre
Collaborators From the Centre for Eye Research, St Vincent's Institute and St Vincent's Hospital
LSCC staff Dr Gayle Philip

Dr Philip coordinates the bioinformatics on a range of genomics projects. Data from the projects has been processed and analysed using the best practice pipelines written and maintained by LSCC staff for processing data in an automated, reproducible manner. Additionally, a number of groups from the Precinct have attended the expertise meetings at the VLSCI for help with project design, as well as for advice about solving problems encountered during data analysis. Multiple PIs have also been given access to the VLSCI clusters with data storage allocation and several thousand hours of CPU time. In addition, the VLSCI pipelines have been made available to researchers who have wanted to undertake running the analyses themselves. Training and capacity building for the Precinct has been delivered in the form of Galaxy workshops, variant detection workshops and Unix courses.

The subscription to VLSCI has been transformational in bringing a sea change to the availability and implementation of bioinformatics on this campus. The project-specific emphasis allows individual engagement, and the conduit provided by Gayle to the full range of expertise available at the VLSCI, is very enabling.

PAT-SEQ ANALYSIS METHODS AND TOOLS

Institution Monash University
Collaborator Dr Traude Beilharz
LSCC staff Dr David Powell

I have developed a novel assay based on high-throughput sequencing. I required the development of new software to process the data, assistance with bioinformatics analysis, and help with training postdocs and students in its use. We now have a piece of software called TailTools which takes my raw data and produces summarised results. We are now moving on to downstream bioinformatics analysis to answer more fundamental biological questions.

The subscription model allowed me to get access to a team of expert bioinformaticians at a fractional appointment within my budget. It was a low risk, high gain process.

**The full report has been presented to the LSCC Executive and is available from A/Prof. Andrew Lonie, Head, LSCC*

A/Prof. Andrew Lonie
Head, LSCC

IBM RESEARCH
COLLABORATORY FOR LIFE SCIENCES–MELBOURNE

The VLSCI stimulated collaboration between UoM, Vanderbilt University and IBM researchers due to the capability of combining high level molecular dynamic studies with experimental data.

Prof. Frances Separovic, Head, School of Chemistry, University of Melbourne

2013 IN REVIEW

In addition to continuing work on existing research projects, the IBM Research Collaboratory for Life Sciences-Melbourne (the Collaboratory) also began a number of new and important collaborations in 2013.

One of the most exciting new opportunities is a **deep collaboration 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: building and simulating molecular models of cellulose synthase like proteins in collaboration with Dr Monika Doblin at the Melbourne node; modelling cellulose microfibrils and polysaccharide interactions in the context of building a computational model of the plant cell wall, in collaboration with Dr Tony Bacic, UoM node and Dr Mike Gidley at the Brisbane node; and using molecular modelling and dynamics to investigate evolutionary adaptation of substrate specificity in ß-glucanases with Dr Geoff Fincher at the Adelaide node.

The Collaboratory also began working on Apolipoprotein E (apoE), an important blood protein involved in lipoprotein clearance and metabolism. The protein exists as three major isoforms that differ by single amino acid substitutions at position 112 and 158. The apoE4 (112R/158R) isoform is a major risk factor for late onset Alzheimer's disease (LOAD) with E4/4 homozygotes having a >95% chance of developing LOAD by the age of 65. Work has commenced with collaborators at La Trobe University, A/Prof. Matthew Perugini and PhD student Shane Gordon, **looking at the poorly understood molecular mechanisms of this genetic link in this form of Alzheimer's**.

IBM Collaboratory researchers are involved in many of the large-scale projects which are allocated resources on VLSCI systems through the peer review process. These projects are listed amongst the active projects in 2013 on page 62 of this Report.

Finally, as part of an ongoing collaboration with A/Prof. Ross Bathgate and Dr Daniel Scott at the Florey Institute of Neuroscience and Mental Health, and Prof. Stan Skafidas, UoM, Dr Natalie Gunn, structural biologist, IBM Research Australia, has been performing small angle x-ray scattering (SAXS) using the Australian Synchrotron in order to better understand the shape and size of the detergent corona surrounding the solubilised g-protein coupled receptors (GPCRs) being studied. SAXS is the only technique that can yield the structure of the entire protein-detergent complex, and can be used to rapidly screen for the stability of GPCRs in detergents, as well as validate the high-resolution molecular models which have been developed. This new work adds an exciting new approach to IBM's drug discovery platform development, and represents **the first time an IBM researcher has used the Australian Synchrotron directly**.

Collaboratory staff continued to be involved in a wide range of teaching, skills development, student mentoring and supervision and communications and outreach activities at VLSCI. Specific roles are listed below. Outreach activities and internships are incorporated with others documented from page 44.

IN THE COMMUNITY

IBM staff contribute to the research community at the University of Melbourne through the following roles:

John Wagner

- Senior Fellow. Department of Electrical and Electronic Engineering, School of Engineering, 20 Feb 2012 to 8 Jul 2014.
- Honorary Fellow. Department of Mathematic and Statistics, Faculty of Science, 2 Aug 2010 to 31 Dec 2014.
- IBM-University of Melbourne Partnership Committee.
- Scientific Committee Member. Centre for Neural Engineering, Aug 2011 to Aug 2014.

Stephen Moore

- Honorary Fellow. Department of Mechanical Engineering, Faculty of Engineering, Aug 2010 to 31 Dec 2013.

Matthew Downton

- Honorary Fellow. Department of Physics, Faculty of Science, Aug 2010 to 31 Dec 2013.

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

(from l-r) Director, IBM Research Australia, Dr Glenn Wightwick, A/Prof. Matthew Perugini, La Trobe University, A/Prof. Ashley Buckle, Monash University, Dr John Wagner. Image: Casamento photography

VLSCI has very quickly forged itself as an essential organisation to support the high performance computing requirements of researchers state-wide in Victoria, including La Trobe University where I am located. I am absolutely thrilled with the support and outcomes that VLSCI has provided in 2013, and I look forward to developing stronger links with the organisation in the immediate and distant future.

A/Prof. Matthew E. Perugini, Associate Professor, ARC Future Fellow, Faculty of Science, Technology and Engineering, School of Molecular Sciences, Department of Biochemistry, La Trobe University.

AUSTRALIAN HPC AT **SUPERCOMPUTING 2013**

VLSCI Communications, with assistance from NCI, iVEC (Pawsey Centre) and V3 alliance, planned, coordinated, implemented and staffed the Australian HPC booth at Supercomputing 2013 in Denver, Colorado, USA from 17-22 November.

With other partners from Monash University's MASSIVE facility, Swinburne University's Centre for Astrophysics and Supercomputing, RMIT and La Trobe Universities' Trifid system and CSIRO, over 25 representatives from high-end computing organisations in Australia joined over 10,000 participants. VLSCI's Senior Systems Engineer, Chris Samuel, presented in the SPXXL (international IBM Facility user group) program on the July installation and commissioning of VLSCI's latest high-memory IBM iDataplex x86 system 'Barcoo', which initiated a move across to the new scheduling system 'Slurm' for all machines. Key staff from VLSCI, NCI and iVEC presented at the booth's Tim Tam Talks and fielded enquiries from researchers, technical experts and prospective employees and students. The Communications team were part of a session entitled: High Performance Communication for High Performance Computing (hpc-hpc), sharing a short video and report about the Melbourne Knowledge Week event held on 30 October: Personalised Medicine - the Hope and the Hype. Throughout the week social media activity was generated through a series of news items, including documenting the live demonstration of the transfer from the Aspera booth of a 10Gb file to the University of Queensland in less than a minute.

With the SC13 Top500* announcements, Avoca remained in the Top500, and is now at 48. Avoca also retained its equal 7th ranking in the Graph 500, the official benchmark for data intensive supercomputers, with IBM's three major BlueGene centres taking the top three places.

*[*for details re Top500, refer page 16 of this Report – Supercomputer Systems]*

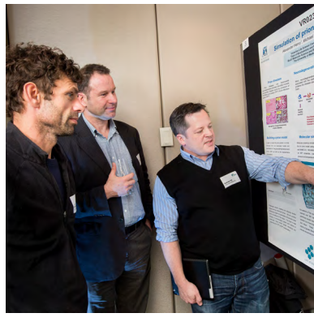
RESEARCH SHOWCASE
3 October 2013

At the request of the Resource Allocation Scheme Committee (RAS Committee) Thursday 3 October became a showcase of research being conducted through VLSCI.

Included in the program for The University's Festival of Ideas, the first hour of the day was opened to the public, with four lively presentations made by four high profile researchers using substantial VLSCI resource allocations. They demonstrated how supercomputing has impacted their research to an audience of 60 stakeholders and 40 members of the public and including Victoria's newly appointed Lead Scientist, Dr Leonie Walsh and Steering Committee Chair, Prof. John Zillman. The public presentations included:

- John Hopper, *A novel method for genome-wide scanning of regions associated with breast cancer risk*
- Tania Kameneva, *Computational neuroscience approach to the challenges of retinal prostheses*
- Robin Gasser, *Parasite Genomics & Genetics Program*
- Michael Kuiper, *Modelling pore-forming toxins and drug design*

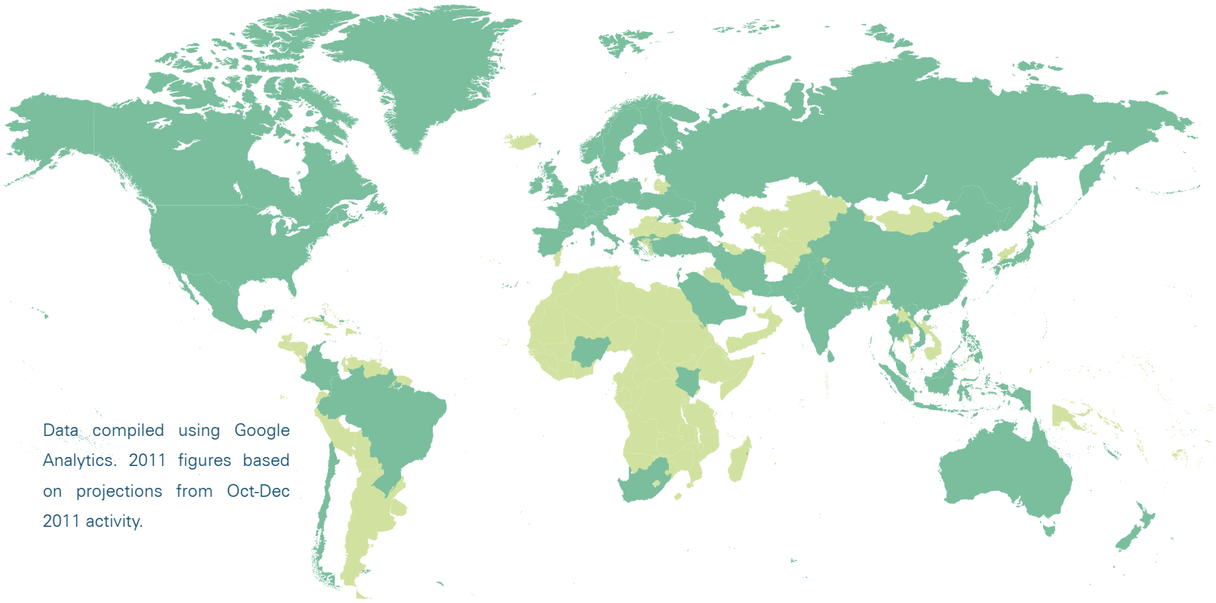
These talks were followed by a networking session to allow the audience to speak further with the presenters. The remainder of the day involved impressive oral and poster presentations of research outcomes by almost 50 project leaders with RAS allocations in 2013 to an audience of the VLSCI RAS Committee and various research peers. It was a very lively and successful day.



INTERACTIONS

61% INCREASE IN WORLDWIDE WEBSITE VISITORS

Website Visitors



Data compiled using Google Analytics. 2011 figures based on projections from Oct-Dec 2011 activity.

TOTAL WEBSITE VISITORS

- **2011**.....22,388 visitors
- **2012**.....31,082 visitors
- **2013**.....36,004 visitors

UNIQUE WEBSITE VISITORS

- **2011**.....10,380 visitors
- **2012**.....14,769 visitors
- **2013**.....17,705 visitors

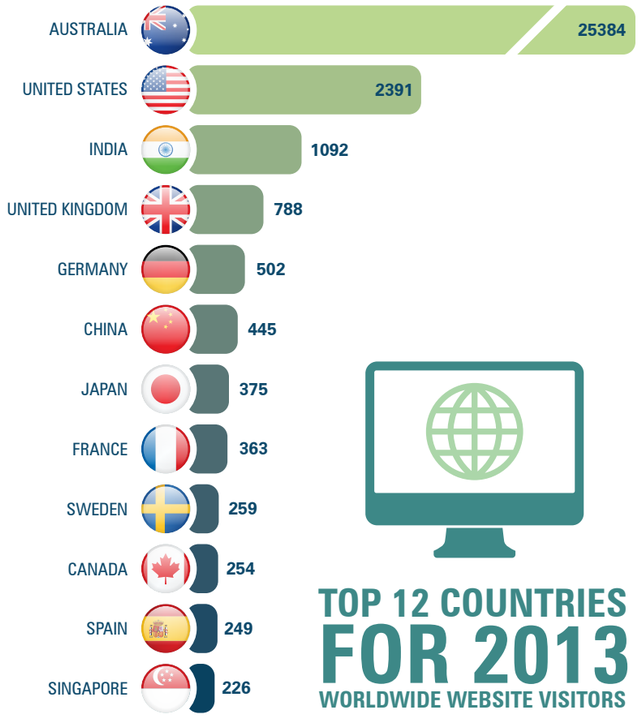
WEBSITE PAGE VIEWS

- **2011**.....64,388 page views
- **2012**.....92,204 page views
- **2013**.....96,506 page views

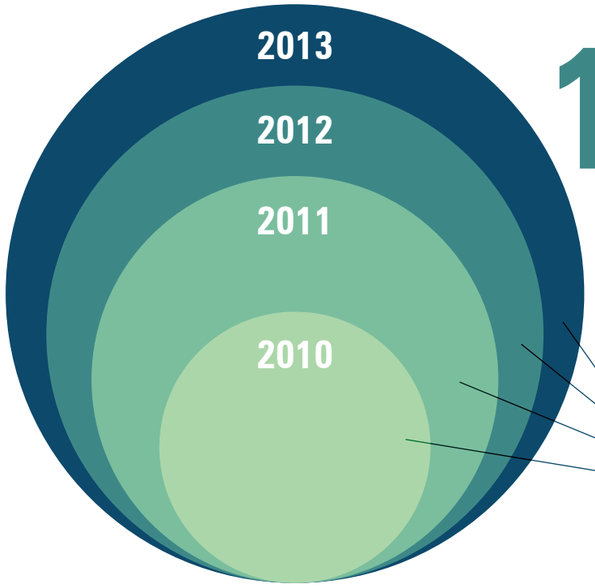
AVERAGE WEBSITE VISITS

- **2011**.....61 per day
- **2012**.....85 per day
- **2013**.....99 per day

70% OF VISITORS TO OUR WEBSITE VLSCI.ORG.AU WERE FROM AUSTRALIA IN 2013



TOP 12 COUNTRIES FOR 2013 WORLDWIDE WEBSITE VISITORS



113% INCREASE IN eNEWS SUBSCRIBERS

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

- 640 subscribers *(December '13)*
- 550 subscribers *(December '12)*
- 450 subscribers *(December '11)*
- 300 subscribers *(December '10)*

TOP 5 MOST VISITED WEBSITE PAGES

VLSCI Homepage.....*vlsci.org.au*

Opportunities.....*vlsci.org.au/page/outreach*

System Documentation.....*vlsci.org.au/page/documentation*

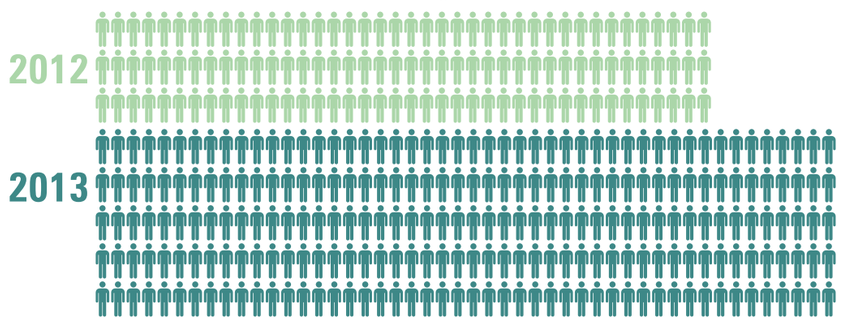
LSCC Resources.....*vlsci.org.au/lscc*

Upcoming Events.....*vlsci.org.au/page/upcoming-events*

100% INCREASE IN TWITTER FOLLOWERS

The VLSCI twitter account, @vlsci, is one 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 2013, VLSCI also hosts and maintains the @australianhpc twitter account.



IN THE **NEWS**

Public and media interest in VLSCI's supercomputers and the Victorian researchers working on them remained strong throughout 2013. Ongoing public interest in the Victorian Infectious Diseases Laboratory's (VIDRL) exciting enterovirus work (which includes the poliovirus) led to a front page and accompanying feature story in the Fairfax media's *Melbourne Magazine*'s April 2013 edition. Published in several Australian States, its circulation in Melbourne alone reached over 150,000 people. This was followed in August by a feature on VIDRL's work on ABC TV's science show *Catalyst*.

Additional media included in particular, two features in the biotechnology industry journals *Australasian Biotechnology* and *Australian Life Sciences*, a six minute feature on *ABC TV's 7:30 report*, several opinion pieces submitted by Director, Prof. Peter R. Taylor and science stories in major daily newspapers including the national circulation *Financial Review*.

ESTIMATED MEDIA VALUE

National television	$90,000*
Major daily newspapers	$132,600
National radio	$17,000
Industry news	$46,000
TOTAL	**$285,600**

**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.*

$285,600
ESTIMATED MEDIA VALUE

Kind permission to reproduce Melbourne Magazine images granted from Fairfax syndication

3 APRIL, ABC TV 7:30 REPORT

Endangered tortoises in Western Australia have been given a fighting chance with the help of a Melbourne based supercomputer

Dr Michael Kearney, University of Melbourne ecologist working with Nicola Mitchell and Matthew Hipsey from the University of Western Australia was featured in this story about the environmental modelling he had contributed to this search for relocation options for the critically endangered Western Swamp Tortoise. The study was published in the international journal *Biology*.

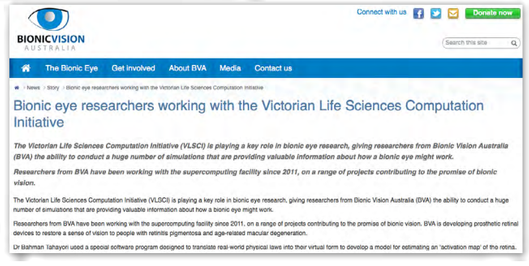
Dr Michael Kearney fronts the cameras for the ABC TV story.

27 FEBRUARY, THE AUSTRALIAN

Visit by Allan Jones, CEO, Allen Institute for Brain Science to launch the Victorian node of the International Neuroinformatics Coordinating Facility.

22 MAY, AUSTRALIAN LIFE SCIENTIST

Feature article written by LSCC Head, A/Prof. Andrew Lonie



23 JULY, WWW.BIONICVISION.ORG.AU

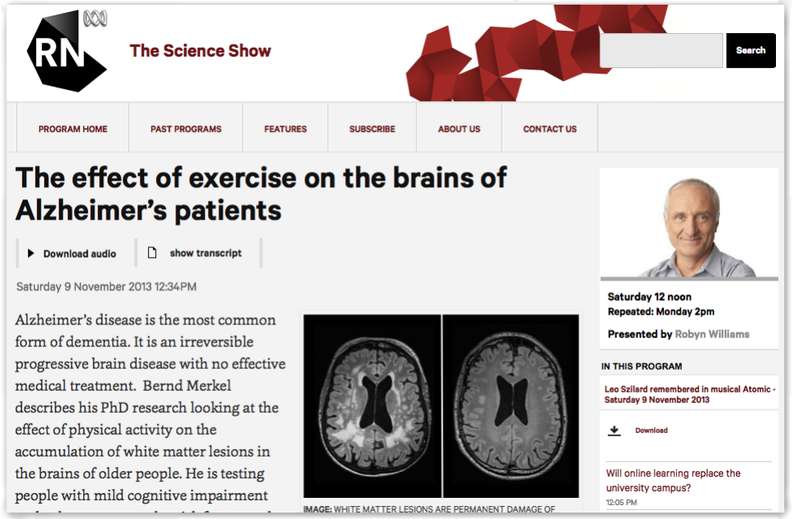
Bionic Vision Australia published an online story explaining VLSCI's role in an important part of the work of this major ARC-funded project.

13 SEPTEMBER, WWW.UNIMELB.EDU.AU

Australia's Chief Scientist visited the University of Melbourne's Faculty of Science before spending time at VLSCI learning about operations and discussing Australia's future needs in Science, Technology, Engineering and Mathematics.

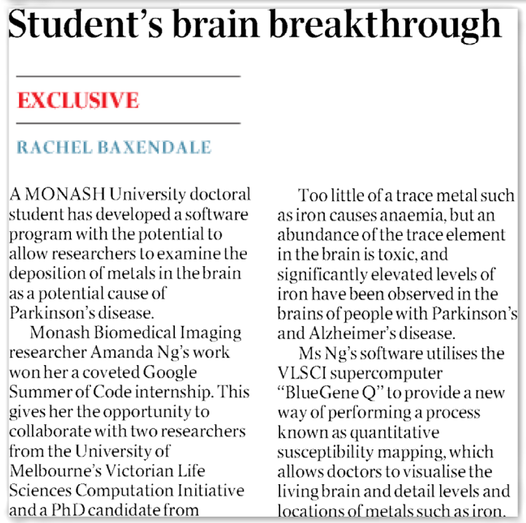
12 AUGUST, GENERAL MEDIA COVERAGE

VLSCI systems user Dr Kat Holt's work in genetics, maths and supercomputers led to her being awarded a L'Oreal Women in Science award.



9 NOVEMBER, ABC RADIO NATIONAL, SCIENCE SHOW

Recipient of VLSCI PhD top-up scholarship Bernd Merkel talked about his work studying causes of Alzheimer's disease with host Robin Williams.



