Michelle Mary Kuttel

Department of Computer Science
University of Cape Town
Private Bag X3, 7702
Cape Town, South Africa

Tel: +27 (0) 21 6505107 *(W)*
mkuttel@cs.uct.ac.za

Research Profile

My research is in the general area of Computational Science: the development of research software and its application to solve problems in scientific disciplines. Within this broad field, I work in the areas of:

1. *Computational Chemistry*: my focus is on computational glycochemistry, using molecular modelling methods to investigate the conformation and interactions of bacterial carbohydrates playing key roles in infection;
2. *Computational Astronomy*: development of software and computational methods to support the South African Square Kilometre Array radio telescope initiative;
3. *Parallel and High Performance Computing*: using parallel architectures to accelerate compute-intensive algorithms;
4. *Research Programming*: the development of software tools to support research in Chemistry and Astronomy; and
5. *Visualisation*: using visualisation methods to generate novel effective visualisations of large, complex scientific data sets.

Personal Details

Date of Birth	3 September 1974
Nationality	South African
Marital Status	married
Children	2

Qualifications

2003	Ph.D *Computational Chemistry*	University of Cape Town Thesis title: *Simulations of Carbohydrate Conformational Dynamics and Thermodynamics*
1999	MSc *Computational Chemistry* (awarded with distinction)	University of Cape Town Thesis title: *Developing Analytical Tools for Saccharides in Condensed Phases*
1996	BSc(Hons) (First Class), *Computer Science*	University of Cape Town
1995	BSc, *Chemistry* (distinction in chemistry)	University of Cape Town

Employment

Jan 2012 to present
Associate Professor (Permanent Post)
Computer Science Department, University of Cape Town, Cape Town, South Africa

Jan 2006 to Dec 2011
Senior Lecturer (Permanent Post)
Computer Science Department, University of Cape Town, Cape Town, South Africa

Jan 2003 to Dec 2005
Lecturer (Contract)
Computer Science Department, University of Cape Town, Cape Town, South Africa

Projects

I have a number of key collaborative research projects, as follows.

Anti-bacterial Vaccines

For many bacterial species, the external capsular polysaccharides which surround the cells are essential for bacterial virulence and vaccine-induced serum antibodies against capsular polysaccharides can confer resistance to pneumococcal disease. **Prof. Neil Ravenscroft** (UCT Chemistry) and I have developed joint research project in investigation of bacterial polysaccharides important for the development of modern vaccines [2,3], combining NMR experiments with molecular modelling methods to predict polysaccharide conformations. Our current focus on pneumococcus and meningococcus. This work is now funded with a grant from Pfizer Inc.

CarbBuilder

Characterisation of carbohydrate molecular conformation remains a central problem in glycobiology and molecular models are increasingly used to interpret experimental results, or in the absence thereof. I have a long-standing collaboration with NMR experimentalist **Prof. Göran Widmalm** (U. Stockholm, Sweden) to develop and test our CarbBuilder research software for the building of carbohydrate models from primary structure information using effective heuristics [1,30]. CarbBuilder can generate a wide variety of carbohydrate structures, ranging from monosaccharides to large, branched polysaccharides. Future developments will focus on increasing the range of monosaccharides building blocks supported, as well as extending to automated building of glycoproteins and glycolipids.

Biofilms

Microorganisms often organise in biofilms, where a matrix immobilises cells in close proximity to each other. Biofilms are implicated in persistent infections, particularly nosocomial infections that are difficult to eradicate. I collaborate with carbohydrate experimentalists **Prof. Roberto Rizzo** and **Prof. Paola Cescutti** of University of Trieste, Italy) to investigate the conformation, dynamics and interactions of carbohydrate components of biofilms through simulation. This collaboration builds on a previous, related joint project, on determination of the conformation of two bacterial exopolysaccharides [7]. This collaboration has now been extended to include **Prof. John Brady** of Cornell University, U.S.A - we aim to expand the scope of the project to create a viable model of bacterial bioflims. Fleshing out the details of this work and establishing a work plan is the purpose of my proposed three-week visit to Cornell University.

AstroComp

I have a long-term ongoing collaboration with **Dr. Sarah Blyth** (UCT Astronomy) to develop high performance computing software solutions for the new international SKA radio telescope [4, 23-25]. This project has expanded to include **Dr Anja Schroeder (SAAO)** and evolved to focus primarily on detection and mitigation of radio frequency interference.

SciVis

I have a strong interest in the principles and practice of visualisation, particularly the use of scientific visualisation to facilitate research. This interest cuts across all my projects listed above: scientific visualisation is increasingly important for exploring large data sets to test hypothesis and propose new ones. I have collaborated with research software developer **John Stone** (UIUC, USA) to develop novel visualisations of molecules [11,13] and with **Dr Sarah Blyth** to develop visualisations of data cubes [4]. In addition, I have taught a Honours-level visualization course for six years, which in 2017 will develop into a Masters-level course for the M.Sc. in Data Science.