4 OCTOBER, THE AUSTRALIAN

Monash Biomedical Imaging researcher working on Google Summer of Code project involving the BG/Q.

INDUSTRY ENGAGEMENT

Australian Bioinformatics Network *member*

Ausbiotech *member*
VLSCI stories published in Australasian Biotech and Australian Life Sciences journals

Bio21 Cluster's Innovating for Victoria's Health Exhibition *contributing exhibitor*
Displayed in Federation Square, Melbourne during Melbourne Knowledge Week

BioMelbourne Network *member*

eResearch Australasia 2013 *sponsor and exhibitor at Brisbane in October*

GVL NeCTAR-funded Genomics Virtual Laboratory *partner*

HPC500 *High Performance Computing industry body accepted as member*

IBM Deep Computing Institute *Director attended as Board Member*

ICT for Life Sciences Forum *sponsor of Forum and Graeme Clark Oration*

IDC International Data Corporation *subscriber*

INCF *Co-sponsor with MASSIVE of Victorian node under 3 year joint agreement, and co-sponsor of node launch event held in February*

ISC2013 International Supercomputing Conference 2013
Presentation by Communications Manager, Facility Manager attended, Leipzig, Germany in June

MASSIVE *Host to Computational Bioimaging theme in conjunction with Monash Biomedical Imaging*

NCI National Computational Infrastructure *Director attended Board meetings as member*

Supercomputing 2013 *Australian HPC booth, Denver, USA in November Attendance by Director, Facility Manager, Systems Administrator & Communications team*

Tertiary Education Manager's Conference *represented by Business Manager Hobart, September*

Texas Advanced Computing Center *Director attended Strategic Advisory Board Meeting as member Denver, USA in November*

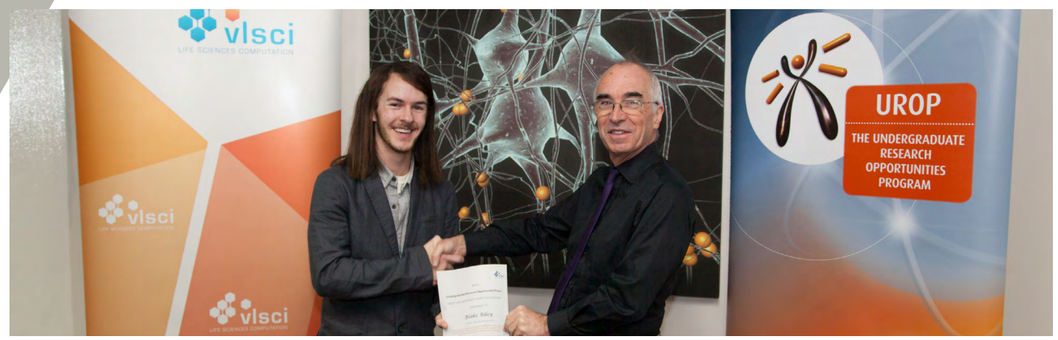
Victorian Government's Technology Voucher Program *registered provider*

Victorian Platform Technologies Network *member and exhibitor*
Inaugural VPTN industry showcase, Melbourne Town Hall, October

CAREER DEVELOPMENT
FOR COMPUTATIONAL BIOLOGISTS

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

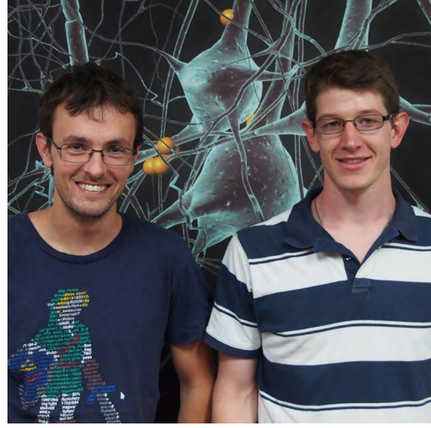
- PhD top-ups - supporting exceptional students with annual stipends
- M.Sc. (Bioinformatics) - providing student bursaries to projects
- Internships - hosting talented postgraduates over their Summer recess
- Undergraduate Research Opportunities Program (UROP) - co-sponsoring Program and providing direct stipend support to computational biology projects for undergraduates
- Sponsorship of conferences & meetings
- Travel grants
- Workshops

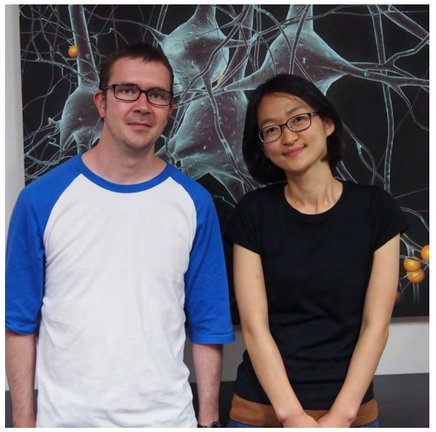


UROP

VLSCI provides substantial funding towards the administration of the Undergraduate Research Opportunities Program as well as direct support to numerous projects through student stipends. The largest ever field of applications was received in the first round of 2013, with 277 students vying for 48 projects - 16 of which comprised computational or bioinformatics research. Across the two rounds in 2013, VLSCI provided a part-stipend to 11 projects. The University of Melbourne and its affiliated research institutes, Monash University and its affiliates, Deakin University, Swinburne University, RMIT and various industry groups were engaged in the Program. Over 100 people attended the UROP Conference Day on 10 July, including the Minister for Technology, The Hon. Gordon Rich-Phillips, who opened the proceedings and keynote speaker, Prof. John Carroll, Head of the School of Biomedical Sciences, Monash University.

"Through this internship, I got valuable experience in life science and learnt how interesting it is to work in the bioinformatics field. Therefore, I can say that this internship has provided me with more options to choose my career path."
Sori Kang



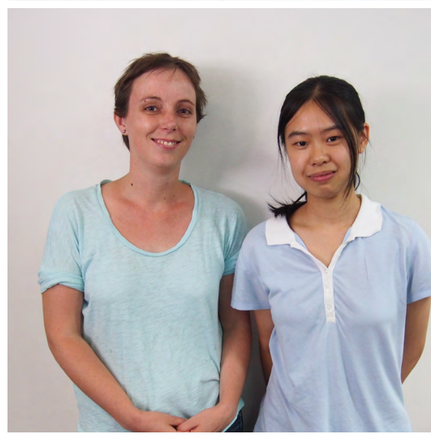


"The internship was overall a very positive experience which enabled me to learn a lot in a short period of time. This project has proved an incredibly useful starting point to my PhD project."
Brett Sheil

INTERNSHIPS 2012-2013

LEFT TO RIGHT, TOP TO BOTTOM: Igor Grossman (Monash University) delivers his internship research project findings; Supervisor Ira Cooke and Intern Brett Sheil (La Trobe University); Supervisor Bernard Pope and Intern Sori Kang (VLSCI, University of Melbourne); Intern Lee Yeoh and Supervisor Nathan Hall (La Trobe University); Intern Alexander Henry and Supervisor Michael Kuiper (VLSCI); Supervisor Clare Sloggett and Intern Jessica Chung (VLSCI/NICTA). OPPOSITE: Blake Riley receives his 'Best Life Sciences Computation Presentation' Award at the 2013 UROP Conference Day from VLSCI Director, Peter Taylor.

"This internship has helped me learn a variety of programming and computational techniques. It has also introduced me to the world of computational biology and molecular modelling, which is now an interesting career option for me."
Alexander Henry



PHD TOP-UPS, SUMMER INTERNSHIPS, UROP STIPEND SUPPORT AND PROJECT PLACEMENTS

Refer Glossary (p.96) for all abbreviations used in all tables in this Report.

STUDENT	HOST RESEARCH INSTITUTION, DEPARTMENT	PRIMARY SUPERVISOR/S	PROJECT
		PHD TOP-UP STUDENTSHIPS	
Jason Shiller	La Trobe, Botany	Kim Plummer	Determination of virulence factors in the apple scab fungus
Monther Al Hamdoosh	La Trobe, Computer Science	Dianhui (Justin) Wang	Regulatory Motifs Identification Using Machine Learning Techniques.
Sarah Diepstraten	La Trobe, Genetics	Adam Hart	A new experimental model for analysis of Human globin gene switching during embryonic stem cell differentiation
Cyril Reboul	Monash, Biochemistry & Molecular Biology	James Whisstock, Ashley Buckle	Structural aspects of the pore-forming protein, Perforin
Emma Hodges	Monash, Chemical Engineering/ Engineering	Ravi Jagadeeshan	Mesoscopic simulations and experimental observations of cell adhesion in hydrodynamic flow
Samuel Forster	Monash, Faculty of Medicine	Paul Hertzog	Systems biology of the Type 1 IFN response
Jian D.L Yen	Monash, Faculty of Science	Ralph Mac Nelly	Thermodynamic ecology: theoretical and empirical approaches.
Phillip Ward	Monash, IT	David Dowe, David Barnes, Parnesh Raniga, Gary Egan	Quantification of vasculature damage and microbleeds using susceptibility weighted imaging with application to normal ageing and Alzheimer's disease
Woldeamanuel Birru	Monash, MIPS	Colin Pouton	Molecular Dynamics Simulations of Lipid Drug Delivery Systems
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
Luisa Teasdale	Museum Victoria, Terrestrial Invertebrates, Sciences	Adnan Moussalli	Using 'next generation' sequencing to resolve deep phylogenetic relationships in the land molluscs (Panpulmonata)
Xiao Zheng Mu	RMIT, School of Applied Sciences	Peter Smooker	ID of virulence and colonization factors of campylobacter
James Pham	UoM, Bio21	Stuart Ralph, Matt Perugini, Ren Dobson	Cysteinyl-tRNA synthase as a potential antimalarial target
Lee Yeoh	UoM, Biochemistry & Molecular Biology	Stuart Ralph	The identification and characterization of alternatively- spliced genes and their regulation in Plasmodium falciparum and Toxoplasma gondii.
Nafise (Nina) Erfanian Saeedi	UoM, Electronic Engineering	David Grayden	Neural Network model of Auditory Perception
David Kaplan	UoM, Florey Neuroscience Institute	Steven Petrou	The dynamic action potential clamp as a tool for investigating anti-epileptic drugs.
Felicity Jackling	UoM, Genetics	Belinda Appleton	A genetic investigation of commercially important traits in alpacas
Rahul Vivek Rane	UoM, Genetics	Sui Fai (Ronald) Lee, Ary Hoffmann, John Oakeshott	Genomic basis of adaptation
Simon Sadedin	UoM, MCRI	Alicia Oshlack, Terry Speed, Andrew Sinclair	Improving detection of disease causing variants in targeted NGS data
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
Danielle Ingle	UoM, Microbiolology & Immunology	Roy Robins-Browne, Kathryn Holt, Marija Tauschek, Timothy Stinear	Virulence within atypical enteropathogenic E. coli
Daniel Brown	UoM, Pathology	Theo Mantamadiotis	Investigating signalling pathways in glioma stem cells
Scott Ritchie	UoM, Pathology, MDHS	Michael Inouye, Gad Abraham, Paul Waring	Preservation of Disease Modules across biological networks
Stefano Mangiola	UoM, Veterinary Faculty	Robin Gasser	Design and application of advanced bioinformatic tools to explore the parasitic worms system biology
Brendan Ansell	UoM, Veterinary Science	Aaron Jex, Malcolm McConville	Investigating mechanisms of drug resistance in Giardia
Daniel Cameron	UoM, WEHI	Tony Papenfuss, Terry Speed	Detecting somatic indels and other structural variants using high-throughput genomic sequencing
Peter Hickey	UoM, WEHI	Terry Speed, Peter Hall	The statistical analysis of data from high-throughput assays for studying DNA methylation
Ehtesham Mofiz	UoM, WEHI/MDHS	Tony Papenfuss	Scabies mite genome project
		MSC (BIOINFORMATICS) BURSARY RECIPIENTS	
Michael Zhang *VLSCI bursary*	CERA/UoM	Paul Baird	Variants associated with eye diseases
Yu Wan *VCCC bursary*	LSCC	Chol-Hee Jung	Breast cancer epigenome-wide association study
Serene Siah	LSCC	Torsten Seemann	Genomic analysis of a novel marine mycobacterium
Anna Trigos *VCCC bursary*	Peter Mac	David Goode	Gene expression patterns between tumour cells and eukaryotes
Jumana Yousef *Peter Mac bursary*	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
Erica Plummer *VLSCI bursary*	RWH	Sepehr Tabrizi	Effect of probiotic supplementation on microbiota of preterm infants
		VLSCI SUMMER INTERNS 2013-2014	
Jocelyn Penington	LSCC La Trobe intern - Completed Grad Dip Bioinformatics, RMIT	Brian Smith	BioPPSy / Solubility: An extensible program for calculating parameters to predict solubility (or other things)
Yuri Benovitski	LSCC Monash intern - Current PhD Student, Bionics Institute/La Trobe	David Barnes	Visualising MRI Scans on a Virtual Environment (CAVE2)
Adrian Hecker	LSCC UoM intern - Completed BSc(Hons) Mathematics, RMIT	Bernard Pope, Kathryn Holt, Michael Inouye	Characterising and predicting effects of nsSNPs on protein structure
Luke Shillabeer	LSCC UoM intern - Current student, MSc(Bioinformatics), UoM	Bernard Pope, Daniel Park, Tu Nguyen-Dumont	Design and analysis of primers within a high-plex PCR protocol
		RHD STUDENTS WITH VLSCI SUPERVISION	
Gourav Singhai	La Trobe, MSc	Nathan Hall, Matthew Perugini	Predicting lysing inhibition in bacterial DHDPS enzymes

STUDENT	HOST RESEARCH INSTITUTION, DEPARTMENT	PRIMARY SUPERVISOR/S	PROJECT
Fiona Durand	La Trobe, PhD	Ira Cooke, Nick Hoogenraad	Differential Expression of Membrane Proteins under Heat Shock
Brett Shiel	La Trobe, PhD	Nathan Hall, Ira Cooke, Jan Strugnell	Understanding of abalone heat stress through transcriptomics
Shakira Johnson	La Trobe, PhD	Nathan Hall, Kim Plummer	Genomics and transcriptomic studies of Venturia host-pathogen responses
Shane Gordon	La Trobe, PhD	Matthew Downton (IBM), John Wagner (IBM)	Investigations into Binding Modes of Substrates and Small Molecules to Bacterial Dihydrodipicolinate Synthase
Saad Alsunbal	Monash , PhD	Jeff Tan (IBM)	Secure network and protocol architecture
Mark Creado	Monash , PhD	Jeff Tan (IBM)	Basic security primitives for operating systems
Kirill Tsyganov	UoM, BSc(Hons)	David Powell, Traude Beilharz	Bioinformatic investigation into 3'UTR elements that mediate cytoplasmic polyadenylation
Serene Siah	UoM, MSc(Bioinf)	Torsten Seemann, Tim Stinear	Genomic analysis of a novel marine mycobacterium
David Edwards	UoM, MSc(Bioinf)	Bernard Pope, Kathryn Holt	A Next-Generation Sequencing Analysis Pipeline for Bacterial Genomics
Lilly Yuen	UoM, MSc(Bioinf)	Dieter Bulach	A next generation sequencing approach for the detection of drug resistant hepatitis B virus in the clinical setting
David Edwards	UoM, MSc(Bioinf)	Bernard Pope	A Next-Generation Sequencing Analysis Pipeline for Bacterial Genomics
Kian Ho	UoM, PhD	Michael Kuiper, Rao Kotagiri	Protein folding
Dan Brown	UoM, PhD	Andrew Lonie, Theo Mantamadiotis	Genomic characterisation of Glioblastoma multiforme (GBM) subtypes
Sehrish Kanwal	UoM, PhD	Andrew Lonie, Richard Sinnot	Informatics platforms for clinical genomics
Sabrina Rodriguez	UoM, PhD	Andrew Lonie, Richard Huggins	Predicting Phenotypes through Pathway Analysis using Conditional Independence and Central Subspaces
Melissa Yeow	UoM, PhD	Dieter Bulach, Melissa Southey	Using a high throughput sequencing strategy to detect microbial agents (viral or bacterial) associated with prostate cancer
Ehtesham Mofiz	UoM, PhD	Torsten Seemann, Tony Papenfuss	Scabies mite genome project
Shabnam Khatibi	UoM, PhD	John Wagner (IBM)	TGF-Beta and IL-6 signalling in cancer
James Korte	UoM, PhD	Stephen Moore (IBM), John Wagner (IBM)	Continuous waveform MRI
IBM SUMMER INTERNS 2013-2014			
Tao Nelson	La Trobe University Honours student	Matthew Downton, John Wagner (IBM)	Pi-stacking in the allosteric inhibition of Vitis vinifera dihydrodipicolinate synthase
Jake Parker	University of Adelaide PhD student	Daniel Oehme (IBM)	Substrate specificity in two barley beta-glucan endohydrolases
Daniel Weber	UoM PhD student	Matthew Downton (IBM)	Modelling the interaction of Equinatoxin II with micelles
GOOGLE SUMMER OF CODE INTERNSHIP			
Timothy Roberts	LSCC Monash supervisors - Cambridge University student	Amanda Ng, David Barnes, Bernard Pope, Steve Moore (IBM)	Algorithm improvements to diffusion guided quantitative susceptibility mapping

STUDENT	HOST RESEARCH INSTITUTION, DEPARTMENT	PRIMARY SUPERVISOR/S	PROJECT
UROP STUDENTS			
David Hughes	MIMR	Ross Chapman	Factors Regulating the expression of Interferon regulated genes; data mining of the INTERFEROME database
Blake Riley	Monash	Ashley Buckle	Molecular Simulation and modelling
Dominic Long	Monash	Natalie Borg	The transfer of ubiqitin to a cellular substrate
Preethi Jeeva	Monash	Sheena McGowan	Molecular simulation of the PlyC phage lysin, a novel antimicrobial scaffold
Stella Ying	NICTA, UoM	Tatiana Kamaneva	Using control theory tool in neuroprosthetics
Robert Fuller	Peter Mac / WEHI	Mark Shackleton	Understanding evolutionary change in human melanoma
Tony Jialun Wei	RCH	Morgan Sangeux	Muscle activity during walking for children with cerebral palsy
Yaniv Kaufman	UoM	David Grayden	Parallelising finite element model code for epilespsy research
John Gilbertson	UoM	Nicholas Geard	Computational Simulation and mathematical modelling of infectious disease dynamics
Daniel Williams	UoM	Christos Pantelis	Development of a gene based classifier for the diagnosis of schizophrenia
Edward Chmiel	UoM, MBC	Chris French	Realistic Neural Network Computation – Applications to Epilepsy and Drug Effect Modelling
Rama Lokon	WEHI	Jarney Choi	Data mining the hematopoietic expression atlas
Charles Grey	WEHI	Kurt Lackovic	Cheminformatic dissection of biological pathways
Catherine Phillips	WEHI	Mathew Ricthie	Statistical methods for next generation genomics
Jessica Tran	WEHI	Shalin Naik	Determining the transcriptomes of individual dendritic cell progenitors
Damian Pavlyshyn	WEHI	Andrey Kan	Computational Immunology
BEST UROP PRESENTATION IN COMPUTATIONAL BIOLOGY WINNER			
Blake Riley	Monash	Ashley Buckle	Chemokine receptor sulfation: Parameterising novel residues for molecular dynamics
WORK EXPERIENCE STUDENTS			
Ben Harper	Camberwell High School	Michael Kuiper	
Joe Toce	St Leonard's College	Various	
Lachlan Grant	University High School	Daniel Oehme (IBM)	

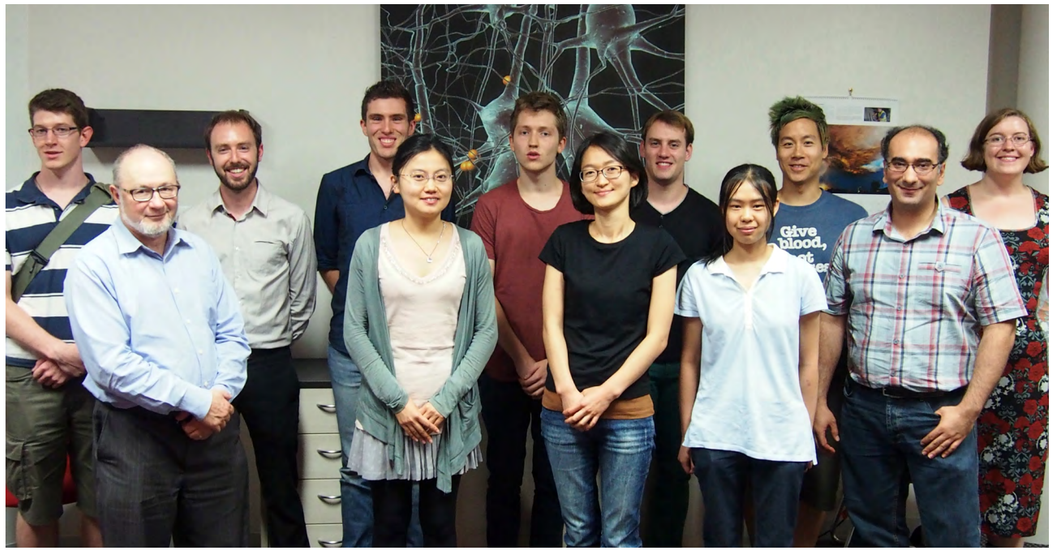
SKILLS DEVELOPMENT

A recent recruit to the LSCC, Harriet Dashnow, is a perfect example of how VLSCI provides opportunities for life scientists to develop skills to equip them for a career in bioinformatics.

With an undergraduate background in Genetics, Biochemistry, Molecular Biology and Psychology, Harriet became increasingly aware that to make a real contribution to biology she would need to embrace increasingly high throughput technologies. Harriet actively sought out internships that provided hands-on experience in both the laboratory and data analysis aspects of next-generation sequencing. This included a VLSCI Summer Internship at Bio21, working in a team with expertise in bioinformatics, pathogenomics and computer science to developing software that detects resistance genes in next-generation sequencing data from pathogenic bacteria. This gave Harriet the opportunity, so early in her career, to make a real contribution to the public health community. Her research continued after being offered work as a Research Assistant, which broadened her previous experience that included a year-long autoimmune disease project at SVI as part of the VLSCI-funded UROP scheme.

During her time enrolled in the Master of Science (Bioinformatics) program, Harriet and was awarded a VLSCI bursary for her excellent marks, and as part of the program she was able to build on her long-term laboratory Technical Assistant position at MCRI with a research placement with leading Bioinformatician, Alicia Oshlack. This research project continues today as part of a subscription by the ANU and MCRI with the LSCC, where Harriet was employed as a Bioinformatician in 2013.

Harriet is now developing a set of current best practice guidelines, including protocols to assess the quality of pipeline components, in particular variant callers. The hope is to evaluate the clinical bioinformatics pipeline being developed by the Melbourne Genomics Health Alliance - a collaboration of seven organisations in the Parkville precinct - to implement clinically driven exome sequencing. The demonstration project involves patients with epilepsy, acute myeloid leukemia, hereditary colorectal cancer, Charcot-Marie-Tooth disease and childhood syndromes, and Harriet has been working with genetic counsellors and physicians to develop a list of appropriate genes to analyse.



OPPOSITE: Harriet (far right) with the group of 2012-2013 VLSCI Summer Interns

M.Sc. (BIOINFORMATICS) **GRADUATES**

Refer Glossary (p.96) for all abbreviations used in all tables in this Report.

STUDENT	PROJECT	SUPERVISOR	INSTITUTION
Tulio Campos	Parasite genomics	Prof. Robin Gasser	UoM
Peter Diakumis	Detection of rare disease causing genetic variants in two families using whole exome sequencing data	Dr Melanie Bahlo	WEHI
Andrew Bakshi	In silico models of genomics instability in tumours	Dr David Goode	Peter Mac
Josua Troesch	Predicting peptide fragmentation using machine learning algorithms	Dr Nick Williamson	WEHI
Tane Hunter	Identifying TP53 mutations in ctDNA from high grade serous ovarian cancer patients using ultra-deep sequencing.	Dr Maria Doyle	Peter Mac
Lilly Yuen	A next generation sequencing approach for the detection of drug resistant hepatitis B virus in the clinical setting	Dr Dieter Bulach	VLSCI
Long Chen	Investigating the influence of different parameters in copy number detection using PennCNV and QuantiSNP	A/Prof. Paul Baird	CERA
Harriet Dashnow	Monogamy is in your genes: Genotyping microsatellites in next generation sequencing data	Dr Alicia Oshlack, Prof. Simon Eastel (ANU)	MCRI
Serene Siah	Genomic Analysis of a Novel Marine Mycobacterium	Dr Torsten Seemann, A/Prof. Tim Stinear	VLSCI, UoM

INVITED SEMINARS AND **PRESENTATIONS**

Refer Glossary (p.96) for all abbreviations used in all tables in this Report.

EVENT	SUBJECT	PERSONNEL	LOCATION	DATE
SPXXL Winter 2013 Workshop	VLSCI Site Update	Bernard Pope	Hawaii, USA	January
UoM Science Experience	A career in life sciences computation	Christina Hall	Victoria, Australia	January
Linux Conference Australia 2013	Enabling Compute Clusters atop OpenStack	Enis Afgan	ACT, Australia	January
Linux Openstack Conference 2013	Enabling Compute Clusters atop OpenStack	Enis Afgan	ACT, Australia	January
Huntington's Disease and Tandem Repeat Disorders Satelite Meeting	Functional changes during working memory in Huntington's disease - Longitudinal 30 months data from the IMAGE-HD study	Govinda Poudel	Victoria, Australia	February
Lorne Proteomics Conference 2013	Galaxy as a Platform for Proteomics	Ira Cooke	Victoria, Australia	February
CSIRO FOAM 2013	The Genomics Virtual Lab: progress	Andrew Lonie	Victoria, Australia	March
CSIRO Focus on Analytical Methods : Bioinformatics	Bridging the gap between computer scientist and biologists	Nathan Hall	Victoria, Australia	March
La Trobe University Chemistry Departmental Seminar	Modelling proteins on ice	Michael Kuiper	Victoria, Australia	April
Big Data	Galaxy and the GVL workshop	Andrew Lonie	Victoria, Australia	April
Illumina Asia Pacific Science Summit	Clinical bacterial pathogen genomics	Torsten Seemann	Phuket, Thailand	April
SHE++ Women in IT Event	Panel discussion	Vera Hansper	Victoria, Australia	May
Applied Bioinformatics and Public Health Microbiology	Using Prokka for rapid annotating microbial genomes	Torsten Seemann	Cambridge, UK	May
International Symposium on Footrot	Genomics of D.nodosus	Dieter Bulach	Oslo, Norway	May
UK Midlands Bioinformatics Day	Microbial tutorials in Galaxy	Simon Gladman	Birmingham, UK	May
UK Midlands Bioinformatics Day	Genomics analysis of foot-rot in Norway	Dieter Bulach	Birmingham, UK	May
UK Midlands Bioinformatics Day	Prokka, Nesoni, VelvetOptomiser & VAGUE	Torsten Seemann	Birmingham, UK	May
BioIT Asia 2013	The Australian Genomics Virtual Lab	Andrew Lonie	Singapore	May
RMH Lecture Series	Modelling in the age of high capacity computing	Michael Kuiper	Victoria, Australia	May
La Trobe University Biochemistry Departmental Seminar	Backup your Precious Data: Avoiding the data dragons	Andrew Robinson	Victoria, Australia	June
Monash University Microbiology Seminar	Bioinformatics on the command line	Paul Harrison	Victoria, Australia	June
Doing Data Better Mini-conference	VLSCI capabilities	Bernard Pope	Victoria, Australia	June
CSC-IT Center for Science visit	The Victorian Life Sciences Computation Initiative	Vera Hansper	Helsinki, Finland	June
Galaxy Community Conference 2013	Advances in the GVL	Enis Afgan	Oslo, Norway	June
Melbourne Conversations	Science City: Has Melbourne got what it takes?	Peter Taylor	Victoria, Australia	June
International Supercomputing Conference	Communications in HPC	Helen Gardiner	Leipzig, Germany	June
IMB Winter School	Assembling NGS Data	Torsten Seemann	Queensland, Australia	July
Galaxy Community Conference 2013	A Galaxy of learning: Bioinformatics tutorials based on Galaxy	Simon Gladman	Oslo, Norway	July
Galaxy Community Conference 2013	BioBlend	Clare Sloggett	Oslo, Norway	July
EMBL Australia PhD Symposium	Molecular Simulation in Structural Biology	Michael Kuiper	Victoria, Australia	July
EMBL Australia PhD Symposium	Genome assembly	Torsten Seemann	Victoria, Australia	July
UoM CIS Doctoral Symposium	Life Sceinces Panel	Bernard Pope	Victoria, Australia	July
4th Workshop on Computational Modelling of Proteins & Membranes	Modelling in the age of high capacity computing	Michael Kuiper	Victoria, Australia	July
BOSC 2013	BioBlend	Clare Sloggett	Berlin, Germany	July
BOSC 2013	CloudMan+Hadoop+HTCondor	Enis Afgan	Berlin, Germany	July
BOSC 2013	Visualising RNA-Seq results with DGE-Viz	David Powell	Berlin. Germany	July
EuroSciPy 2013	Learn to segment n-dimensional images with GALA	Juan Nunez-Iglesias	Brussels, Belgium	August
RMIT Chemistry Lecture Series	Modelling proteins on ice	Michael Kuiper	Victoria, Australia	August
MHTP Seminar Series	Introduction to Bioinformatics	David Powell	Victoria, Australia	September
La Trog - Bundoora Genomics Group	RNAseq Project Design	Nathan Hall	Victoria, Australia	October
Molecules to Medicine Postdoctoral Program	Convergence of Software and Health	Michael Kuiper	Victoria, Australia	October
SPXXL SC13 Meeting	VLSCI Site Update	Chris Samuel	Denver, USA	November
Computer Science for High School Workshop	Secretly teaching the foundations of computing with steganography	Bernard Pope	Victoria, Australia	November

TRAINING WORKSHOPS

Refer Glossary (p.96) for all abbreviations used in all tables in this Report.

WORKSHOP TITLE	DATE	PRESENTER	ATTENDED	PARTICIPANTS' INSTITUTES
Movie Making for Molecular Modelling (3hr)	25 Jan	Michael Kuiper	5	VIDRL, SVI, MIPS
Using Unix effectively (3x3hr)	6 March 20 March 26 March	Bernard Pope	8 15 15	UoM, Monash, Deakin, WEHI, Peter Mac
Using Unix effectively	9 April	Bernard Pope	11	Peter Mac
Introduction to high performance computing at VLSCI (3hr)	17 April	Andrew Isaac Simon Wail Mark Nelson	14	UoM, WEHI, Monash, MCRI
Introduction to molecular modelling and visualisation for life sciences (3hr)	24 April	Michael Kuiper	15	RMIT, Monash, UoM, La Trobe
Variant Detection (Full day)	29 April	Charlotte Anderson Torsten Seemann Andrew Lonie	20	MCRI
Intermediate molecular modelling and visualisation for life sciences (3hr)	01 May	Michael Kuiper	15	La Trobe, Monash, RMIT, UoM
Introduction to molecular modelling and visualisation for life sciences (3hr)	14 May	Michael Kuiper	18	University of Melbourne MSc (Bioinformatics) students
Computational Modelling of Proteins & Membranes (1hr)	9 July	Michael Kuiper	80	National – participants of the 4th Workshop on Computational Modelling of Proteins & Membranes (at RMIT)
Python for Bioinformatics 1 (1.5hr)	14 August	Dieter Bulach Simon Gladman Torsten Seemann David Powell Bernard Pope	10	Monash
Python for Bioinformatics 2 (1.5hr)	21 August	Dieter Bulach Simon Gladman Torsten Seemann David Powell	8	Monash
Introduction to bacterial genomics (4hr)	28 August	Dieter Bulach Simon Gladman	20	Monash
Introduction to Bioinformatics (1hr)	10 September	David Powell	27	Monash Health Translation Precinct
Introduction to Galaxy (1hr)	11 September	Simon Gladman	10	School of Biological Sciences, Monash
Introduction to Galaxy Workflows – Intermediate Galaxy (1hr)	18 September	Simon Gladman	10	School of Biological Sciences, Monash
Python for Life Sciences (3hr)	26 September	Bernard Pope	20	COMBINE postgrads/early career researchers from UoM, WEHI, NICTA, Deakin
Introduction to Bacterial Genomics (4hr)	October	Dieter Bulach	35	Fukuoka University, Japan
Python for Bioinformatics 3 (1.5hr)	23 October	Dieter Bulach Simon Gladman Torsten Seemann David Powell	7	Monash
Programming Languages Workshop	4 December	Bernard Pope	50	UoM
Preliminary Analysis of RNAseq data (3hr)	5 December	Nathan Hall	12	La Trobe
Introduction to CLCbio (6hr)	10 December	Nathan Hall	20	La Trobe
Introduction to Galaxy & RNAseq analysis (3hr)	11 December	Simon Gladman Dieter Bulach Juan Nunez-Inglesias	26	Monash Central Clinical School
Melbourne Scala Users Group	Monthly	Bernard Pope	Varied	Varied

VLSCI **STAFF CONTRIBUTIONS** TO UNIVERSITY TEACHING

Refer Glossary (p.96) for all abbreviations used in all tables in this Report.

COURSE	YEAR LEVEL	FACULTY, UNIVERSITY	LECTURER/S
MSc(Bioinformatics)	Postgraduate	MGSS, UoM	Andrew Lonie (Coordinator) Michael Kuiper Dieter Bulach Torsten Seemann
Algorithms for Functional Genomics	Graduate / Postgraduate	Computing & Information Systems, UoM	Clare Sloggett (Coordinator in 2013) Bernard Pope Juan Nunez-Iglesias Gayle Philip David Powell Dieter Bulach Simon Gladman Torsten Seemann
Foundations of Computing	Undergraduate	Computing & Information Systems, UoM	Bernard Pope (Coordinator)
Introduction to Bioinformatics	Undergraduate	Medicine, Nursing & Health Sciences, Monash	Dieter Bulach
Genetics (GEN3EEG & GEN3HMG)	Undergraduate	La Trobe	Nathan Hall
Computational Fluid Dynamics (ENGR0024)	Graduate/Postgraduate	Engineering, UoM	Steve Moore (IBM)
Applied High Performance Computing (MCEN90031)	Graduate/Postgraduate	Engineering, UoM	Steve Moore (IBM)
Parallel and Multicore Computing (COMP90025)	Graduate/Postgraduate	CIS, UoM	John Wagner (IBM)
Neural Information Processing (BMEN90002)	Graduate/Postgraduate	Engineering, UoM	John Wagner (IBM)

CONFERENCE AND **TRAVEL GRANTS**

Refer Glossary (p.96) for all abbreviations used in all tables in this Report.

GRANT RECIPIENT	POSITION	INSTITUTION	DESTINATION
Lee Yeoh	Postgraduate student	Bio21/UoM	EBI-Wellcome Trust Summer School in Bioinformatics, England, Wellcome Trust Sanger Institute, University of Glasgow
Arun Konagurthu	Snr Lecturer	Monash	ISMB2013 and 3D-SIG2013, Germany
James Collier	Postgraduate student	Monash	ISMB2013, 3D-SIG2013, and Student Council Symposium Germany
Yousef Kowsar	Postgraduate student	UoM	MIPRO 2013 Conference, Croatia
Patrick Charchar	Postgraduate student	RMIT	ONETEP Masterclass workshop, University of Cambridge, UK
Nina Erfanian Saeedi	Postgraduate student	UoM	Conference on Implantable Auditory Prostheses, California, USA
Bernd Merkel	Postgraduate student	UoM	ISMRM Conference, SLC, USA
Cyrus Keong	Software Engineer	VeRSI	Winter School in Mathematical and Computational Biology, Brisbane
Jane Hawkey	Postgraduate student	UoM	Introduction to Phylogenetics Analysis Workshop, University of Sydney
Danielle Ingle	Postgraduate student	UoM	Introduction to Phylogenetics Analysis Workshop, University of Sydney
Andrew Lonsdale	Postgraduate student	UoM	European Conference on Computational Biology, Switzerland
Mahtab Mirmomeni	Postgraduate student	UoM	Genome Informatics 2013 & SC13, USA
Hernan Morales	Postgraduate student	Monash	BioInfoSummer 2013, Adelaide
Ashish Saini	Postgraduate student	Deakin	BioInfoSummer 2013, Adelaide
COMBINE representative	Postgraduate student	COMBINE	BioInfoSummer 2013, Adelaide

SPONSORSHIPS
AND CONFERENCES

Refer Glossary (p.96) for all abbreviations used in all tables in this Report.

DATE	ACTIVITY (LOCATION)	TYPE OF SPONSORSHIP	TOTAL PARTICIPANTS
30 January-1 February	International Brain Research Organisation/ Asia Pacific Regional Committee (IBRO/APRC) Advanced Computational Imaging Workshop *(Monash Biomedical Imaging)*	Fully funded accommodation and catering for students.	24 postgraduate students
9-13 February	38th Lorne Conference on Protein Structure and Function *(Mantra Lorne)*	Primary sponsor, attended with info booth to announced new VLSCI MM theme.	422
22 February	Sponsorship of the Victorian node of the International Neuroinformatics Coordinating Facility (INCF), including the Inaugural Neuroinformatics Launch/Workshop	Primary co-sponsor of INCF over 3 years, including sponsorship of international guest speaker at Launch/Workshop.	75
29 April	Graeme Clark Oration activities *(Melbourne Convention and Exhibition Centre)*	Sponsored event, hosted a group of UROP students at Oration and Oration Dinner.	1800 Oration attendees, 600 Dinner attendees
1-2 June	GovHack	Provided Prize.	900 nationally
8 July	Computing & Information Systems Doctoral Symposium *(University of Melbourne)*	Provided/Awarded Prizes.	130
10 July	UROP Conference Day *(Monash University)*	In addition to ongoing UROP sponsorship, provided a prize for Best Computational Biology Presentation. Of the 4 staff attending the event, including participating in the judging panel.	100 attendees 27 presenters
11 July	12th Melbourne Protein Group Student Symposium *(LIMS, La Trobe University)*	Sponsored program of careers talks.	150 attendees from 29 universities, research institutes and companies
20-24 October	eResearch Australasia *(Brisbane)*	Information booth, 4 staff attended.	450 delegates
25-27 October	HealthHack *(Thoughtworks, Melbourne)*	Provided prizes.	50 participants including researchers, software developers
30 October	Personalised Medicine dinner presentation, Knowledge Week event *(William Angliss Institute)*	Organised and funded event.	50 public 15 researchers
30 October	SOBR Student Brain Symposium 2013 *(Monash Institute of Pharmaceutical Sciences)*	Provided monetary support, and sponsored Best Computational Imaging Poster prize.	181
4-5 November	Biochemists And Molecular Biologists Bio21 Institute Graduate Retreat *(Bio21 Institute)*	Provided canvas bags.	80
13 November	PC4G – Programming Challenge for Girls *(UoM)*	Sponsored catering for female high school students, staff member lectured/tutored.	22 students from 7 schools
24-27 November	Australian Society for Biophysics Conference *(RMIT)*	Covered travel expenses for international guest speaker.	167
27 November	Metagenomics@Melbourne Symposium *(Bio21 Institute)*	Sponsored event, provided VLSCI information booth.	192 registrants from hospitals, government agencies, universities.
28 November-1 December	4th Australasian Cognitive Neuroscience Conference *(Monash University)*	Best PhD Student Oral Presentation in Computational Neuroscience.	267 registrants from 50 national/international research institutes & organisations.






Ms Helen Gardiner
Communications and Development Manager

SCIENCE STORY 10

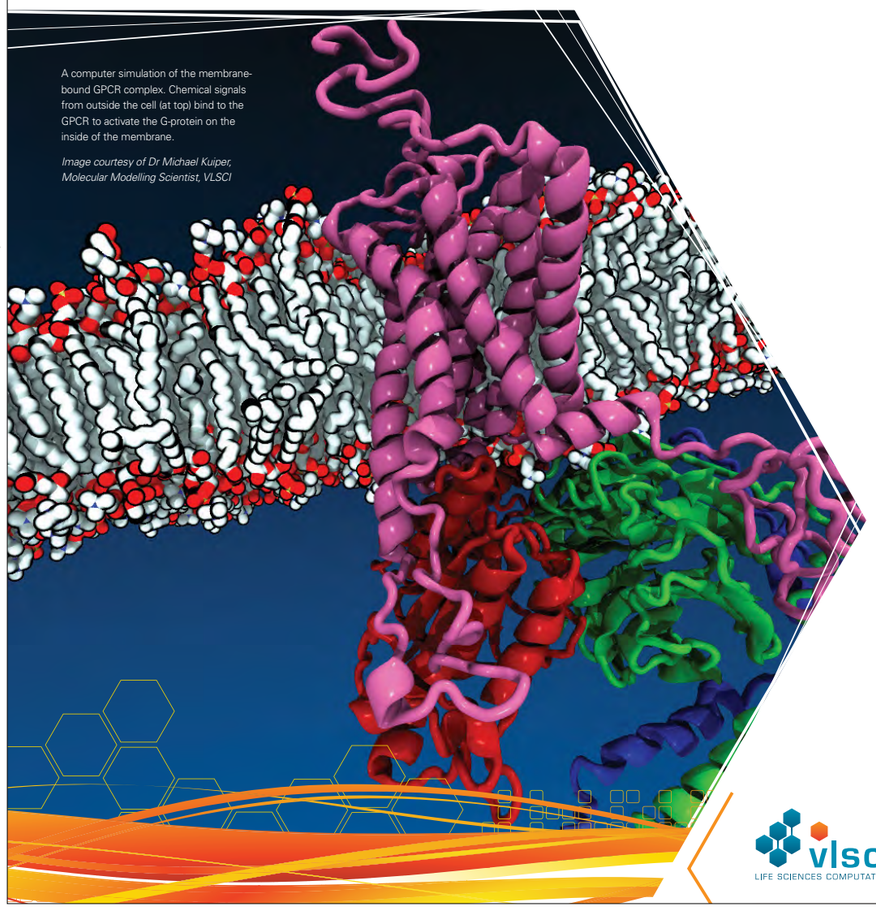
Continuing our Science Story Series (refer Current Research on the VLSCI website for the entire series)

VLSCI SCIENCE STORY 10

UNDERSTANDING DRUG INTERACTIONS AT THE MOLECULAR LEVEL

Almost half of the currently available medicines act on a single group of molecules - G protein-coupled receptors (GPCRs), which can trigger cellular responses to a wide range of ailments such as heart disease, infections, respiratory disorders, digestive and other conditions. New drugs are predicted to emerge from a deeper understanding of GPCRs at the molecular level. The race is on.

Tim Thwaites, Science Writer



A computer simulation of the membrane-bound GPCR complex. Chemical signals from outside the cell (at top) bind to the GPCR to activate the G-protein on the inside of the membrane.

Image courtesy of Dr Michael Kuiper, Molecular Modelling Scientist, VLSCI

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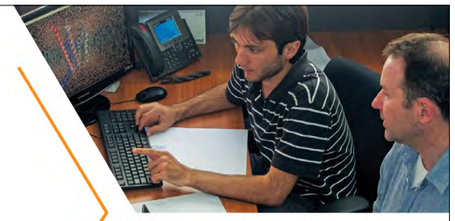
LIFE SCIENCES COMPUTATION

"These computer simulations to test different docking models used to take six weeks – now they take a couple of days."



Dr Thomas Coudrat (left) is a Post Doctoral Fellow who has come from France to join Professor Sexton's group in Melbourne to carry out the complex computational modelling work for this project. He is seen here getting advice from Dr Michael Kuiper, VLSCI's Molecular Modelling Scientist.
Image credit: VLSCI

Monash University researchers are using the unique number-crunching power of supercomputers to look at aspects of GPCRs in a way that would have been unimaginable even a few years ago. And the research has attracted the interest of the large European pharmaceutical group, Servier.