HPC

High Performance Computing (HPC) is another area of direct relevance to Computational Science: without the use of parallel computers and parallel software, much of the research I perform would be impracticable. However, I also have a direct interest in developing parallel software. I have a long-standing collaboration with **Dr Robert Best** (NIH, Washington, USA) to develop efficient high performance software for simulation of protein-protein interactions on Graphics Processing Units.

Publications

Book chapters

2018 *The role of molecular modeling in predicting carbohydrate antigen conformation and understanding vaccine immunogenicity.* M. M. Kuttel, N. Ravenscroft. *In* **Carbohydrate-Based Vaccines: From Concept to Clinic**, Chapter 7,139-173, *ACS Symposium Series, Vol. 1290.* (July 2018)

Journal Articles (* denotes corresponding author)

2018 *Conformations of Neisseria meningitidis serogroup A and X polysaccharides: the effects of chain length and O-acetylation.* J. Hlozek, M. M. Kuttel, N. Ravenscroft*, **Carbohyd. Res.**, 465: 44-51 (2018). DOI: 10.1016/j.carres.2018.06.007

2017 *Genetic and structural elucidation of capsular polysaccharides from Streptococcus pneumoniae serotype 23A and 23B, and comparison to serotype 23F.* N. Ravenscroft*, A. Omar, J. Hlozek, C. Edmonds-Smith, R. Follador, F. Serventi, M. M. Kuttel, P. Cescutti, A. Faridmoayer, **Carbohyd. Res.**, 450:19-29 (2017) DOI:10.1016/j.carres.2017.08.006

\+ *Cross protection in Neisseria meningitides serogroups Y and W polysaccharides: a comparative conformational analysis.* M. M. Kuttel*, Z. Timol, N. Ravenscroft, **Carbohyd. Res.**, 446-447,40-47 (2017) DOI:10.1016/j.carres.2017.05.004

\+ *Fluorescence and NMR spectroscopy together with molecular simulations reveal amphiphilic characteristics of a Burkholderia biofilm exopolysaccharide* M. M. Kuttel, P. Cescutti, M. Distefano, R. Rizzo*, **J. Biol. Chem.**, 292,11034-11042 (2017) DOI:10.1074/jbc.M117.785048.

2016 *CarbBuilder: Software for Building Molecular Models of Complex Oligo- and Polysaccharide Structures.* M. M. Kuttel*, J. Ståhle, and G. Widmalm, **J. Comput. Chem.**, 37(22),2098-2105 (2016).

2015 *Capsular polysaccharide conformations in pneumococcal serotypes 19F and 19A.* M. M. Kuttel*, G. E. Jackson, M. Mafata, N. Ravenscroft, **Carbohydr. Res.**, 406, 27-33 (2015).

2014 *Comparative simulation of pneumococcal serogroup 19 polysaccharide repeating units with two carbohydrate force fields.* M. M. Kuttel*, M. Gordon, N. Ravenscroft, **Carbohydr. Res.**, 390,20-27 (2014).

\+ *Scalable desktop visualization of very large radio astronomy data cubes.*, S. Perkins, J. Questiaux, S. Finniss, R. Tyler, S. Blyth, M. M. Kuttel*, **New Astron.**,30,1-7 (2014).

2013 *Towards Realistic and Interactive Sand Simulation: A GPU-based Framework.*, J.-P. Longmore*, P. Marais, M. Kuttel, **Powder Technol.**, 235, 983-1000 (2013).

2012 *Efficient Compression of Molecular Dynamics Trajectory Files*, P. Marais*, J. Kenwood, K. Carruthers Smith, M. M. Kuttel, J. Gain, **J. Comput. Chem.**, 33(27), 2131-2141 (2012).

\+ *Conformational properties of two exopolysaccharides produced by Inquilinus limosus, a cystic fibrosis lung pathogen.*, M. Kuttel*, N. Ravenscroft, M. Foschiatti, P. Cescutti, R. Rizzo, **Carbohydr. Res.** 350, 40-48 (2012).

2011 *Conformational Free Energy of Carbohydrates*, M. M. Kuttel, **Mini-Reviews in Organic Chemistry**, 8(3), 256-262 (2011)

2010 *Simulation of Coarse-Grained Protein-Protein Interactions with Graphics Processing Units*, I. Tunbridge, R. Best, J. Gain, M. M. Kuttel*, **J. Chem. Theory Comput.**, 6(11), 3588-3600 (2010).

\+ *Exhaustive computational search of ionic-charge clusters that mediate interactions between mammalian cytochrome P450 (CYP) and P450-oxidoreductase (POR) proteins*, A. Zawaira, M. Gallotta, N. Beeton-Kempen, L. Coulson, P. Marais, M. Kuttel, J. Blackburn, **Comput. Biol. Chem.**,34(1),42-52, (2010).