The body's capacity to adapt to environmental conditions such as heat and cold are well understood at the physiological level – shivering heats up the muscles, sweating cools them down. That is Biology 101. But what happens at the cellular level is less obvious: how is information about the external environment transmitted to the cells to trigger a response that can adapt the whole body to the ambient temperature? The story of how this is done, and the role played by this large and complex class of proteins (GPCRs) formed the substance of the 2012 Nobel Prize for Chemistry. GPCRs form a communication link between the external and internal environment of cells and as such are targets of nearly 50% of current pharmaceuticals. Drugs outside the cell can act on GPCRs sitting within the membrane to stimulate internal cellular responses and treat many common health complaints.

What makes the development of new drugs difficult is getting that ground level understanding of these proteins is hard, due to their complex crystal structure. GPCRs are made up of a set of seven linked helices each of which spans the cellular membrane and this complexity has meant that most of the thousands of GCPRs encoded by the human genome have remained a mystery.

A research group at the Monash Institute of Pharmaceutical Sciences (MIPS) in Parkville, advised by 2012 Nobel Laureate Professor Brian Kobilka who won the Prize for his work in GPCRs, is using the supercomputing resources of the Victorian Life Sciences Computation Initiative (VLSCI) to expand our knowledge of these complex molecules and their interactions.

"We're hoping to create predictive models of GPCRs which allow us to understand how certain ligands (binding molecules) bind to them," says Professor Patrick Sexton, leader of the Drug Discovery Biology group at MIPS. "That could allow us to predict other ligands that might bind, and possibly to pick out new drug leads."

Building and testing those models demands a lot of computer power. Previously, running computer simulations to test different docking models could take six weeks – now with the VLSCI supercomputers, this computing time has been slashed to a couple of days. All of this work has not gone unnoticed. In 2012, MIPS signed a significant agreement with Les Laboratoires Servier, to collaborate on GPCRs research. The agreement provides researchers with access to substantial funding and resources, while allowing them to apply their expertise to identify novel GPCRs targets and design new ligands to modify the activity of drugs already of interest to the company.

Prof. Patrick Sexton, Theme Leader, Drug Discovery Biology, Professor of Pharmacology, Monash Institute of Pharmaceutical Sciences (MIPS)
Image credit: MIPS

For further information about this research contact Professor Patrick Sexton at patrick.sexton@med.monash.edu.au.

To contact VLSCI go to www.vlsci.org.au

This article first appeared in the October 2013 edition of Australasian Biotechnology.

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LIFE SCIENCES COMPUTATION

ACTIVE PROJECTS IN 2013

All projects allocated resources through the Research Allocation Scheme Committee process which were active in 2013 are listed here (refer Current Research on the VLSCI website for exact dates for each)

Refer Glossary (p.96) for all abbreviations used in all tables in this Report.

NO.	PROJECT TITLE	CHIEF INVESTIGATORS	INSTITUTE	VLSCI SERVICE UNITS
ROUND 5				
VR0069	Examination of the Specific Mechanisms of Vaccine-Derived Poliovirus Antiviral Drug Interactions	Mr Jason Roberts Dr Bruce Thorley Dr Andrew Hung	VIDRL VIDRL RMIT	2400000
	PRESENTATIONS	**PUBLICATIONS**		
	Roberts, J. A., Supercomputer Simulation of Viruses, The Merging of Art and Science, Institute of Medical and Biological Illustrators, "Illuminate" biennial conference., Australia. Roberts, J. H., Molecular Dynamics Simulation of Viruses, RMIT University, 4th Workshop On Computational Modelling of Proteins and Membranes., Australia. Roberts, J. H., Refinement of the wild poliovirus capsid structure by atomistic molecular dynamics simulation of a complete virion., CSIRO Computational and Simulation Sciences and eResearch Annual Conference., Australia. Roberts, J. H., Supercomputer Simulation of Newly Discovered and Novel Enteroviruses., Australian Institute for Bioengineering and Nanotechnology Special Seminar, Australia. Roberts, J. H., Atomistic Molecular Dynamics Simulation of Viruses, RMIT University invited lectures, Australia.	Four publications currently in preparation.		
VR0148	High-resolution electron microscopy studies of the insulin and insulin-like growth factor receptor	A/Prof. Michael Lawrence	WEHI	1600000
VR0212	Calculating Climatic Constraints on Animals	Dr Michael Kearney	UoM	400000
	PRESENTATIONS	**PUBLICATIONS**		
	Kearney, M. R., The Thermodynamic Niches of Tropical Ectotherms, The Biological Impacts of Tropical Climate Warming for Ectothermic Animals, Puerto Rico. Kearney, M. R., The Thermodynamic Niche – physiologically based models of climatic constraints on animals, Invited Departmental Seminar, The University of Otago, New Zealand. Kearney, M. R., The Thermodynamic Niche – physiologically based models of climatic constraints on animals, (Plenary) - The International Biogeography Society Early Career Conference, Australia.	Kearney, M. R., Isaac, A. P. & Porter, W. P., microclim: Global estimates of hourly microclimate based on long-term monthly climate averages, (in preparation). Kearney, M. R., Isaac, A. P. Porter, W. P. & Huey, R. B., Body size constraints on the ability of lizards to go out in the midday sun, (in preparation). Kearney, M. R., Activity restriction and the mechanistic basis for extinctions under climate warming, Ecology Letters. Mitchell, N., Hipsey, M. R., Arnall, S., McGrath, G., Bin Tareque, H., Kuchling, G., Vogwill, R., Sivapalan, M., Porter, W. P. & Kearney, M. R., Linking eco-energetics and eco-hydrology to select sites for the assisted colonisation of Australia's rarest reptile, Biology.		

NO.	PROJECT TITLE	CHIEF INVESTIGATORS	INSTITUTE	VLSCI SERVICE UNITS
VR0224	Enabling Next Generation Drug Screening	Prof. Stan Skafidas Dr Stefan Harrer Dr Ross Bathgate Dr Daniel Scott Dr John Wagner	UoM IBM Florey Florey IBM	1750000
	PRESENTATIONS	**PUBLICATIONS**		
	Kannam, S. K., Downton, M. T., Gunn, N., Kim, S. C., Rogers, P. R., Schieber, C.,Baldauf, J. S., Wagner, J. M., Scott, D., Bathgate, R., Skafidas, S. & Harrer, S., Nanosensors for next generation drug screening, SPIE Micro+ Nano Materials, Devices, and Applications, Australia.	Sridhar, K., Kim, S. C., Rogers, P., Gunn, N., Wagner, J., Harrer, S. & Downton, M., Sensing of protein molecules through nanopores: A molecular dynamics study, Nanotechnology. Kim, S. C., Kannam, S. K., Harrer, S., Downton, M. T., Moore, S. & Wagner, J. M., Geometric dependence of the conductance drop in a nanopore due to a particle, Physical Review E.		
VR0225	Molecular modelling of plasma albumin for development of brain drug delivery	Prof. Norman Saunders	UoM	2000800
	PRESENTATIONS	**PUBLICATIONS**		
	Saunders, N. R., Barrier mechanisms in the developing brain, University Da Minho, Portugal. Saunders, N. R., Dziegierleska, K. M., Koehn, L. & Kuiper, M., Transport Mechanisms in the developing choroid plexus, Cerebrovascular Biology 2013, Canada. Saunders, N. R., Transport mechanisms in the developing choroid plexus, University of Bern, Switzerland.	Kuiper, M., Boding, J. & Koehn, L., 3-dimensional modelling of potential choroid plexus transport proteins, Frontiers in Neuroscience, (in preparation).		
ROUND 6				
VR0001	Structural dynamics of myxoma virus peptide for cancer therapy	Dr Alexe Bojovschi Dr Elena Pirogova	RMIT RMIT	40000
VR0003	Computational Neuroscience: Modelling the brain at microscopic, mesoscopic and macroscopic levels	A/Prof. David Grayden Prof. Anthony Burkitt Prof. Dragan Nesic A/Prof. Leigh Johnston Prof. Mark Cook	UoM UoM UoM UoM UoM	990000
	PRESENTATIONS	**PUBLICATIONS**		
	Spencer, J., McLachlan, N. M. & Grayden, D., A computational model of sound recognition used to analyze the capacity and adaptability in learning vowel classes, International Symposium on Auditory and Audiological Research 2013, Denmark. Erfanian Saeedi, N., Blamey, P., Burkitt, A. N., & Grayden, D. B., Model-based evaluation of speech processing strategies in pitch discrimination tasks, Conference on Implantable Auditory Prostheses 2014, USA.	Erfanian Saeedi, N., Blamey, P. Burkitt, A. N. & Grayden, D.B., Application of a pitch perception model to investigate the effect of stimulation field spread on the pitch ranking abilities of cochlear implant recipients, Hearing Research, (in preparation). Spencer, J., McLachlan, N. M. & Grayden, D., Neurobiologically Inspired Computational Model of Auditory Recognition Mechanisms, (in preparation). Kuhlmann, L., Hauser-Raspe, M., Manton, J. H., Grayden, D. B., Tapson, J. & van Schaik, A., Approximate, Computationally Efficient Online Learning in Bayesian Spiking Neurons, Neural Computation. Kerr, R., Burkitt, A. N., Thomas D, A., Gilson M & Grayden D. B., Delay selection by spike-timing-dependent plasticity in recurrent networks of spiking neurons receiving oscillatory inputs, PLOS Computational Biology. Kerr, R. R., Grayden, D. B., Thomas D. A., Gilson, M. & Burkitt, A. N., Coexistence of reward and unsupervised learning during the operant conditioning of neural firing rates, PLOS ONE.		

NO.	PROJECT TITLE	CHIEF INVESTIGATORS	INSTITUTE	VLSCI SERVICE UNITS
VR0004	Computational Drug Formulation	Dr David Chalmers Prof. Colin Pouton	Monash Monash	2400000

PRESENTATIONS

Birru, W. A., Warren, D. B., Benameur, H., Porter, C. J. H., Pouton, C. W. & Chalmers, D. K., Phase Behaviour of POPC and Lyso PC With Bile Salt Using Molecular Dynamics Simulations.

Birru, W. A., Warren, D. B., Williams, H. D., Benameur, H., Porter, C. J. H., Pouton, C. W. & Chalmers, D. K., Phase behaviour of digested and undigested phospholipids and bile salt in blank simulated intestinal fluids.

PUBLICATIONS

Warren, D. B., King, D., Benameur, H., Pouton, C. W. & Chalmers, D. K., Glyceride lipid formulations: molecular dynamics modelling of phase behavior during dispersion and molecular interactions between drugs and excipients, Pharmaceutical Research.

NO.	PROJECT TITLE	CHIEF INVESTIGATORS	INSTITUTE	VLSCI SERVICE UNITS
VR0007	Parasite Genomics and Genetics Program	Prof. Robin Gasser	UoM	432000

PUBLICATIONS

Jex, A. R., Liu, S., Li, B., Young, N. D., Hall, R.S., Li, Y., Yang, L., Zeng, N., Xu, X., Xiong, Z., Chen, F., Wu, X., Zhang, G., Fang, X., Kang, Y., Anderson, G.A., Harris, T., Campbell, B.E., Vlaminck, J., Wang, T., Cantacessi, C., Schwarz, E.M., Ranganathan, S., Geldhof, P., Nejsum, P., Sternberg, P.W., Yang, H., Wang, J., Wang, J. & Gasser, R.B., *Ascaris suum* draft genome, Nature.

Young, N.D., Jex A.R., Li, B., Liu, S., Yang, L., Xiong, Z., Li, Y., Cantacessi, C., Hall, R.S., Xu, X., Chen, F., Wu, X., Zerlotini, A., Oliveira, G., Hofmann, A., Zhang, G., Fang, X., Kang, Y., Campbell, B. E., Loukas, A., Ranganathan, S., Rollinson, D., Rinaldi, G., Brindley, P.J., Yang, H.M., Wang, J., Wang, J. & Gasser, R.B., Whole-genome sequence of *Schistosoma haematobium*, Nature Genetics.

Tang, Y. T., Gao, X., Rosa, B. A., Abubucker, S., Hallsworth-Pepin, K., Martin, J., Tyagi, R., Heizer, E., Zhang, X., Bhonagiri-Palsikar, V., Minx, P., Warren, W. C., Wang, Q., Zhan, B., Hotez, P. J., Sternberg, P. W., Dougall, A., Torres-Gaze, S., Mukvenna, J., Sotillo, J., Ranganathan, S., Rabelo, E. M., Wilson, R. K., Felgner, P. L., Bethony, J., Hawdon, J. M., Gasser, R. B., Loukas, A. & Mitreva, M., Genome of the human hookworm *Necator americanus*, Nature Genetics.

NO.	PROJECT TITLE	CHIEF INVESTIGATORS	INSTITUTE	VLSCI SERVICE UNITS
VR0009	Toxin Binding to Membrane Proteins: Towards Novel Treatments in Neuropathology	Dr Andrew Hung Prof. David Adams	RMIT RMIT	1600000

PRESENTATIONS

Kompella, S. N., Hung, A., Clark, R. J., David J. & Adams, D. J., alpha-Conotoxin RegIIA targeting nAChRs: mutagenesis studies improving selectivity and potency, Biophysical Society Meeting, USA.

van Lierop, B. J., Robinson, S. D., Kompella, S. N., McArthur, J. R., Hung, A., MacRaild, C. A., Adams, D. J., Norton, R. S. & Robinson, A. J. , Dicarba alpha-Conotoxin Vc1.1 Analogues with Differential Selectivity for Nicotinic Acetylcholine and GABAB Receptors, Lorne Protein Conference, Australia.

PUBLICATIONS

Grishin, A. A., Cuny, H., Hung, A., Clark, R. J., Brust, A., Akondi, K., Alewood, P. F., Craik, D. J. & Adams, D. J., Identifying Key Amino Acid Residues that Affect alpha-Conotoxin AuIB Inhibition of alpha3alpha4 Nicotinic Acetylcholine Receptors, Journal of Biological Chemistry.

van Lierop, B. J., Robinson, S. D., Kompella, S. N., Belgi, A., McArthur, J. R., Hung, A., MacRaild, C. A., Adams, D. J., Norton, R. S. & Robinson, A. J., Dicarba alpha-Conotoxin Vc1.1 Analogues with Differential Selectivity for Nicotinic Acetylcholine and GABAB Receptors, ACS Chemical Biology.

Kompella, S. N., Hung, A., Clark, R. J., Mari, F. & Adams, D. J., alpha-Conotoxin RegIIA targeting nAChRs: mutagenesis studies improving selectivity and potency, Journal of Biological Chemistry.

Suresh, A., Adams, D. & Hung, A., Molecular basis of conotoxin selectivity for neuronal nAChR subtypes - simulation studies, (in preparation).

NO.	PROJECT TITLE	CHIEF INVESTIGATORS	INSTITUTE	VLSCI SERVICE UNITS
VR0010	Mesoscopic Simulation Of Cell Transport and Cell Adhesion In Hydrodynamic Flow	Dr Ravi Jagadeeshan	Monash	200000

PRESENTATIONS

Sasmal, C., Mehrotra, A., Patricia, S., Duenweg, B., Prabhakar, R. & Prakash, J. R., Optimization of the Smooth Particle Mesh Ewald (SPME) Algorithm for Treating Long-ranged Hydrodynamic and Electrostatic Interactions, Proc. 6th Pacific Rim Conference on Rheology, Australia.

Ramesh, K. V., Prabhakar, R., Prakash, J. R., & Thaokar, R. M., Significance of thermal fluctuations in receptor-ligand mediated micro-particle adhesion, International conference on Discrete simulation of fluid dynamics, India.

Ramesh, K. V., Prabhakar, R., Prakash, J. R. & Thaokar, R. M., Significance of thermal fluctuations in receptor-ligand mediated micro-particle adhesion, Fluid Structure Interactions in Soft Matter Systems, Italy.

Jain, A., Hartkamp, R., Sasmal, C., Mehrotra, A. S., Todd, B. D., Prabhakar, R. & Prakash J. R., Brownian dynamics simulations of semidilute polymer solutions undergoing planar mixed flow, The Society of Rheology, 85th Annual Meeting, Canada.

PUBLICATIONS

Ramesh, K. V., Prabhakar, R., Prakash, J. R. & Thaokar R. M., Significance of thermal fluctuations in receptor-ligand mediated micro-particle adhesion, (in preparation).

Jain, A., Hartkamp, R., Sasmal, C., Mehrotra, A. S., Todd, B. D., Prabhakar, R. & Prakash, J. R., Brownian dynamics simulations of semidilute polymer solutions undergoing planar mixed flow, (in preparation).

Soysa, W. C., Duenweg, B. & Prakash, J. R., Static and Dynamic properties of dilute salt free polyelectrolyte solutions, (in preparation).

Jain, A., Sunthar, P., Dünweg B. & Prakash, J. R., Optimization of a Brownian dynamics algorithm for semidilute polymer solutions, (in preparation).

Jain, A., Duenweg, B. & Prakash, J. R., Dynamic crossover scaling in polymer solutions, Physical Review Letters.

NO.	PROJECT TITLE	CHIEF INVESTIGATORS	INSTITUTE	VLSCI SERVICE UNITS
VR0011	A Multi-Scale Quantitative Kidney Model	Dr Edmund Kazmierczak Dr Linda Stern	UoM UoM	10000

PRESENTATIONS

Gale, T., A network model of a whole kidney, Doctoral Colloquium, University of Melbourne, Australia.

Gale, T., Generating the Arterial Structure of a Rat Kidney, Doctoral Colloquium Bioengineering, University of Melbourne, Australia.

PUBLICATIONS

Gale, T., Kazmierczak, E. & Stern, L., Generating the Arterial Structure of a Rat Kidney, (in preparation).

NO.	PROJECT TITLE	CHIEF INVESTIGATORS	INSTITUTE	VLSCI SERVICE UNITS
VR0018	A Computational Model for Heat Transfer and Blood Flow through Multi-Stenosis Arteries	Prof. Andrew Ooi Prof. Hugh M Blackburn	UoM Monash	1600000

PUBLICATIONS

Saha, S., Klewicki, J. C., Ooi, A. & Blackburn, H. M., Scaling properties of pipe flows with sinusoidal transversely-corrugated walls, (in preparation).

Saha, S., Klewicki, J. C., Ooi, A. & Blackburn, H. M., Comparison of thermal scaling properties between turbulent pipe and channel flows via DNS, (in preparation).

Saha, S., Klewicki, J., Ooi, A., Blackburn, A. & Wei, T., Scaling properties of the equation for passive scalar transport in wall-bounded turbulent flows, International Journal of Heat and Mass Transfer.

NO.	PROJECT TITLE	CHIEF INVESTIGATORS	INSTITUTE	VLSCI SERVICE UNITS
VR0021	Modelling pore-forming toxins	Prof. Michael Parker	SVI	4400400

PRESENTATIONS

Parker, M. W., Membrane pores – twists and turns, 2nd Membrane Protein Symposium, Academia Sinica, Taiwan.

PUBLICATIONS

Feil, S. C., Ascher, D. B., Kuiper, M. J., Tweeten, R. K. & Parker, M. W., Structural Studies of Steptococcus pyogenes Streptolysin O provide Insights into the early steps of membrane penetration, Journal of Molecular Biology.

NO.	PROJECT TITLE	CHIEF INVESTIGATORS	INSTITUTE	VLSCI SERVICE UNITS
VR0023	Shear induced platelet aggregation: characterising shear forces in in-vitro geometries.	Dr Kris Ryan Dr Josie Carberry	Monash Monash	3215000

PRESENTATIONS

Arthur, J. F., Pinar, I., Facey, A., Fouras, A., Ryan, K., Andrews, R. K., Carberry, J. & Gardiner, E. E., Medicine Meets Mathematics: Measuring ADAM10 Activity Directly on a Forming Thrombus, American Society of Hematology 2013, USA.

PUBLICATIONS

Arthur, J.F., Pinar, I., Facey, A., Fouras, A., Ryan, K., Andrews, R. K., Carberry, J. & Gardiner E. E., Medicine Meets Mathematics: Measuring ADAM10 Activity Directly on a Forming Thrombus, Blood.

Pinar, I., Arthur, J., Andrews, R., Gardiner, E., Carberry, J. & Ryan, K., Pulsatilty effects on shear dependent thrombus growth, (in preparation).

NO.	PROJECT TITLE	CHIEF INVESTIGATORS	INSTITUTE	VLSCI SERVICE UNITS
VR0024	Computational Modelling of G protein-coupled receptors	Prof. Patrick Sexton Prof. Arthur Christopoulos	Monash Monash	1500000

PRESENTATIONS

Sexton, P. & Wootten, D., The molecular control of ligand-biased signalling at Family B GPCRs, GPCR workshop, Hawaii, USA.

Christopoulos, A., Recent mechanistic insight into GPCR allostery, GPCR Workshop, Hawaii, USA.

Coudrat, T., Wootten, D. & Sexton, P. M., Modelling of G Protein-Coupled Receptor (GPCR): method evaluation, Drug Discovery Biology (DDB) annual student symposium, Australia.

PUBLICATIONS

Wootten, D., Simms, J., Miller, L. J., Christopoulos, A. & Sexton, P. M., Polar transmembrane interactions drive formation of ligand-specific and signal pathway-biased family B G protein-coupled receptor conformations., Proceedings of the National Academy of Sciences of the USA.

Abdul-Ridha, A., Oacutepez L., Keov P., Thal D. M., Mistry, S. N., Sexton, P. M., Lane, J. R., Canals, M. & Christopoulos, A., Molecular Determinants of Allosteric Modulation at the M1 Muscarinic Acetylcholine Receptor, Journal of Biological Chemistry.

NO.	PROJECT TITLE	CHIEF INVESTIGATORS	INSTITUTE	VLSCI SERVICE UNITS
VR0025	Exploiting unique mechanical responses of cells for disease diagnosis and management	Dr Gregory Sheard	Monash	320000

PRESENTATIONS

Vo, T., Sheard, G. & Montabone, L., How barotropic and stable are differential-rotation cylindrical flows, APS-DFD13, November 2013, USA.

Sheard, G. J., Tsai, T. K., Hussam, W. K., Wong, K. Y. & King, M. P., Heat transfer and stability of horizontal convection with a moving forcing boundary, APS-DFD13, November 2013, USA.

Tsai, T. K., Hussam, W. K. & Sheard, G. J., Stability of horizontal convection with different temperature profiles, 8th Australasian Natural Convection Workshop, Sydney, Australia.

Hussam, W. K., Tsai, T. K. & Sheard, G .J., Horizontal convection in a rotating cylinder, 8th Australasian Natural Convection Workshop, Sydney, Australia.

PUBLICATIONS

Henon, Y. N., Sheard, G. J. & Fouras, A., Erythrocyte deformation in a microfluidic cross-slot channel, (in preparation).

Hussam, W. K., Tsai, T. K. & Sheard, G. J., Radial horizontal convection in a rotating cylindrical container, (in preparation).

Sheard, G. J. & King, M. P., Forced and free convection regimes in horizontal convection with mechanical forcing, (in preparation).

Tsai, T. K., Hussam, W. K. & Sheard, G. J., Stability of horizontal convection driven by imposed temperature profile, (in preparation).

Henon, Y. N., Sheard, G. J. & Fouras, A., Effect of erythrocyte membrane stiffness on the distribution of cells in microchannel flows, (in preparation).

Hussam, W. K. & Sheard, G. J., Heat transfer in a high Hartmann number MHD duct flow with a circular cylinder placed near the heated side-wall, International Journal of Heat and Mass Transfer.

NO.	PROJECT TITLE	CHIEF INVESTIGATORS	INSTITUTE	VLSCI SERVICE UNITS
VR0028	Protein self-assembly on surfaces, interfaces and nanoparticles	Dr Nevena Todorova Prof. Irene Yarovsky	RMIT RMIT	840000

PRESENTATIONS

Todorova, N., Chiappini, C., Mager, M., Simona, B., Stevens, M. M. & 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, ICONN2014, Australia.

Todorova, N., Chiappini, C., Mager, M., Simona, B., Stevens, M. M. & Yarovsky, I., Functional peptides structure and surface presentation regulates cell internalisation of TAT conjugated nanoparticles, Nanobionics Symposium, Australia.

PUBLICATIONS

Todorova, N., Chiappini, C., Mager, M., Simona, B., Stevens, M. M. & Yarovsky, I., Surface presentation of functional peptides determines cell internalization efficiency of TAT conjugated nanoparticles, (in preparation).

Andresen, H., Mager, M., Grießner, M., Charchar, P., Todorova, N., Bell, N., Theocharidis, G., Bertazzo, S., Yarovsky, I. & Stevens, M. M., Single-step immunoassays utilising epitope-tagged gold nanoparticles: On the mechanism, feasibility, and limitations..., (in preparation).

Todorova, N., Makarucha, A. J., Hine, N. D. M., Mostofi, A. A. & Yarovsky, I., Dimensionality of Carbon Nanomaterials Determines the Binding and Dynamics of Amyloidogenic Peptides: Multiscale Theoretical Simulations, PLOS Computational Biology.

Todorova, N., Yeung, L., Hung, A. & Yarovsky, I., Janus Cyclic Peptides: A New Approach to Amyloid Fibril Inhibition?, PLOS ONE.

NO.	PROJECT TITLE	CHIEF INVESTIGATORS	INSTITUTE	VLSCI SERVICE UNITS
VR0030	Development of Molecular Dynamics Drug Docking	Dr Michael Kuiper A/Prof. Matthew Wilce	VLSCI Monash	3000800

PRESENTATIONS

Kuiper, M., Molecular modelling in the age of high capacity computing, RMIT 4th Workshop on Computational Modelling of Proteins & Membranes.

Kuiper, M., Molecular Modelling & Visualisation training courses (Introduction and Intermediate), VLSCI.

Kuiper, M., Advanced modelling training course, VLSCI.

NO.	PROJECT TITLE	CHIEF INVESTIGATORS	INSTITUTE	VLSCI SERVICE UNITS
VR0031	In silico modelling of protein dynamics and drug design	Dr David Wilson	La Trobe	2900000

PRESENTATIONS

Buskes, M. J., Gilson, P. R., Crabb, B. S., Deady, L. W., Wilson, D. J. D. & Abbott, B. M., Investigation and development of novel PKA inhibitors as antimalarials: Modelling and synthesis of isoquinoline analogues, Frontiers in Med Chem, USA.

Buskes, M. J., Gilson, P. R., Crabb, B. S., Deady, L. W., Wilson, D. J. D. & Abbott, B. M., Development of Novel inhibitors of PKA, CRC Biomarker Translation Student Conference, Australia.

PUBLICATIONS

Buskes, M. J., Brzozowski, M., Oehme, D. P., Abbott, B. M. & Wilson, D. J. D., Assessment of solvation effect on MM-PB(GB)SA calculated binding free energies, (in preparation).

O'Brien, N. J., Brzozowski, M., Wilson, D. J. D., Deady, L. W. & Abbott, B. M., Synthesis of substituted 2-anilino-7H-deazapurines as potential PDK1 inhibitors, (in preparation).

Brzozowski, M., O'Brien, N. J., Wilson, D. J. D. & Abbott, B. M., Synthesis of substituted 4-(1H-indol-6-yl)-1H-indazoles as potential PDK1 inhibitors, Tetrahedron.

Oehme, D. P., Brownlee, R. T. C. & Wilson, D. J. D., Can cyclic HIV protease inhibitors bind in a non-preferred form? An ab initio, DFT and MM-PB(GB)SA study, Journal of Molecular Modelling.

NO.	PROJECT TITLE	CHIEF INVESTIGATORS	INSTITUTE	VLSCI SERVICE UNITS
VR0052	Modelling, testing and searching human vision	Dr Andrew Turpin	UoM	440000

PRESENTATIONS

McKendrick, A. M., What can vision tell us about cortical excitability in migraine?, 34th Australasian Neuroscience Society meeting 2014, Australia.

Chong, L., McKendrick, A. M. & Turpin, A., Automated stimulus choice in condensed grids for assessment of visual field defects, ARVO 2013, USA.

PUBLICATIONS

Dennis, J., Turpin, A. & McKendrick, A. M., Individualised Structure-Function Mapping for Glaucoma: Practical Constraints on Map Resolution for Clinical and Research Applications, Investigative Ophthalmology and Visual Science.

Chong, L., McKendrick, A. M. & Turpin, A., Automated stimuli placement in perimetry, Investigative Ophthalmology and Visual Science.

Dennis, J., Turpin, A. & 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.

Denniss, J., McKendrick, A.M. & Turpin, A., Towards patient-tailored perimetry: automated perimetry can be improved by seeding procedures with patient-specific structural information, Translational Vision Science and Technology.

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

VR0056	Neuroanatomical changes in childhood-onset epilepsy	Prof. Graeme Jackson Dr David Abbott	Florey Florey	56000

PUBLICATIONS

Pardoe, H. R., Berg, A. T., Archer, J. S., Fulbright, R. K. & Jackson, G. D., A neurodevelopmental basis for BECTS: Evidence from structural MRI, Epilepsy Research.

Pardoe, H. R, Berg, A. T & Jackson, G. D., Sodium valproate use is associated with reduced parietal lobe thickness and brain volume, Neurology.

Pardoe, H. R., Abbott, D. F., Jackson, G. D., Sample size estimates for well-powered cross-sectional cortical thickness studies, Human Brain Mapping.

VR0057	Direct Numerical Simulation of Newtonian and non Newtonian fluid in Wall-bounded Flow	Prof. Ivan Marusic	UoM	500000

PRESENTATIONS

Chin, C., Marusic, I. & Barlis, P., Direct Numerical Simulation of Newtonian and non-Newtonian fluid in constricted circular geometry, VLSCI Presentation Day, Australia.

PUBLICATIONS

Chin, C., Monty, J. P. & Ooi, A., Reynolds number effects in DNS of pipe flow and comparison with channels and boundary layers, International Journal of Heat and Fluid Flow.

VR0058	Dynamic characterization of biomolecular systems	Prof. Phoebe Chen	La Trobe	48000

PUBLICATIONS

Kalyaanamoorthy, S. & Chen, Y. P., Ligand release mechanisms and channels in histone deacetylases, Journal of Computational Chemistry.

Kalyaanamoorthy, S. & Chen, Y. P., Quantum polarized ligand docking investigation to understand the significance of protonation states in histone deacetylase inhibitors, Journal of Molecular Graphics and Modelling.

Kalyaanamoorthy, S. & Chen, Y. P., Energy based pharmacophore mapping of HDAC inhibitors against class I HDAC enzymes, Biochimica et Biophysica Acta-Proteins and Proteomics.

Kalyaanamoorthy, S. & Chen, Y. P., A steered molecular dynamics mediated hit discovery for histone deacetylases, Physical Chemistry Chemical Physics.

NO.	PROJECT TITLE	CHIEF INVESTIGATORS	INSTITUTE	VLSCI SERVICE UNITS
VR0062	Thalamocortical oscillations in epilepsy	Dr Evan Thomas Mr Jordan Chambers Dr David Abramson A/Prof. Steven Petrou	Florey UoM UQ Florey	415000
VR0063	Computational Studies of Prion Proteins to Reveal Secrets of Immunity to Prion Diseases	Dr Jiapu Zhang	FedUni	500000

PRESENTATIONS

Zhang, J., Mathematical optimization models of molecular structures in the unstructured region of prion proteins, Seminar Report, Chinese Agricultural University.

Zhang, J., Molecular Dynamics (MD), Quantum Mechanics / Molecular Mechanics (QMMM), and Molecular Modelling (MM) Studies of Prion Proteins and Prions, Seminar Report, Swinburne University of Technology.

Zhang, J., Computational studies of prion proteins to reveal secrets of immunity to prion diseases, Poster, VLSCI Presentation Day.

Zhang, J., Introduce prion diseases to school kids, and introduce the Lennard-Jones function to school kids, CSIRO Scientists In Schools Program, Ascot Vale School.

Zhang, J., An implication from the molecular structure principle for the anti-prion drug GN8, Medicinal Chemistry 2013, USA.

PUBLICATIONS

Zhang, J. et al., Molecular dynamics studies on the NMR and X-ray structures of rabbit prion protein wild-type and mutants, Journal of Theoretical Biology.

Zhang, J. et al., Molecular dynamics studies on 3D structures of the hydrophobic region PrP(109-136), Acta Biochimica et Biophysica Sinica (Shanghai).

Zhang, J., Recent advances in the immunity research of rabbits to prion diseases, Biochemistry & Pharmacology.

Zhang, J., A survey on the studies of rabbit prion proteins, Rabbits: Biology, Diet and Eating Habits and Disorders.

Zhang, J., Simulated annealing: in mathematical global optimization computations, hybrid with local or global search and practical applications in crystallography & molecular modelling of prion amyloid fibrils, Simulated Annealing: Strategies, Potential Uses and Advantages.

VR0064	Modelling of antifreeze proteins at the ice water interface	Dr Angus Gray-Weale Dr Michael Kuiper	UoM VLSCI	3200000

PRESENTATIONS

Kuiper, M. J., Antifreeze proteins, La Trobe University Chemistry Department Seminar.

Kuiper, M. J., Modelling in the age of High Capacity Computing, Royal Melbourne Hospital Departmental Seminar.

Kuiper, M. J., Modelling proteins on ice, RMIT Chemistry Seminar.

PUBLICATIONS

Kuiper, M. J., Elizabeth, S., Morton, C. & Gray-Weale, A, Molecular insights into the antifreeze mechanism, (in preparation).

VR0067	Project Overview Simulations of HIV reverse transcriptase	A/Prof. Gilda Tachedjian	Burnet	2000800
VR0069	Molecular Modelling of Novel Enterovirus Proteins Associated With Acute Flaccid Paralysis	Dr Jason Roberts Dr Andrew Hung Dr Bruce Thorley	VIDRL RMIT VIDRL	4800000

PRESENTATIONS

As reported in Round 5

VR0071	Understanding dynamic events at the immune synapse	A/Prof. Ashley Buckle	Monash	9000000

PRESENTATIONS

Buckle, A. M., Epitope Flexibility and Dynamic Footprint Revealed by Molecular Dynamics of a pMHC-TCR Complex, Coral Gables symposium on immunogenicity, USA.

Buckle, A. M., Understanding dynamic events at the immune synapse, Dept Chemistry seminar, University of Canterbury, New Zealand.

Kass, I., Investigating the 3D Structure of Proteins in 4D, Dept Biochemistry seminar, Hebrew University of Jerusalem, Israel.

PUBLICATIONS

Kass, I., Buckle, A. M. & Borg, N. A., A Molecular Simulation Based Approach To Understanding The Dynamics Of The Immune Synapse, (in preparation).

NO.	PROJECT TITLE	CHIEF INVESTIGATORS	INSTITUTE	VLSCI SERVICE UNITS
VR0082	Population genomics of bacterial pathogens	Dr Kathryn Holt Dr Matthias Reumann A/Prof. Tim Stinear	UoM IBM UoM	640000

PRESENTATIONS

Inouye, M. T., Dashnow, H., Raven, L., Pope, B. J., Schultz, M., Zobel, J. & Holt, K. E., Short read sequence typing: rapid analysis of genome data for public health labs, Molecular Microbiology Meeting, Australia.

Ingle, D., Phylogeny and virulence of atypical enteropathogenic Escherichia coli, Lorne Infection and Immunity, Australia.

PUBLICATIONS

Inouye, M. T., Dashnow, H., Raven, L., Pope, B. J., Schultz, M., Zobel, J. & Holt, K. E., Short read sequence typing: rapid analysis of genome data for public health labs, (in preparation).

Holt, K. E., Thieu Nga, T. V., Thanh, D. P., Vinh, H., Kim, D. W., Vu Tra, M. P., Campbell, J. I., Hoang, N. V., Vinh, N. T., Minh, P. V., Thuy, C. T., Nga, T. T., Thompson, C., Dung, T. T., Nhu, N. T., Vinh, P. V., Tuyet, P. T., Phuc, H. L., Lien, N. T., Phu, B. D., Ai, N. T., Tien, N. M., Dong, N., Parry, C. M., Hien, T. T., Farrar, J. J., Parkhill, J., Dougan, G., Thomson, N. R. & Baker, S., Tracking the establishment of local endemic populations of an emergent enteric pathogen, Proceedings of the National Academy of Sciences of the USA.

Howden, B. P., Holt, K. E., Lam, M. M., Seemann, T., Ballard, S., Coombs, G. W., Tong, S. Y., Grayson, M. L., Johnson, P. D. & Stinear, T. P., Genomic Insights to Control the Emergence of Vancomycin-Resistant Enterococci, mBio.

Hawkey, J. Edwards, D. J. Dimovski, K. Hiley, L. Billman-Jacobe, H. Hogg, G. Holt, K. E. Evidence of microevolution of Salmonella Typhimurium during a series of egg-associated outbreaks linked to a single chicken farm, BMC Genomics.

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 Methicillin Resistant Staphylococcus aureus, Genome Biol Evol.

VR0088	Investigation of de-novo assembly on massively parallel, distributed memory supercomputers	Prof. Justin Zobel Dr Matthias Reumann Dr Thomas Conway	UoM UoM UoM	23000

PRESENTATIONS

Mirmomeni, M., Resolving Ambiguity in Genome Assembly using High Performance Computing, Genome informatics conference, USA.

Mirmomeni, M., Resolving genome assembly ambiguity using HPC, Supercomputing conference, USA.

Mirmomeni, M., Conway, T., Reumann, M. & Zobel, J., Resolving ambiguity in genome assembly using High Performance Computing, Big data and healthcare analytics, Australia.

VR0089a	Dynamics and docking: DHDPS	A/Prof. Matthew Perugini Prof. Michael Parker Dr John Wagner	La Trobe SVI IBM	2008000

PRESENTATIONS

Wubben, J., Cold Enzymology Offers Insight into Evolution of Enzyme Quaternary Structure, Melbourne Protein Group, Australia.

Perugini, M. A., Multiple Personalities of a Pesticide Target from an Important Plant Pathogen, 21st International AUC Conference, Japan.

Perugini, M. A., From Molecular Evolution to Rational Inhibitor Design of a Promising Antibiotic Target, JSS University, India.

PUBLICATIONS

Atkinson, S. C., Dogovski, C., Downton, M. T., Czabotar, P. E., Dobson, R. C. J., Gerrard, J. A., Wagner, J. & Perugini, M. A., Structural, kinetic and computational investigation of Vitis vinifera DHDPS reveals new insight into the mechanism of lysine-mediated allosteric inhibition, Plant Molecular Biology.

Hor, L., Dobson, R. C. J., Downton, M. T., Wagner, J., Hutton, C. A. & Perugini, M. A., Dimerization of bacterial DAP epimerase is essential for catalysis, Journal of Biological Chemistry.

VR0089b	Dynamics and docking: mechanistic simulations of a viral capsid	Prof. Michael Parker Dr John Wagner	SVI IBM	4004000

NO.	PROJECT TITLE	CHIEF INVESTIGATORS	INSTITUTE	VLSCI SERVICE UNITS
VR0126	Complex Statistical Genome-Wide Association Studies Analyses Related Selected Cancer and Asthma	Prof. John Hopper Dr Matthias Reumann Dr Adam Kowalczyk Dr Daniel Schmidt Dr Enes Makalic A/Prof. Gianluca Severi Dr Guoqi Qian Dr John Wagner Prof. Justin Zobel Dr Michael Inouye	UoM IBM UoM UoM UoM UoM UoM IBM UoM UoM	20030000

PRESENTATIONS

Reumann, M. et. al., Supercomputing enabling exhaustive statistical analysis of genome wide association study data: Preliminary results, Conf Proc IEEE Eng Med Biol Soc, .

Makalic, E., Schmidt, D. & Hopper, J., DEPendence of associations on the number of Top Hits (DEPTH), 26th Australasian Joint Conference on Artificial Intelligence, New Zealand.

Makalic, E., Schmidt, D. & Hopper, J., DEPendence of associations on the number of Top Hits (DEPTH), Invited presentation at the Alfred Hospital for VicBiostats, Australia.

Makalic, E., Schmidt, D. & Hopper, J., Supercomputing and Genomics of Breast Cancer, MENDEL Short Course, Australia.

Hopper, J., DEPendence of associations on the number of Top Hits (DEPTH), VLSCI RAS Symposium, Australia.

Hopper, J., Supercomputing and Genomics of Breast Cancer, Seoul National University, South Korea.

PUBLICATIONS

Goudey, B., Abedini, M., Hopper, J. L., Inouye, M., Makalic, E., Schmidt, D. F. Wagner, J., Zhou, Z., Zobel, J. & Reumann, M., High performance computing enabling exhaustive analysis of higher order single nucleotide polymorphism interaction in Genome Wide Association Studies, (in preparation).

VR0127	Computational studies in beta-sheet folding	Prof. Kotagiri Ramamohanarao	UoM	160000

PRESENTATIONS

Ho, H. K., Computational studies of the protein beta-sheet, PhD Completion Seminar, Australia.

Ho, H. K., Computational studies of the protein beta-sheet, Guest Lecture (COMP90016, UniMelb).

VR0133	Molecular Dynamics Studies of G Protein-Coupled Receptors	Dr David Chalmers Dr Elizabeth Yuriev	Monash Monash	1600000

PRESENTATIONS

Chalmers, D., Computational methods in drug design and development, Monash, Sunway, Malaysia.

Chalmers, D., Computational methods in drug design, University of Malaya, Malaysia.

Thomas, T., Scanlon, M. J., Yuriev, E. & Chalmers, D. K., Ligand binding pathways in fatty acid binding proteins.

Thomas, T., Yuriev, E. & Chalmers, D. K., Molecular dynamics of GPCRs.

La, J., Fang, Y., Tachedjian, G. & Chalmers D., In Silico mapping of potential binding pockets in human immunodeficiency virus type 1 reverse transcriptase.

PUBLICATIONS

Chin, S. P., Buckle, M. J. C., Chalmers, D. K., Yuriev, E. & Doughty, S. W., Towards activated homology models of the human M1 muscarinic acetylcholine receptor: model generation, refinement, enrichment studies and agonist/antagonist selectivity, Journal of Molecular Graphics and Modelling.

Thomas, T., McLean, K. C., McRobb, F. M., Manallack, D. T., Chalmers, D. K. & Yuriev, E., Homology Modelling of Human Muscarinic Acetylcholine Receptors, Journal of Chemical Information and Modelling.

NO.	PROJECT TITLE	CHIEF INVESTIGATORS	INSTITUTE	VLSCI SERVICE UNITS
VR0138	Stimulation Strategies for the Bionic Eye	Prof. Anthony Burkitt A/Prof. David Grayden Dr Hamish Meffin Prof. Nigel Lovell A/Prof. Socrates Dokos	UoM UoM Non-Vic Non-Vic Non-Vic	180000
	PRESENTATIONS	**PUBLICATIONS**		
	Sergeev, E. N., Meffin, H., Tahayori, B., Grayden, D.B. & Burkitt, A. N., Effect of soma polarization on electrical stimulation thresholds of retinal ganglion cells, Proceedings of the 6th IEEE EMBS Neural Engineering Conference, pp. 1131-1134, San Diego, USA. Tahayori, B. & Dokos, S., Challenging the optimality of rectangular pulse stimulation for neuroprosthetic devices, Proceedings of the 6th IEEE EMBS Neural Engineering Conference, pp. 1135-1138, San Diego, USA. Sergeev, E. N., Meffin, H., Tahayori, B., Burkitt, A. N. & Grayden, D. B., A model of retinal ganglion cell axon activation thresholds for suprachoroidal retinal prostheses, NeuroEng 2013: Australian Workshop on Computational Neuroscience, Melbourne, Australia. Meffin, H., Tahayori, B., Sergeev, E. N., O'Sullivan, E., Grayden, D. B. & Burkitt, A. N., Spatial shaping of neural activity for neuroprosthetic devices, 3rd International Conference on Medical Bionics, Australia.	Meffin, H., Tahayori, B., Sergeev, E. N., Grayden, D. B., Mareels, I. M. Y. & Burkitt, A. N., Modelling Extracellular Electrical Stimulation: III. Derivation and interpretation of macro equations, (in preparation). Sergeev, E. N., Meffin, H., Tahayori, B., Mareels, I. M. Y., Burkitt, A. N. & Grayden, D. B., Modelling Extracellular Electrical Stimulation: IV. Analysis of point source solution in an extensive fibre bundle, (in preparation). Tahayori, B., Meffin, H., Sergeev, E. N., Grayden, D. B. & Burkitt, A. N., Modelling Extracellular Electrical Stimulation: V. Experimental versus model res, (in preparation). Maturana, M. I., Kameneva, T., Burkitt, A. N., Meffin, H. & Grayden, D. B., The effect of morphology upon electrophysiological responses of retinal ganglion cells, Journal of Computational Neuroscience.		
VR0142	Rational design of dehalogenase enzymes for use in bioremediation	Dr Del Lucent Dr Tom Peat	CSIRO CSIRO	20014
VR0146	High-Resolution Holographic Imaginging for the Investigation of Micro-organisms Locomotion	Dr Nicolas Buchmann Prof. Julio Soria	Monash Monash	105000
	PRESENTATIONS	**PUBLICATIONS**		
	Buchmann, N. A., Kitsios, V., Atkinson, C. & Soria, J., Investigation of coherent structures and dynamics using POD and DMD of a separated airfoil flow subject to ZNMF jet forcing, International Conference on Instability and Control of Massively Separated Flows, Prato, Italy, Conference. Kitsios, V., Buchmann, N. A., Atkinson, C., Frederiksen, J. S. & Soria, J., Recovery of the DMD modes of a leading-edge separated airfoil flow via a POD rank reduction, International Conference on Instability and Control of Massively Separated Flows, Prato, Italy, Conference. Atkinson, C., Stegeman, P., Hackl, J., Borrell, G. & Soria, J., Lagrangian evolution of fluid particles in the vicinity of the turbulent non-turbulent interface of a turbulent boundary layer, 66th Annual Meeting of the APS Division of Fluid Dynamics, Pittsburgh, Unitied States, Conference.	Buchmann, N. A., Atkinson, C. & Soria, J., Ultra-high-speed tomographic digital holographic velocimetry in supersonic particle-laden jet flows, Measurement, Science and Technology. Buchmann, N. A., Kitsios, V., Atkinson, C. & Soria, J., Investigation of coherent structures and dynamics using POD and DMD of a separated airfoil flow subject to ZNMF jet forcing, (in preparation).		
VR0148	High-resolution electron microscopy studies of the insulin and insulin-like growth factor receptors	A/Prof. Michael Lawrence	WEHI	1732000

NO.	PROJECT TITLE	CHIEF INVESTIGATORS	INSTITUTE	VLSCI SERVICE UNITS
VR0152	Quantitative Magnetic Resonance Image Analysis	Dr Steve Moore A/Prof. Leigh Johnston	IBM UoM	120000
VR0164	Designing new reactions for novel pharmaceutical synthesis	Carl Schiesser	UoM	300000
	PRESENTATIONS	**PUBLICATIONS**		
	Alexander, S. A., Sloggett, R. J., Schiesser, C. H. & Kyi, C. P., Free Radicals, Biofilms and Cultural Materials, 6th Pacific Symposium on Radical Chemistry, Canada. Schiesser, C. H., Constructing Selenium and Tellurium Heterocycles ising Free Radical Chemistry, International Conference on the Chemistry of Selenium and Tellurium, Wales. Schiesser, C. H., The Electronics of Free Radicals: Influence of Lone Pairs and Vacancies, 6th International Conference on Reactive Intermediates and Unusual Molecules, Australia. Hancock, A. N. & Schiesser, C. H., Rate Constants for Intramolecular Addition of Acyl and Oxyacyl Radicals at Alkenes, 6th Pacific Symposium on Radical Chemistry, Canada. Hancock, A. N. & Schiesser, C. H., Theoretical Investigations of Intramolecular Additions of Acyl and Oxyacyl Radicals, Gordon Research Conference on Physical Organic Chemistry, USA.	Horvat, S. M. & Schiesser, C. H., An ab-initio and DFT Study of Some Homolytic Substitution Reactions of Methyoxycarbonyl Radicals at Silicon, Germanium and Tin, New Journal of Chemistry. Hancock, A. N., & Schiesser, C. H., Carbonyl Radical Cyclizations: Arrhenius Parameters for Unimolecular Radical Clocks, (in preparation).		
VR0165	Molecular systematics of Australian plants and fungi	Dr Daniel Murphy Dr Elizabeth James	RBG RBG	49200
	PUBLICATIONS			
	Birch, J. L. & Keeley, S. C., Dispersal pathways across the pacific: The historical biogeography of Astelia s.l. (Asteliaceae, Asparagales), Journal of Biogeography. Stefani, F. O. P., Jones, R. H. & May, T., Concordance of seven gene genealogies compared to phenotypic data reveals multiple cryptic species in Australian dermocyboid Cortinarius (Agaricales), Molecular Phylogenetics and Evolution. James, E. A., Jordan, R. & Griffin, P. C., Spatial genetic analysis of two polyploid macrophytes reveals high connectivity in a modified wetland , Freshwater Biology. James, E. A. & McDougall, K. L., Spacial genetic structure reflects extensive clonality, low genotypic diversity and habitat fragmentation in Grevillea renwickiana (Proteaceae), a rare, sterile shrub from southeastern Australia, Annals of Botany. Bell, K. L., Rangan, H., Fowler R., McConvell, P., Saunders, T., Sproncke, S., Kull C. A. & Murphy, D. J., New genetic and linguistic analyses show ancient humans shaped baobab evolution in Australia over thousands of years, (in preparation).			
VR0189	Glycogen structure in healthy and diseased organisms	Dr Angus Gray-Weale	UoM	370000
VR0191	Identifying genes involved in plant wall biosynthesis and regulation during development and stress	Prof. Tony Bacic Dr Ute Roessner	UoM UoM	140000
	PUBLICATIONS			
	Cassin, A., Doblin, M., Schultz, C., Bacic, A. & Johnson, K., Evolution of Arabinogalactan proteins: from algae to flowering plants, (in preparation). Zeng, W., Doblin, M., Bacic, A. & Cassin, A., Arabinoxylan synthesis: investigation of glycosyltransferase genes, (in preparation). Lampugnani, E. R., Moller, I. E., Cassin, A., Jones, D. F., Koh, P. L., Ratnayake, S., Beahan, C. T., Wilson, S. M., Bacic, A. & Newbigin, E., In Vitro Grown Pollen Tubes of Nicotiana alata Actively Synthesise a Fucosylated Xyloglucan, PLOS ONE.			

NO.	PROJECT TITLE	CHIEF INVESTIGATORS	INSTITUTE	VLSCI SERVICE UNITS
VR0200	Charged protein-lipid interactions and the regulation of membrane ion channel function.	A/Prof. Toby Allen	RMIT	2400000

PUBLICATIONS

Boiteux, C., Vorobyov, I. & Allen, T. W., Ion conduction and conformational flexibility of a bacterial voltage-gated sodium channel., Proceedings of the National Academy of Sciences, USA.

Vorobyov, I., Olson, T. E., Kim, J. H., Koeppe II, R. E., Andersen, O. S. & Allen, T. W., Ion-induced defect permeation of lipid membranes, Biophysical Journal.

Li, L. B., Vorobyov, I. & Allen, T. W., The Different Interactions of Lysine and Arginine Side Chains with Lipid Membranes, Journal of Physical Chemistry B.

Maresa, L. J., Garcia, A., Rasmussen, H. H., Cornelius F., Mahmmoud, Y. A., Berline, J. R., Lev, B., Allen, T. W. & Clarke R. J., Identification of Electric-Field-Dependent Steps in the Na+,K+-Pump Cycle. Biochimica et Biophysica Acta, Bioenergetics, Biochimica et Biophysica Acta, Bioenergetics.

Yarov-Yarovoy, V., Allen, T. W. & Clancy, C. E., Computational Models for Predictive Ion Channel Pharmacology, Drug Discovery Today: Disease Models.

VR0202	Exploring protein - surface interactions for engineering nanomaterials for biomedical applications	Dr George Yiapanis Prof. Irene Yarovsky	RMIT RMIT	320000

PRESENTATIONS

Christofferson, A. J., Yiapanis, G., Ren, J., Qiao, G. & Yarovsky, I., Structure of Cyclic Poly(methyl methacrylate) Stereocomplexes Determined by Molecular Dynamics Simulation, ICONN 2014, Australia.

PUBLICATIONS

Tran, D. N. H., Prime, E. L., Plazzer, M., Leung, A. H. M., Yiapanis, G., Christofferson, A. J., Yarovsky, I., Qiao, G. G. & Solomon, D. H., Molecular Interactions behind the Synergistic Effect in Mixed Monolayers of 1?Octadecanol and Ethylene Glycol Monooctadecyl Ether, Journal of Physical Chemistry B.

Yiapanis, G., Christofferson, A. J., Plazzer, M., Weir, M. P., Prime, E. L., Qiao, G. G., Solomon, D. H. & Yarovsky, I., Molecular Mechanism of Stabilization of Thin Films for Improved Water Evaporation Protection, Langmuir.

VR0203	Structure-Function Relationships for Materials-binding Peptides via Advanced Conformational Sampling	A/Prof. Tiffany Walsh	Deakin	4170878

PRESENTATIONS

Walsh, T. R., Can we be smarter than a coccolithophore? Taking lessons in advanced materials from nature, ICT for Life Sciences Forum, Austraila.

Palafox-Hernandez, J. P. & and Walsh, T. R., Towards An Atomistic Understanding of Binding Principles for Gold-Binding Peptides, MRS (Materials Research Society) Fall Conference, USA.

Sultan, A. & Walsh, T. R., Peptide-Surface Interactions at the Aqueous Titania Interface, MRS (Materials Research Society) Fall Conference, USA.

Wright, L. B., Palafox-Hernandez, J. B., Hughes, Z. E. & Walsh, T. R., Modelling Materials-Selective Binding of Biomolecules on Artificial Substrates, 4th Annual Symposium on Nanobionics, Australia.

PUBLICATIONS

Tang, Z., Palafox-Hernandez, J. P., Law, W. C., Hughes, Z. E., Swihart, M. T., Prasad, P. N., Knecht, M. R. & Walsh, T. R., Biomolecular Recognition Principles for Bionanocombinatorics: An Integrated Approach to Elucidate Enthalpic and Entropic Factors, ACS Nano.

VR0204	Assessing thermal effects of electromagnetic fields on people in realistic environmental conditions	Prof. Andrew Wood Dr Steve Moore Dr Robert McIntosh Mr Steve Iskra	Swinburne IBM Swinburne Swinburne	80000

NO.	PROJECT TITLE	CHIEF INVESTIGATORS	INSTITUTE	VLSCI SERVICE UNITS
VR0207	Prediction and Imaging of Vulnerable Plaque Evolution and Rupture	Prof. Kerry Hourigan	Monash	800000

PUBLICATIONS

Rao, S., Thompson, M. C., Leweke, T. & Hourigan, K., The flow past a circular cylinder translating at different heights above a wall, Journal of Fluid Mechanics.

Rao, A., Leontini, J., Thompson, M. C. & Hourigan, K., Three-dimensionality in the wake of a rapidly rotating cylinder in uniform flow, Journal of Fluid Mechanics.

Griffith, M. D., Leontini, J., Thompson, M. C & Hourigan, K., Effect of Small Asymmetries on Axisymmetric Stenotic Flow, Journal of Fluid Mechanics.

Rao, A., Thompson, M. C., Leweke, T. & Hourigan, K., Dynamics and stability of the wake behind tandem cylinders sliding along a wall, Journal of Fluid Mechanics.

VR0208	Multiscale three-dimensional model of Plant Cell Walls	Dr Natalie Gilka Prof. Geoff Fincher Dr John Wagner Prof. Mike Gidley Prof. Tony Bacic	UoM Non-Vic IBM Non-Vic UoM	100000

PRESENTATIONS

Gilka, N., Computational Modelling of Plant Cell Walls, Seminar at the Centre for Plant Integrative Biology, Nottingham, UK.

Oehme, D., Multi-scale Computational Modelling of Plant Cell Walls: An Update, ARC CoE in Plant Cell Walls Retreat, Australia.

Oehme, D., Building Homology Models of Csl Proteins, ARC CoE in Plant Cell Walls Node Meeting, Australia.

Bacic, T., 8th Annual Georgie Glycoscience Symposium, USA.

PUBLICATIONS

Schwerdt, J. G., Harvey, A. J., Shirley, N. J., Burton, R. A., Wright, F., MacKenzie, K., Schreiber, M., Halpin, C., Zimmer, J., Oehme, D., Wagner, J., Marshall, D. F., Waugh, R. & Fincher, G. B., Ancient Recombination Events and Differential Selection Pressure During the Evolution of the Cellulose Synthase Gene Superfamily in Grasses, (in preparation).

VR0209	How enteric neural circuits mediate mixing and propulsive motor patterns in the intestine	Mr Jordan Chambers Dr Evan Thomas Prof. Joel Bornstein	UoM Florey UoM	200000

PRESENTATIONS

Chambers, J. D., Bornstein, J. C., Gwynne, R. M., Koussoulas, K. & Thomas, E. A., A computational model of intrinsic sensory neurons of the gut, ANS, Australia.

VR0222	Molecular design and computational development of scaffold proteins	Dr Ming Liu	CSIRO	200000
VR0225	Project Overview Molecular modelling of plasma albumin for development of brain drug delivery	Prof. Norman Saunders	UoM	2400800
VR0226	Biosensors of kinase signalling in leukaemia	Dr Terry Mulhern	UoM	2040400
VR0227	Understanding influenza antiviral drug resistance by computational analysis	Dr Aeron Hurt	VIDRL	3200800
VR0229	Investigating the molecular dynamics of TRP ion channel protein structures	Dr Nicholas Veldhuis Prof. Peter McIntyre	Monash RMIT	2700000
VR0230	Simulations of prion protein folding in a domain critical for infectious prion formation	Prof. Andrew Hill	UoM	2600000

PRESENTATIONS

Hill, A. F., Update on Prion Research in Australia, Australian National CJD Support Group Network Annual Conference, Australia.

Hill, A. F., Role of Exosomes in Neurodegenerative Diseases, Adelaide RNA Group, Australia.

NO.	PROJECT TITLE	CHIEF INVESTIGATORS	INSTITUTE	VLSCI SERVICE UNITS
VR0232	Transitions in Biopolymers: The buckling of DNA	Prof. Aleks Owczarek	UoM	45000

PRESENTATIONS

Dagrosa, E., Applying torque to twist storing lattice polymers, AustMS 2013, Australia.

Dagrosa, E., Applying torque to twist storing lattice polymers, SM^2 2013, Australia.

PUBLICATIONS

Dagrosa, E., Writhe-induced knotting in a lattice polymer, (in preparation).

Dagrosa, E., PhD Thesis, University of Melbourne.

VR0236	Modelling post operative arrhythmogensis in Tetralogy of Fallot patients	Dr Andreas Pflaumer Dr Christopher Butler Dr Matthias Reumann Dr John Wagner	RCH IBM IBM IBM	6832670

PRESENTATIONS

Reumann, M., Butler, C., Pflaumer, A., Draeger, E. W., Glosli, J. N., Kim, C., Magerlein, J. H., Mirin, A. A., Liang, S., Danani, B., Wagner, J., Gurev, V., Richards, D. F. & Rice, J. J., Big Data challenges in predictive modelling for treatment using biophysical cardiac models, HISA Big Data 2013 Conference, Australia.

Butler, C., Pflaumer, A. & Reumann, M. et al, Cardioid cardiac simulation: Big data and compute challgenges, IBM A/NZ RTE, Australia.

Pflaumer, A., Butler, C., Jones, B., Rice, J., Gurev, V. & Reumann, M., Development of a whole heart model in patients with Tetralogy of Fallot, AEPC Helsinki 2014, Finnland.

PUBLICATIONS

Richards, D. F., Glosli, J. N., Draeger, E. W., Mirin, A. A., Chan, B., Fattebert, J.-L., Krauss, W. D., Oppelstrup, T., Butler, C. J., Gunnels J. A., Gurev, V., Kim, C., Magerlein J., Reumann, M., Wen, H.-F. & Rice, J. J., Toward Real-Time Simulation of Cardiac Electrophysiology in a Human Heart at Ultra-High Resolution., Computer Methods in Biomechanics and Biomedical Engineering.

VR0240	Statistical Imputation of HLA and KIR Alleles and Studies of Disease in Diverse Human Populations	Dr Stephen Leslie	MCRI	369000

PUBLICATIONS

Leslie, S. & Vukcevic, D. et al., Statistical Imputation of KIR Alleles from SNP data, American Journal of Human Genetics (submitted).

VR0250	Modelling protein-carbohydrate recognition	Dr Elizabeth Yuriev Dr Paul Ramsland	Monash Burnet	900000

PRESENTATIONS

Yuriev, E., Sugar footprints in the snow: In silico mapping of carbohydrate ensembles in protein binding sites, Boston Glycobiology Discussion Group, USA.

Thomas, T., Scanlon, M., Yuriev, E. & Chalmers, D. K., Ligand binding pathways in fatty acid-binding proteins, 37th Annual Conference of the Australian Society for Biophysics, Australia.

PUBLICATIONS

Thomas, T., McLean, K. C., McRobb, F. M., Manallack, D. T., Chalmers, D. & Yuriev, E., Homology Modelling of Human Muscarinic Acetylcholine Receptors, Journal of Chemical Information and Modelling.

VR0251	Investigating targeted drug delivery through optimising release points	Prof. Andrew Ooi Dr Steve Moore A/Prof. David Prior Prof. Mark Cook	UoM IBM SVI SVH	200000

PUBLICATIONS

Zhu, S. J., Poon, E., Ooi, A. & Moore, S., Enhanced Targeted Drug Delivery Through Controlled Release in a 3D Vascular Tree, (in preparation).

VR0252	The hydrophobic effect and protein folding	Dr Angus Gray-Weale Dr Sneha Abraham Prof. Paul Mulvaney	UoM UoM UoM	3100000

PRESENTATIONS

Liu, M., Besford, Q., & Gray-Weale, A., An explanation for the hydrophobic effect, Invited and travel paid by Forschungszentrum Julich (not a conference), Germany.

Liu, M., Besford, Q., & Gray-Weale, A., An explanation for the hydrophobic effect, RACI Phys Chem Meeting, Australia.

Liu, M., Besford, Q., & Gray-Weale, A., An explanation for the hydrophobic effect, University of Sydney invited talk, Australia.

PUBLICATIONS

Gray-Weale, A., The role of dispersion forces in solvophobic effects, Journal of Physical Chemistry Letters.

Beattie, J. K. & Gray-Weale, A. et al., pH dependence of surface tension, Journal of Colloid and Interface Science.

NO.	PROJECT TITLE	CHIEF INVESTIGATORS	INSTITUTE	VLSCI SERVICE UNITS
VR0253	Next Generation Sequencing to identify key genes for defence against a fungal pathogen of canola.	Dr Rohan Lowe Prof. Barbara Howlett	UoM UoM	41000

PUBLICATIONS

Lowe, R. G. T., Cassin, A., Clark, B., Van de Wouw, A. P., Grandaubert, J., Rouxel, T. & Howlett, B. J., Complement of Carbohydrate Active Enzyme genes and transcriptomes of partners in the Leptosphaeria: Brassica napus interactions reflect different fungal lifestyles during disease, (in preparation).

Grandaubert, J., Lowe, R., Soyer, J., Schoch, C., Van de Wouw, A., Robbertse, B., Lapalu, N., Links, M., Barbe, V., Mangenot, S., Cruaud, C., Borhan, H., Howlett, B, Balesdent, M.-H. & Rouxel, T., Transposable Element-assisted evolution and adaptation within members of the Leptosphaeria maculans/biglobosa species complex of fungal plant pathogens, (in preparation).

Van de Wouw, A. P., Lowe, R. G., Elliott, C. E., Dubois, D. J. & Howlett, B. J., An avirulence gene, AvrLmJ1, from the blackleg fungus, Leptosphaeria maculans, confers avirulence to Brassica juncea cultivars., Molecular Plant Pathology.

VR0254	The genome sequence of the parasitic dinoflagellate Hematodinium	Dr Ross Waller Dr Sebastian Gornik	UoM UoM	515000

PRESENTATIONS

Gornik, S. G., Marsa, F., Cassin, A., Pain, A. & Waller, R.F., Endosymbiosis undone: the early-branching parasitic dinoflagellate Hematodinium sp. forfeits its plastid., International Congress of Protistology (ICOP XIV), Canada.

Gornik, S. G., Could an eukaryotic phylum have abandoned histones? - the unusual biochemistry of the nuclei of dinoflagellates., Seminar Series Computational Bioscience Research Center, KAUST, Saudi Arabia.

PUBLICATIONS

Gornik, S. G., Marsa, F., Buchanan, H., Otto, T., Cassin, A., Pain, A. & Waller, R. F. , Endosymbiosis undone: the early-branching parasitic dinoflagellate Hematodinium sp. forfeits its plastid, (in preparation).

Gornik, S. G., Ganesan, P., Pain, A. & Waller, R. F., Hematodinium micro RNAs and their role in transcription control and differentiation from dinospore to trophont, (in preparation).

Gornik, S. G., Otto, T., Pain, A. & Waller, R. F., The deviant genome of the dinoflagellate parasite Hematodinium sp.: insights into alveolate genome evolution., (in preparation).

Bachvaroff, T. R. et al, Dinoflagellate phylogeny revisited: Using ribosomal proteins to resolve deep branching dinoflagellate clades, Molecular Phylogenetics and Evolution.

Danne, J. C., Gornik, S. G., Macrae, J. I., McConville, M. J. & Waller, R. F., Alveolate Mitochondrial Metabolic Evolution: Dinoflagellates Force Reassessment of the Role of Parasitism as a Driver of Change in Apicomplexans, Molecular Biology and Evolution.

VR0255	Optimising blood flow in stented arteries: a fluid mechanics approach incorporating optical coherenc	A/Prof. Peter Barlis Prof. Andrew Ooi Dr Daniel Chung Dr Olivier Cabrit Dr Stephen Moore	UoM UoM UoM UoM IBM	2000000
VR0256	Molecular simulation of actin dynamics in the malaria parasite: the track of parasite gliding motor	Dr Wilson Wong	WEHI	2600000

PRESENTATIONS

Baum, K., Kuiper, M. J. & Wong, W., Structural insights into actin filament disassembly from the malaria parasite, Grenoble, CNRS, France.

Baum, K., Kuiper, M. J. & Wong, W., Structural insights into actin filament disassembly from the malaria parasite, Curie Institute, Paris, France.

Baum, K., Kuiper, M. J. & Wong, W., Structural insights into actin filament disassembly from the malaria parasite, WEHI Institute Seminar, Australia.

Baum, K., Kuiper, M. J. & Wong, W., Structural insights into actin filament disassembly from the malaria parasite, Regensberg Actin Meeting 2014, Germany.

VR0257	Simulations of the Bacteriophage Lysin PlyC	Dr Sheena McGowan	Monash	1000000

PRESENTATIONS

McGowan, S., Molecular Dynamics Simulations of the Bacteriophage Lysin PlyC, VLSCI presentation day, Australia.

PUBLICATIONS

Reboul, C., Cowieson, N. P., Jeeva, P. & McGowan, S., Use of molecular dynamics simulations to elucidate the solution structure of PlyC., (in preparation).

NO.	PROJECT TITLE	CHIEF INVESTIGATORS	INSTITUTE	VLSCI SERVICE UNITS
VR0258	Examining the connection between defective mRNA splicing and colon cancer	A/Prof. Joan Heath	WEHI	13800
	PRESENTATIONS			
	Love, C., Sakthianandeswaren, A., Doggett, K., Boglev, Y., Cloonan, N., Sieber, O. & Heath, J. K., Examining the connection between defective mRNA splicing and colon cancer, AMATA 2013, Australia.			
VR0259	Interactions of Chemokines with Sulfated Tyrosine Residues in Chemokines Receptors	A/Prof. Martin Stone	Monash	1200000
VR0260	Determinants of the substrate specificity of the complement initiating proteases	Prof. Robert Pike	Monash	50000
	PUBLICATIONS			
	Wijeyewickrema, L. C., Yongqing T, Tran, T. P., Thompson, P. E., Viljoen, J. E., Coetzer, T. H., Duncan, R. C., Kass, I., Buckle, A. M. & Pike, R. N., Molecular determinants of the substrate specificity of the complement-initiating protease, C1r., Journal of Biological Chemistry.			
VR0261	Co-Evolutionary Dynamics of Culture and Social Structure	Prof. Garry Robins Prof. Yoshihisa Kashima Dr Alex Stivala	UoM UoM UoM	240000
	PRESENTATIONS	**PUBLICATIONS**		
	Stivala, A. & Robins, G., Ultrametric distribution of cultural vectors in an extended Axelrod mo, INSNA 2013, China. Stivala, A., Wang, P., Koskinen, J., Robins, G. & Rolls, D., Many snowballs make light work: a technique for large networks, INSNA Sunbelt XXXIV, USA.	Stivala, A., Robins, G., Kashima, Y. & Kirley, M., Ultrametric distribution of culture vectors in an extended Axelrod model, Scientific Reports. Stivala, A., Wang, P., Koskinen, J., Robins, G. & Rolls, D., Snowball sampling for estimating exponential random graph models for large networks, (in preparation).		
VR0262	Examination of the Specific Mechanisms of Vaccine-Derived Poliovirus Antiviral Drug Interactions	Mr Jason Roberts	VIDRL	1200000
	PRESENTATIONS	**PUBLICATIONS**		
	Roberts, J. A., Supercomputer Simulation of Viruses, The Merging of Art and Science, Australian Institute of Medical and Biological Illustrators, "Illuminate" biennial conference, Australia. Roberts, J. A., Kuiper, M. J., Thorley, B. R., Smooker P. M. & Hung, A., Refinement of the wild poliovirus capsid structure by atomistic molecular dynamics simulation of a complete virion, CSIRO Computational and Simulation Sciences and eResearch Annual Conference, Australia. Roberts, J. A., Computational Biophysics. Case study: In-Silico Reconstruction of Poliovirus., AMSI Summer Symposium in Bioinformatics, Australia. Roberts, J. A., Supercomputer Modelling of a Complete Human Viral Pathogen: Poliovirus., Centers for Disease Control and Prevention, Bioinformatics Seminar Series, United States. Roberts, J. A., Supercomputer Modelling of a Complete Human Viral Pathogen: Poliovirus., Theoretical and Computational Biology Group, Beckman Institute, University of Illinois, United States.	(in preparation)		
VR0263	Whole-genome characterisation of the genetic landscape of colorectal cancer	Dr Oliver Sieber	WEHI	194000
	PUBLICATIONS			
	Mouradov, D., Sloggett, C. & Sieber, O. M., Colorectal cancer cell lines are representative models of the main molecular subtypes of primary cancer, (in preparation). Sakthianandeswaren, A., Mouradov, D. & Sieber, O. M., Haploinsufficiency at the fragile site locus MACROD2 is associated with impaired DNA strand break repair in colorectal cancer, (in preparation).			

NO.	PROJECT TITLE	CHIEF INVESTIGATORS	INSTITUTE	VLSCI SERVICE UNITS
VR0264	A longitudinal study of brain volume and cognitive decline following stroke	Dr Heath Pardoe Prof. Geoffrey Donnan Prof. Graeme Jackson Dr Amy Brodtmann Dr Toby Cumming	Florey Florey Florey Florey Florey	30000
	PRESENTATIONS	**PUBLICATIONS**		
	Cumming, T., Physical activity is associated with cognition after stroke, but only for tasks presented visually, the 6th Congress of The International Society for Vascular Behavioural and Cognitive Disorders, Canada. Werden, E., Ipsilesional hippocampal atrophy occurs within the first year after ischaemic stroke., the 6th Congress of The International Society for Vascular Behavioural and Cognitive Disorders, Canada.	Li, Q., Pardoe, H., Brodtmann, A., Cumming, T. & Werden, E., Cortical thickness estimation in longitudinal stroke studies: a comparison of 3 measurement methods., (in preparation). Brodtmann, A., Li, Q., Cumming, T., Werden, E., Jackson, G., Donnan, G. & Pardoe, H., Charting cognitive and volumetric trajectories after stroke: the Cognition And Neocortical Volume After Stroke (CANVAS) Study, (in preparation).		

ROUND 7

VR0010	Cytoadhesive dynamics of parasitized red blood cells	Prof. Ravi Jagadeeshan Prof. Brian Cooke	Monash Monash	800000
VR0011	A Multi-Scale Quantitative Kidney Model	Dr Edmund Kazmierczak Dr Linda Stern	UoM UoM	22000
VR0024	Computational Modelling of G protein-coupled receptors	Prof. Patrick Sexton Prof. Arthur Christopoulos	Monash Monash	2400000
VR0057	Direct Numerical Simulation of Newtonian and non Newtonian fluid in Constricted Circular Geometery	Dr Cheng Chin Prof. Ivan Marusic	UoM UoM	500000
VR0165	Molecular systematics of Australian plants and fungi	Dr Daniel Murphy Dr Elizabeth James	RBG RBG	115000
VR0208	Multiscale three-dimensional model of Plant Cell Walls	Dr Natalie Gilka Prof. Tony Bacic Prof. Mike Gidley Dr John Wagner	UoM UoM Non-Vic IBM	200000
VR0210	Optimising blood flow in stented arteries: a fluid mechanics approach incorporating OCT	Dr Eric Poon A/Prof. Peter Barlis Prof. Andrew Ooi Dr Stephen Moore Dr Daniel Chung Dr Cheng Chin	UoM UoM UoM IBM UoM UoM	4040000
	PRESENTATIONS	**PUBLICATIONS**		
	Poon, E., Ooi, A., Pan, W., Liu, Y., Ye, Y., Xue, Y., Barlis, P. & Moore, S., Numerical simulations of the hemodynamics impact of stent-malapposition in a circular idealized coronary artery, APS DFD 2013, USA.	Poon, E., Barlis, P., Moore, S., Pan, W.-H., Liu, Y., Ye, Y., Xue, Y., Zhu, S. J. & Ooi, A., Numerical investigations of the hemodynamic changes associated with stent malapposition in an idealised coronary artery, (in preparation).		
VR0212	Calculating Climatic Constraints on Animals	Dr Michael Kearney	UoM	400000
VR0224	Enabling Next Generation Drug Screening	Prof. Stan Skafidas Dr Stefan Harrer A/Prof. Ross Bathgate	UoM IBM Florey	3020000
VR0251	Investigating on targeted drug delivery through optimising release position	Prof. Andrew Ooi A/Prof. David Prior Dr Steve Moore	UoM SVI IBM	1220000
VR0257	Molecular Dynamics Simulations of the Bacteriophage Lysin PlyC	Dr Sheena McGowan	Monash	2000000
VR0270	Molecular Simulation of Water/DMSO/NaCl solutions	Dr Tiffany Walsh A/Prof. Zak Hughes	Deakin Deakin	20000
	PUBLICATIONS			
	Hughes, Z. E. & Walsh, T. R., Molecular Simulations of ternary mixtures of water-DMSO-NaCl, (in preparation).			

NO.	PROJECT TITLE	CHIEF INVESTIGATORS	INSTITUTE	VLSCI SERVICE UNITS
VR0271	The effects of SIFT on the reproducibility and biological accuracy of the structural connectome	Dr Robert Smith	Florey	36000
	PRESENTATIONS	**PUBLICATIONS**		
	Smith, R. E., Tournier, J-D., Calamante, F. & Connelly, A., Towards robust structural connectomics, Epilepsy Melbourne Retreat, Australia. Smith, R. E., Tournier, J-D., Calamante, F. & Connelly, A., Evidence for the improved biological interpretability of white matter connectivity derived following tractogram filtering using SIFT, Proceedings of the ISMRM, USA. Smith, R. E., Tournier, J-D., Calamante, F. & Connelly, A., The effects of SIFT on the reproducibility of the structural connectome, Proceedings of the ISMRM Diffusion Workshop, Croatia.	Smith, R. E., Tournier, J-D., Calamante, F. & Connelly, A., The effects of SIFT on the reproducibility and biological accuracy of the structural connectome, (in preparation).		
VR0272	Determination of a cell death gene expression signature for zebrafish intestinal mutants	A/Prof. Joan Heath	WEHI	115000
VR0273	Membrane structure of equinatoxin II	Prof. Frances Separovic	UoM	402000
	PRESENTATIONS	**PUBLICATIONS**		
	Weber, D. K., Yao, S., Anderluh, G., Lybrand, T. P., Downton, M. T., Wagner, J. & Separovic, F., Modelling the interactions of equinatoxin II with micelles, 5th Asia-Pacific NMR Symposium (APNMR5), Australia. Weber, D. K., Yao, S., Anderluh, G., Lybrand, T. P., Downton, M. T., Wagner, J. & Separovic, F., Modelling the interactions of equinatoxin II with micelles, The 37th Annual Conference of the Australian Society for Biophysics, Australia. Weber, D. K., Yao, S., Anderluh, G., Lybrand, T. P., Downton, M. T., Wagner, J. & Separovic, F., Modelling the interactions of equinatoxin II with micelles, 58th Annual Meeting of the Biophysical Society, USA.	Weber, D. K., Yao, S., Anderluh, G., Paulic, N., Lybrand, T. P., Downton, M. T., Wagner, J. & Separovic, F., On the lines of - NMR and Molecular Dynamics study of the binding of Equinatoxin II with micelles, (in preparation).		
VR0274	Infectious diseases modelling and simulation	Dr James McCaw Dr Nicholas Geard A/Prof. Jodie McVernon	UoM UoM UoM	2280000
	PRESENTATIONS	**PUBLICATIONS**		
	Geard, N., Glass, K., McCaw, J. M., McVernon, J., Modelling the impact of vaccine coverage on maternal measles immunity, 20th International Congress on Modelling and Simulation, Australia. Petrie, S., Butler, J., Hurt, A., McVernon, J. & McCaw, J. M., Quantifying the relative fitness of two different influenza strains, 20th International Congress on Modelling and Simulation, Australia. Petrie, S., McVernon, J. & McCaw, J. M., Disentangling within-host and transmission fitness in competitive-mixtures experiments, Infectious Diseases Modelling AMSI workshop, Australia. Geard, N., Black, A., Ross, J., McCaw, J. M. & McVernon, J., A microsimulation model of pandemic influenza surveillance strategies, Infectious Diseases Modelling AMSI workshop, Australia.	Five publications currently in preparation.		
VR0275	Free Energy Simulations of Ion Channels and Transporters	A/Prof. Serdar Kuyucak	Non-Vic	2000000
	PUBLICATIONS			
	Heinzelmann, G. & Kuyucak, S., Molecular Dynamics Simulations of the Mammalian Glutamate Transporter EAAT3, PLOS ONE.			

NO.	PROJECT TITLE	CHIEF INVESTIGATORS	INSTITUTE	VLSCI SERVICE UNITS
NCMAS (projects awarded access to 15% of BlueGene/Q made available to NCMAS)				
NCd30	Theoretical studies of mass spectrometric fragmentations, the formation of cumulenes and biomolecules, molecular dynamic simulation, and bioinformatics	Prof. John Bowie Dr Tianfang Wang Dr Scott Cummins	UoA UoSC UoSC	7500
	PUBLICATIONS			
	Wang, T. & Liu, X., Design of a peptide based interleukin 10 inhibitor by computational modelling and molecular dynamics simulations, (in preparation).			
NCdq3	Understanding the structural basis of pathogenic modulation of the immune response	Dr Mark Agostino	Curtin	1000000
	PUBLICATIONS			
	Agostino, M., Anggayasti, W. L., Helmerhorst, E. & Mancera R. L., Structural insights into the multimerization of HMGB1, Lorne Proteins 2014. Agostino, M., Fernández-Recio, J., Mancera R. L. & Ramsland, P. A., Prediction of immunoglobulin-protein interactions involved in immune response evasion by microorganisms, Lorne Proteins 2014. Agostino, M., Fernández-Recio, J., Mancera R. L. & Ramsland, P. A., Redefining C domain regions leads to improved binding mode prediction of Fc-binding proteins and a possible general framework for protein-protein docking, (in preparation).			
NCdq9	Molecular dynamics simulations of the process of Tau protein aggregation	Dr Neha Gandhi	Curtin	276000
NCdw0	Design and optimization of Bandwidth-Efficient High-Speed Underwater Acoustic Communication Systems	Dr Defeng (David) Huang	UWA	40000
	PRESENTATIONS	**PUBLICATIONS**		
	Yang, J., Guo, Q., Huang, D. & Nordholm, S., Exploiting cyclic prefix for joint detection, decoding and channel estimation in OFDM via EM algorithm and message passing, IEEE International Conference on Communications (ICC), 2014, Australia. Yang, J., Guo, Q., Huang, D. & Nordholm, S., Exploiting cyclic prefix in Turbo FDE systems using factor graph, IEEE Wireless Communications and Networking Conference (WCNC), 2013, China. Yang, J., Guo, Q., Huang, D. & Nordholm, S., Enhanced data detection in OFDM systems using factor graph, IEEE International Conference on Wireless Communications and Signal Processing (WCSP), 2013, China.	Yang, J., Guo, Q., Huang, D. & Nordholm, S., Exploiting cyclic prefix for iterative OFDM receiver design via message passing based EM algorithm, IEEE Transactions on Communications. Yang, J., Guo, Q., Huang, D. & Nordholm, S., A factor graph approach to exploiting cyclic prefix for equalization in OFDM systems, IEEE Transactions on Communications.		
NCdz0	New models and analyses for social networks and criminal careers	Dr Murray Aitkin	UoM	10000
NCe90	Theoretical studies of protein-surface interaction under non-equilibrium conditions	Dr Nevena Todorova Prof. Irene Yarovsky	RMIT RMIT	200000
	PRESENTATIONS	**PUBLICATIONS**		
	Makarucha, A. J., Todorova, N., Hine, N. D. M., Mostofi, A. A. & Yarovsky, I., Dimensionality of carbon nanomaterials effect on amyloidogenic peptide aggregates: theoretical simulation study, 4th Asia-Pacific Symposium on Nanobionics, Australia. Todorova, N., Makarucha, A. J., Hine, N. D. M., Mostofi, A. A. & Yarovsky, I., Interactions of nanomaterials with amyloidogenic peptides: insights from multiscale computational calculations, ONETEP Masterclass University of Cambridge, UK. Makarucha, A. J., Todorova, N., Yarovsky, I., 'Dimensionality of carbon nanomaterials effect on amyloidogenic peptide aggregates: theoretical simulation study, 37th Annual Conference of the Australian Society for Biophysics, Australia. Todorova, N., Chiappini, C., Mager, M., Simona, B., Stevens, M. M. & 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., Chiappini, C., Mager, M., Simona, B., Stevens, M. M. & Yarovsky, I., Surface presentation of functional peptides determines cell internalization efficiency of TAT conjugated nanoparticles, (in preparation). Andresen, H., Mager, M., Grießner, M., Charchar, P., Todorova, N., Bell, N., Theocharidis, G., Bertazzo, S., Yarovsky, I. & Stevens, M. M., Single-step immunoassays utilising epitope-tagged gold nanoparticles: On the mechanism, feasibility, and limitations, (in preparation). Todorova, N., Makarucha, A. J., Hine, N. D. M., Mostofi, A. A. & Yarovsky, I., Dimensionality of Carbon Nanomaterials Determines the Binding and Dynamics of Amyloidogenic Peptides: Multiscale Theoretical Simulations, PLOS Computational Biology. Todorova, N., Yeung, L., Hung, A. & Yarovsky, I., Janus Cyclic Peptides: A New Approach to Amyloid Fibril Inhibition?, PLOS ONE.		

NO.	PROJECT TITLE	CHIEF INVESTIGATORS	INSTITUTE	VLSCI SERVICE UNITS
NCf91	Free Energy SImulations of Ion Channels and Transporters	Dr Serdar Kuyucak	SydneyUni	400000
	PUBLICATIONS			
	Heinzelmann, G., Chen, P-C. & Kuyucak, S., Computation of Standard Binding Free Energies of Polar and Charged Ligands to the Glutamate Receptor GluA2, Journal of Physical Chemistry B.			
NCg15	Simulation studies of biological and synthetic channels	Dr Ben Corry	ANU	600000
	PUBLICATIONS			
	Martin, L., Chao, R. & Corry, B., Molecular dynamics simulation of the partitioning of benzocaine and phenytoin into a lipid bilayer, Biophysical Chemistry.			
NCh77	Electronic Structural Modelling and CPMD Simulation for Molecules of Special Interest	Prof. Feng Wang	Swinburne	60000
	PRESENTATIONS	**PUBLICATIONS**		
	Ahmed, M., Moafi, S., Abouzid, K. A. & Wang, F., Computational investigation of 4¬anilioquinazoline inhibitors with potential anti-EGFR activities. Ahmed, M., Wickrama Arachchilage, A. P., & Wang, F., A QM/MM molecular dynamic simulation and vibrational spectroscopic study of 6-azaCytidine and cytidine.	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. Ahmed, M., Sadek, M. M., Serrya, R. A., Kafafy, A.-H. N., Abouzid, K.A. & Wang, F., Assessment of new anti-HER2 ligands using combined docking, QM/MM scoring and MD simulation, Journal of Molecular Graphics and Modelling. Ahmed, M., Bird, S., Wang, F. & Palombo, E. A., In silico investigation of lactone and thiolactone inhibitors in bacterial quorum sensing using molecular modelling, International Journal of Chemistry. Ahmed, M., Yu, A. & Wang, F., DFT Study on the Conformational and Vibrational Properties of 3′-Deoxycytidine and Its Analogues, International Journal of Chemistry.		
NCq75	Toxin Binding to Membrane Proteins - New Tools for Molecular Neuroscience	Dr Andrew Hung	RMIT	1000000
	PRESENTATIONS	**PUBLICATIONS**		
	Kompella, S. N., Hung, A., Clark, R. J. & Adams, D. J., alpha-Conotoxin RegIIA targeting nAChRs: mutagenesis studies improving selectivity and potency, Biophysical Society Meeting, USA. van Lierop, B. J., Robinson, S. D., Kompella, S. N., McArthur, J. R., Hung, A., MacRaild, C. A., Adams, D. J., Norton, R. S. & Robinson, A. J., Dicarba alpha-Conotoxin Vc1.1 Analogues with Differential Selectivity for Nicotinic Acetylcholine and GABAB Receptors, Lorne Protein Conference, Australia.	Kompella, S. N., Hung, A., Clark, R. J., Mari, F. & Adams, D. J., alpha-Conotoxin RegIIA targeting nAChRs: mutagenesis studies improving selectivity and potency, (in preparation). van Lierop BJ, Robinson SD, Kompella SN, Belgi A, McArthur JR, Hung A, MacRaild CA, Adams DJ, Norton RS, Robinson AJ., Dicarba alpha-Conotoxin Analogues and their Interactions at Nicotinic Acetylcholine Receptors, (in preparation). Suresh, A., Adams, D. J. & Hung, A., Molecular Basis of Conotoxin Selectivity Against nAChR, (in preparation). Grishin, A. A., Cuny, H., Hung, A., Clark, R. J., Brust, A., Akondi, K., Alewood, P. F., Craik, D. J. & Adams, D. J., Identifying Key Amino Acid Residues that Affect alpha-Conotoxin AuIB Inhibition of alpha3alpha4 Nicotinic Acetylcholine Receptors, Journal of Biological Chemistry. van Lierop, B. J., Robinson, S. D., Kompella, S. N., McArthur, J. R., Hung, A., MacRaild, C. A., Adams, D. J., Norton, R. S. & Robinson, A. J., Dicarba alpha-Conotoxin Vc1.1 Analogues with Differential Selectivity for Nicotinic Acetylcholine and GABAB Receptors, ACS Chemical Biology.		

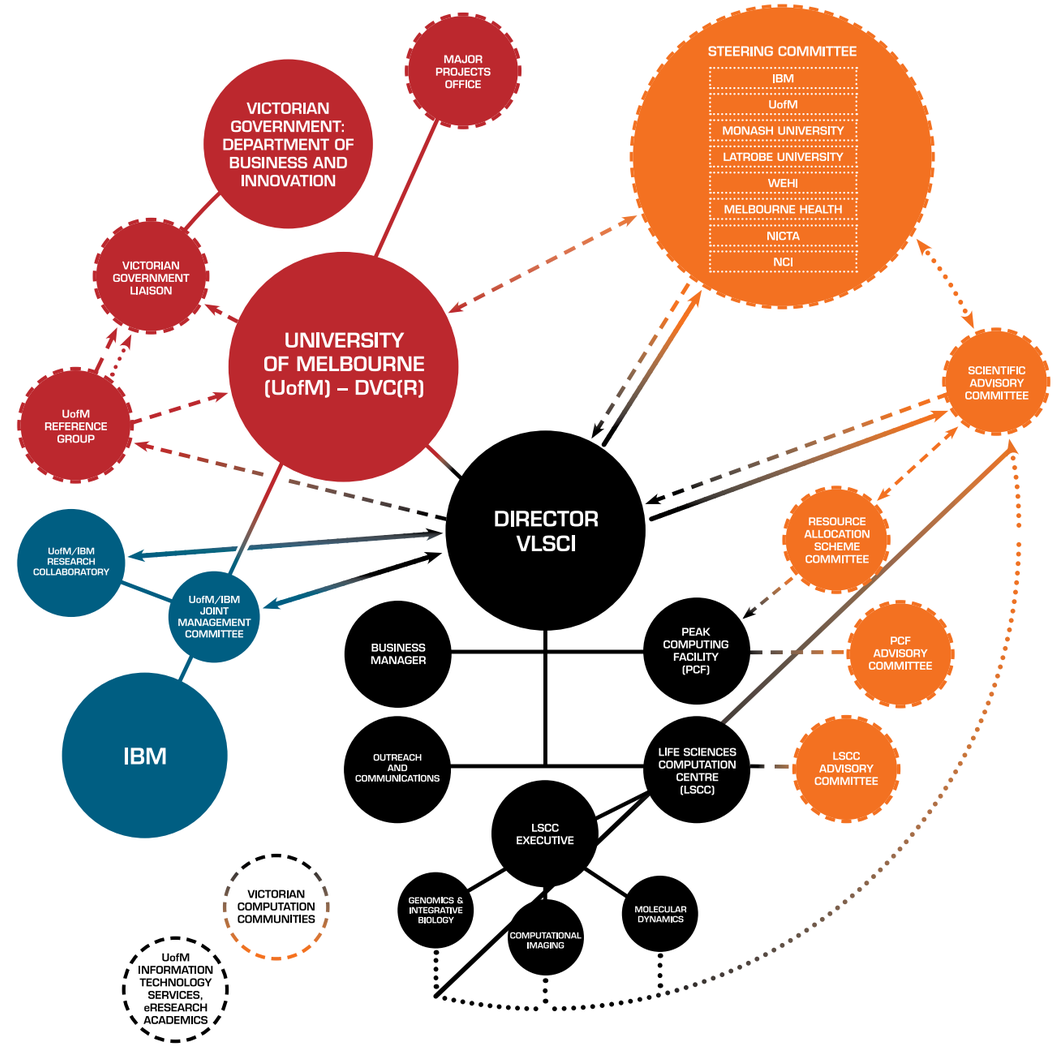
NO.	PROJECT TITLE	CHIEF INVESTIGATORS	INSTITUTE	VLSCI SERVICE UNITS
NCw47	Direct Numerical Simulations and Large Eddy Simulations of Turbulent Combustion	Dr Evatt Hawkes	UNSW	400000
	PRESENTATIONS	**PUBLICATIONS**		
	Karami, S., Talei, M. & Hawkes, E. R., Flame base analysis in a turbulent, partially premixed lifted flame., Thirteenth Mediterranean Combustion Symposium, Turkey. Krisman, A., Bhagatwala, A., Hawkes, E. R., Talei, M. & Chen, J. H., Two-dimensional direct numerical simulations of dimethyl ether lifted jet flames in highly heated co-flow at elevated pressure, Thirteenth Mediterranean Combustion Symposium, Turkey. Karami, S., Talei, M. & Hawkes, E.R., A numerical study of species transport budgets in a turbulent lifted flame, Australian Combustion Symposium 2013, Australia. Talei, M. & Hawkes, E.R., A parametric study of ignition in compositionally and thermally stratified n-heptane/air mixtures, Australian Combustion Symposium 2013, Australia. Karami, S., Talei, M., Hawkes, E. R. & Chatakonda, O., Direct numerical simulation of a partially premixed turbulent, lifted flame, Ninth Asia-Pacific Conference on Combustion, Korea.	Karami, S., Talei, M., Hawkes, E.R. & Yu, H., Edge flame structure in a turbulent lifted flame: a direct numerical simulation study, (in preparation). Talei, M. & Hawkes, E.R., Ignition in compositionally and thermally stratified n-heptane mixtures: a direct numerical simulation study, (in preparation). Behzadi, J., Talei, M., Hawkes, E. R., Lucchini, T., D'Errico, G. & Kook, S., Assessment of conditional moment closure for modelling auto-ignition in compositionally stratified n-heptane/air mixtures using direct numerical simulation, (in preparation). Krisman, A., Hawkes, E. R., Talei, M., Bhagatwala, A. & Chen, J. H., Tribrachial, tetrabrachial and pentabrachial structures in dimethyl ether edge-ames at NTC conditions, (in preparation).		

STARTUP GRANTS FOR TRIAL PROJECTS, allocated at discretion of the PCF Manager

VR0277	Statistical and simulation modelling of emergency animal disease outbreaks	Dr Simon Firestone	UoM	5000
VR0284	Understanding the Spatio-temporal patterns of human mediated plant invasions	Prof. Mark Burgman Mr Aaron Dodd	UoM DEPI	5000
VR0286	New methods for mapping variation in forest water use in time and space	Dr Richard Benyon Dr Dominik Jasierniak	UoM UoM	10000
VR0290	Molecular modelling studies on bromodomain ligands as anticancer agents	Dr Chris Burns	WEHI	5000
VR0292	Formation of Sugar Radical Cations in the Gas Phase	Dr Sandra Osburn	UoM	5000
VR0294	Architectural building blocks of protein three-dimensional structures	Dr Arun Konagurthu	Monash	5000

VLSCI user and Bioinformatician, Dmitri Mouradov, WEHI. Project: Whole-genome characterisation of the genetic landscape of colorectal cancer (VR0263). Image: Casamento Photography.

GOVERNANCE
STRUCTURE & RELATIONSHIPS



COMMITTEES

UNIVERSITY REFERENCE GROUP

The University of Melbourne 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 five times in 2013, in January, February, March, May and June.

Prof. Liz Sonenberg *Pro Vice-Chancellor (Research Collaboration), UoM*
Prof. James McCluskey *Deputy Vice-Chancellor (Research), UoM*
Prof. Peter R Taylor *Director, VLSCI*
Prof. John Zillman *Chair, VLSCI Steering Committee*
Mr John Bruzzaniti *Director, Major Projects, UoM*
Ms Karin Diamond *Business Manager, VLSCI (Observer)*
Ms Fiona Kerr *Executive Officer, VLSCI (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 Department of State Development, Business and Innovation continue to liaise regularly to review the implementation of the approved Business Plan. Three meetings were held in 2013, in May, August and September.

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), UoM*
Prof. Peter R. Taylor *Director, VLSCI*

Dr Mike Sargent, Independent Assessor, attended the September meeting by invitation. Mr Ben Apted and Ms Michelle Faruggia of Strategic Planning Partners (SPP) also attended the September meeting.

Victoria's Lead Scientist Dr Leonie Walsh (far right) with (l:r) VLSCI Director Prof. Peter R. Taylor and key presenters at the RAS Showcase held in October - Dr Michael Kuiper, VLSCI, Prof. John Hopper, MEGA, Dr Tania Kameneva, NICTA, Prof. Robin Gasser, School of Veterinary Science, University of Melbourne. Image: Casamento Photography.

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 2013, in March, May, August 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*
Prof. Liam O'Connor *Division Head, Systems Biology & Personalised Medicine, WEHI*
Dr Ajay Royyuru *Director, Computational Biology Centre, IBM Thomas J. Watson Research Center, New York State, USA*
Prof. Tony Bacic *Chair, VLSCI Scientific Advisory Committee*
Prof. Ian Smith *Pro Vice Chancellor, Research & Research Infrastructure, Monash University*
Prof. Robin Stanton *Deputy Chair, NCI Board*
Prof. Peter R. Taylor *Director, VLSCI*
Prof. Ingrid Winship *Executive Director of Research, Melbourne Health, Chair, Adult Clinical Genetics, Melbourne Health*
Prof. Justin Zobel *Program Leader and Principal Research Fellow, NICTA, Head, Department of Computing and Information Systems, UoM*
Ms Fiona Kerr *Executive Officer, VLSCI (Secretary)*
Ms Amelia King *Senior Policy Officer, CRC Bid Support Program Manager, Technology Policy, Innovation & Technology, DSDBI (Observer)*
Mr Matthew Dummett *Director, Science & Technology Policy, DSDBI (Observer)*
Prof. Liz Sonenberg *Pro Vice-Chancellor (Research Collaboration), UoM (Observer)*

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 met four times in 2013, twice in January, once in March and once in May.

Prof. John Zillman *Chair, VLSCI Steering Committee*
Prof. Peter R Taylor *Director, VLSCI (Chair)*
Dr Mark Kosten *Director, eResearch, La Trobe University*
Prof. Trevor Kilpatrick *Director, Melbourne Neuroscience Institute, UoM*
Prof. Paul Bonnington *Director, eResearch Centre, Monash University*
Ms Fiona Kerr *Executive Officer, VLSCI (Secretary)*

Mr Simon Wilkins and Mr Timothy Morris of SPP attended by invitation the first meeting held in January. Ms Jane Gardam of DSDBI, Mr Simon Wilkins and Mr Timothy Morris attended the second meeting held in January. Ms Amelia King of DSDBI attended the meeting held in March. Ms Amelia King and Mr Matthew Dummett of DSDBI attended the meeting held in May.

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. With the departure of Prof. Saint, Prof. Karen Day, the incoming Dean of Science, The University of Melbourne, subsequently designated Prof. Tony Bacic as Chair. The Committee met once in 2013 in February.

Prof. Robert Saint *(Chair) Dean, Faculty of Science, UoM. (until February 2013)*
Prof. Tony Bacic *(Chair) Director, Bio21 Institute*
Prof. David Bowtell *Head, Cancer Genomics & Genetics, Peter MacCallum Cancer Institute*
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. Rick Stevens *Argonne National Laboratory, The University of Chicago (to February 2013)*
Prof. James Whisstock *ARC Federation Fellow and Honorary NHMRC Research Fellow, Department of Biochemistry and 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 Centre, IBM Thomas J. Watson Research Center, New York State, USA*
Prof. Peter Taylor *Director, VLSCI*
Prof. Justin Zobel* *Program Leader and Principal Research Fellow, NICTA, Head, Department of Computing and Information Systems, UoM*
Prof. Liam O'Connor* *Theme leader, Proteomics, LSCC, Division Head, Systems Biology & Personalised Medicine, WEHI (left end 2012)*
A/Prof. Brian Smith* *Theme leader, Molecular Modelling, LSCC (new in 2013)*
Prof. Gary Egan* *Theme leader, Computational Imaging, LSCC, Director, Monash Biomedical Imaging, Monash University*
Ms Fiona Kerr (Secretary) *Executive Officer, VLSCI.*

*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 (VLSCI PCF Manager) and Dr John Wagner (Manager, IBM Research Collaboratory for Life Sciences – Melbourne) also attended the February meeting.

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 met once in 2013 in May.

Prof. Peter R Taylor *Director, VLSCI (Chair)*
A/Prof. Andrew Lonie *Head, LSCC, VLSCI*
Prof. Justin Zobel *Program Leader and Principal Research Fellow, NICTA, Head, Department of Computing and Information Systems, UoM*
Prof. Gary Egan *Director, Monash Biomedical Imaging (MBI), Monash University*
A/Prof. Brian Smith *Faculty of Science, Technology and Engineering, Deputy Head, La Trobe Institute for Molecular Science, La Trobe University*
Ms Fiona Kerr *Executive Officer, VLSCI (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 2013 in August.

A/Prof. Andrew Lonie *Head, LSCC, VLSCI (Chair)*
Prof. Peter R. Taylor *Director, VLSCI*
Prof. Gary Egan *Director, Monash Biomedical Imaging, Monash University*
A/Prof. Brian Smith *Faculty of Science, Technology and 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 and Information Systems, UoM*
Ms Fiona Kerr *Executive Officer, VLSCI (Secretary)*

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 2013 members provided out-of-session advice and consultation on specific issues as they arose.

Dr Mike Kuiper *Molecular Modelling Scientist, VLSCI*
Dr Vera Hansper *PCF Manager, VLSCI (Chair)*
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 and Pharmaceutical Sciences, Monash University*
Ms Melissa Buskes *Department of Chemistry, La Trobe University*
Mr Colin Hales *Department of Electrical and Electronic Engineering, UoM*
Mr Evan Thomas *Computational neuroscientist, Florey Neuroscience and Mental Health Institute*

Resource Allocation Scheme Committee at Research Showcase day, October 2013.
Back: (l-r) A/Prof. Brian Smith, Dr Jing-Jia Luo, Prof. Richard Huggins, Prof. Debra Bernhardt, A/Prof. Ashley Buckle, Prof. Ben Cocks, Prof. Salvy Russo, Prof. David Abramson, A/Prof. Tiffany Walsh
Front: (l-r) Dr Vera Hansper, Prof. Lindsay Botten (Chair), Prof. Rao Kotagiri
Image: Casamento photography

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 twice in 2013 in May and December.

Prof. Lindsay Botten *(Chair) NCI, Australian National University*
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, VLSCI (Secretary)*
Prof. Richard Huggins *Department of Mathematics & Statistics, UoM*
Prof. Rao Kotagiri *Department of Computing & Information Systems, UoM*
A/Prof. Brian Smith *Faculty of Science, Technology and 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 and Molecular Biology, Monash University*
A/Prof. Tiffany Walsh *Institute for Frontier Materials, Deakin University*

Ms Helen Gardiner (VLSCI Communications and Development Manager), Mr Brett Pemberton (VLSCI PCF Systems Administrator), Dr Andrew Isaac (VLSCI PCF Specialist Programmer) and Ms Fiona Kerr (VLSCI Executive Officer) attended the meeting held in May. Ms Helen Gardiner, Dr Matthew Hodges (VLSCI PCF Systems Administrator), Dr Andrew Isaac and Ms Fiona Kerr attended the meeting held in December.

FINANCIAL
REPORTS

PREAMBLE

VLSCI's funding is sourced from the Department of State Development Business & Innovation (DSDBI) under a $50 million grant from the Victorian Government (the Grant) and a 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 is generated through investment of those funds.

ACCOUNT STRUCTURE

VLSCI CASH FUNDS

Grant Funds from DSDBI reside in a separate project account – that account earns interest at Reserve Bank Rate less 40 basis points. Expenditure from this account is made in accordance with the approved categories of expenditure set out in the Grant: the Peak Computing Facility (PCF), the Life Sciences Computation Centre (LSCC), the Communications, Skill & Outreach Program, and the Directorate.

Cash funding provided by The University ($12.83 million) is made up of a combination of direct funding from Melbourne Research and central Infrastructure Funding. In 2013 income was collected from subscriptions to LSCC services and this amounted to $645,000. These funds were applied to activities of the LSCC and VLSCI. The University's 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. The Framework is provided in a number of documents (the 2009 Annual Report and the 2011 Business Plan - Revised).

2013 FINANCIAL RESULTS

2013 AUDIT

The 2013 accounts have been reviewed by The University's Departments of Financial Operations and Internal Audit. Oakton's have conducted an external audit of the accounts and their audit statement confirming the accuracy of the both the accounts and the in-kind contributions is published as part of the Financial Supplement to this Annual Report.

INCOME

Income to the Initiative in the 2013 year consisted of interest earned from grant funds and direct income support from The University. As noted above, $645,000 of income was also earned by the LSCC as subscription income. Income to the Grant was less than budget due to consistently low interest rates throughout the year. The University Contribution account met budget.

IN-KIND CONTRIBUTIONS

The framework for accounting for in-kind contributions has been devised to capture activities of individuals contributing their time and the resources of their institutions to the VLSCI. It is pleasing to report that in-kind contributions for the 2013 year were 25% over budget for Victorian institutions. 2013 was the first year in which contributions were made from non-Victorian institutions accessing the systems and those contributions amounted to 6.7% measured against total contributions.

As in previous years the most significant contribution ($11.3 million – up from $9.2 million in 2012) is that of individual staff working on LSCC and PCF projects. Data on the contributions of individual staff has been captured, specifically detailing information around the fraction of time spent on the project and individual salary levels. To this, salary on-costs and overheads (to incorporate institutional resources) have been added. A detailed report showing contributions to the LSCC & PCF is available as part of the Financial Supplement to the Annual Report 2013. This report shows activity by quarter, detailing the project, institution, details of individual staff members, 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 $235,265.

INITIATIVE EXPENDITURE

Expenditure from the Grant was made in accordance with the approved categories of expenditure under the Grant and The University's policies and procedures. Overall expenditure was 4% under budget, and not a significant variance.

Expenditure from University Funds was under-expended (43%). During the year planned expenditure on capital equipment of $1 million was set aside, electrical costs were lower than anticipated and there were savings in expenditure on associated ITC equipment and software. As in 2012, this represents a good result, as these funds will need to be managed carefully.

SUMMARY

2013 saw the continuation of major expenditure related to PCF high performance computer equipment, sustained and growing LSCC's activities, significant Outreach and Communications activity and on-going Directorate activity in relation to Business Plans and Sustainability Planning. The Initiative managed the finances in accordance with agreements and budgets and the overall result continues to be sound and pleasing.

GRANT ACCOUNT
STATEMENT

Grant Account Statement of Income & Expenditure for the period - 1 January 2013 to 31 December 2013

CARRY FORWARD CASH BALANCE	**22,235,834.75**
INCOME	
Interest Income Earned	467,639.96
TOTAL INCOME	**467,639.96**
SALARY EXPENDITURE	
LSCC Staff & Overheads	1,331,162.55
Salary Support - Victorian Universities & Institutes	1,071,881.87
Salary Expenditure	**2,403,044.42**
NON SALARY EXPENDITURE	
Advertising	102,213.39
Asset Expense	41.27
Asset Expense >$10,000	47,920.75
Audit Fee Expense	11,800.00
Bursaries & Grants	500.00
Computer Software & Services	38,083.25
Consultants Service Fees	233,800.63
Consumable Supplies	11,227.52
Entertainment & FBT Costs	1,939.10
Expensed Assets	10,150.18
IBM Fitout Supply - Scheduled Payments	4,629,626.00
Network Installation	1,243.79
Printing, Photography / Reprints , Photocopying Charges	528.50
Scholarships	305,611.04
Services Expenses	3,539.78
Staff Training & Development	4,212.49
Subscriptions and Memberships	6,377.90
Travel & Conference	159,871.77
Other (Non-Salary) Expenditure	**5,568,687.36**
TOTAL EXPENDITURE - SALARIES, MAJOR PCF & OTHER	**7,971,731.78**
TOTAL AVAILABLE (CASH)	**14,731,742.93**

UNIVERSITY CONTRIBUTION
ACCOUNT STATEMENT

University Contribution Account Statement of Income & Expenditure for the period - 1 January 2013 to 31 December 2013

CARRY FORWARD CASH BALANCE	**3,935,893.53**
INCOME	
University of Melbourne	1,000,000.00
LSCC Subscriptions	645,439.91
TOTAL INCOME	**1,645,439.91**
EXPENDITURE	
Directorate	
Directorage Salaries & Overheads	536,856.44
Communications & Outreach Salary Expenditure	230,653.98
PCF Salary Expenditure	1,056,424.19
Salary / Consulting Expenditure	**1,823,934.61**
Tax Payments	2,663.70
Consultant Service Fees	161,903.45
Utilities	432,321.00
General Expenses	11,520.42
Rental &Hire Charges	4,892.99
Consumable Materials & Provisions	37,706.35
Travel & Conference	81,565.70
Expensed Assets	61,779.77
Internal Recoveries Expense / Expert Services	31,276.87
Non-Salary (Other Expenditure)	**825,630.25**
TOTAL EXPENDITURE - SALARIES, MAJOR PCF & OTHER	**2,649,564.86**
TOTAL AVAILABLE (CASH)	**2,931,768.58**

Ms Karin Diamond
Business Manager

GLOSSARY

Alfred .....The Alfred Hospital
Austin.....The Austin Hospital
Baker IDI .....Baker IDI Heart and Diabetes Institute
Bio21.....Bio21 Institute
Burnet.....Burnet Institute
Curtin.....Curtin University
CERA.....Centre for Eye Research Australia
Deakin.....Deakin University
DEPI.....Department of Environment & Primary Industries Victoria
FedUni.....Federation University
Florey.....Florey Institute of Neuroscience and Mental Health
GVL.....Genomics Virtual Laboratory
IBM.....IBM Research Collaboratory for Life Sciences - Melbourne
iVEC.....Pawsey Centre
La Trobe.....La Trobe University
LSCC.....Life Sciences Computation Centre – VLSCI
Ludwig.....Ludwig Institute for Cancer Research
Max Planck.....Max Planck Institute of Biochemistry
MASSIVE.....Multi-modal Australian ScienceS Imaging and Visualisation Environment
MBC.....Melbourne Brain Centre
MCRI.....Murdoch Children's Research Institute
Melb Dental.....Melbourne Dental School
MHTP.....Monash Health Translation Precinct
MIMR.....Monash Institute of Medical Research
Monash.....Monash University
Museum Vic.....Museum Victoria
NCI.....National Computational Infrastructure
NCMAS.....National Computational Merit Allocation Scheme
NeCTAR.....National eResearch Collaboration Tools and Resources
NICTA.....National ICT Australia
Oxford.....Oxford University, Britain
PCF.....Peak Computing Facility - VLSCI
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
SVH.....St Vincent's Hospital
SVI.....St Vincent's Institute
Swinburne.....Swinburne University of Technology
SydneyUni.....The University of Sydney
UNSW.....University of New South Wales
UoA.....The University of Adelaide
UoM.....The University of Melbourne
UoSC.....University of the Sunshine Coast
UQ.....The University of Queensland
UWA.....The University of Western Australia
V3 alliance.....V3 alliance (ex VPAC & VERSi)
VABC.....Victorian AgriBiosciences Centre
VCB.....Victorian Cancer Biobank
VIDRL.....Victorian Infectious Diseases Reference Laboratory
VLSCI.....Victorian Life Sciences Computation Initiative
WEHI.....Walter & Eliza Hall Institute of Medical Research

PUBLISHING INFORMATION

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