2009 *Visualisation of Cyclic and Multi-Branched Molecules with VMD*, S. Cross, M. M. Kuttel*, J. E. Stone, J. E. Gain, **J. Mol. Graph. Model.**, 28(2), 131-139 (2009).

2008 *Conformational free energy maps for globobiose (α-D-Gal-(1-4)-β-D-Gal) in implicit and explicit aqueous solution* , M. M. Kuttel, **Carbohyd. Res.**, 343(6), 1091-1098 (2008).

2006 *Techniques for visualization of carbohydrate molecules*, M. Kuttel*, J. Gain, A. Burger, I. Eborn, **J. Mol. Graph. Model.**, 25,380-388 (2006)

Publications

Journal Articles cont. (* denotes corresponding author)

2005 | *Free Energy Surfaces for the α(1-4)-Glycosidic Linkage: Implications for Polysaccharide Solution Structure and Dynamics*, M. Kuttel, K. J. Naidoo, **J. Phys. Chem. B**, 109(15),7468-7474, (2005).

\+ | *Ramachandran Free Energy Surfaces for Disaccharides: Trehalose, a Case Study*, M. M. Kuttel, K. J. Naidoo, **Carbohyd. Res.**, 340, 875-879 (2005).

\+ | *Glycosidic Linkage Rotations Determine Amylose Stretching Mechanism*, M. Kuttel, K. J. Naidoo, **J. Am. Chem. Soc.**, 127, 12-13 (2005).

2002 | *Carbohydrate Solution Simulations: Producing a Force Field with Experimentally-Consistent Hydroxyl Rotational Frequencies and Populations*, M. Kuttel, J. W. Brady, K. J. Naidoo, **J. Comput. Chem.**, 23(13), 1236-1243 (2002).

2001 | *Water Structuring About the Dimer and Hexamer Repeat Units of Amylose from Molecular Dynamics Computer Simulations*, K. J. Naidoo, M. Kuttel, **J. Comput. Chem.**, 22(4), 445-456 (2001).

Peer-Reviewed Conference Proceedings

SAICSIT
26-28 Sept. 2017
Thaba 'Nchu
South Africa

Improving the usability of scientific software with participatory design: a new interface design for radio astronomy visualisation software, Laurisha Rampersad, Sarah Blyth, Ed Elson, Michelle M. Kuttel **SAICSIT '17 Proceedings of the 2017 Annual Research Conference on South African Institute of Computer Scientists and Information Technologists**, doi: 110.1145/3129416.3129899

SAICSIT
26-28 Sept. 2016
Johannesburg
South Africa

Effective Visualization of Tuberculosis Three-Drug Assays: A Design Study, Suganani Silubonde, Digby Warner, Michelle Kuttel, **SAICSIT '16 Proceedings of the 2016 Annual Research Conference on South African Institute of Computer Scientists and Information Technologists**, doi: 10.1145/2987491.2987501

\+

Accelerating Molecular Conformational Searches with Genetic Algorithms, Victor Gueorguiev , Michelle Kuttel, **SAICSIT '16 Proceedings of the 2016 Annual Research Conference on South African Institute of Computer Scientists and Information Technologists**, doi: 10.1145/2987491.2987529

IST-Africa 2016
11-13 May 2016
Durban
South Africa

An eHealth Android Application for Mobile Analysis of Microplate Assays, James Bellairs,. Jason Hlozek, Timothy Egan, Michelle Kuttel, **IST-Africa Week 2016 Conference Proceedings, ISBN: 978-1-905824-54-0** - received conference "**Runner-up Paper award**", doi: 10.1109/ISTAFRICA.2016.7530644

SAICSIT
28-30 Sept. 2015
Stellenbosch
South Africa

Comparison of effectiveness of two mobile application designs for encouraging children to. read, Erin Versveld, James Foster, Michelle Kuttel, **SAICSIT '15 Proceedings of the 2015 Annual Research Conference on South African Institute of Computer Scientists and Information Technologists**, Article No. 38, doi: 10.1145/2815782.2815796

ADASS XXII
5-8 Nov. 2012
Champaign, IL
USA

GPU-based Acceleration of Radio Interferometry Point Source Visibility Calculations in the MEQtrees Framework, Richard J. Baxter, Patrick Marais, Michelle Kuttel, **Astronomical Data Analysis Software and Systems XXII, ASP Conference Series**, 475, p 53-59.

\+

Detection of binary pulsars with GPU-accelerated sinusoidal Hough Transformations, Christopher Laidler, Michelle Kuttel, **Astronomical Data Analysis Software and Systems XXII, ASP Conference Series**, 475, p 83-87.

\+

Acceleration of automated HI source extraction., Scott Badenhorst, Sarah Blyth, Michelle Kuttel, **Astronomical Data Analysis Software and Systems XXII, ASP Conference Series**,475, p 45-49.

IEEE eScience
5-8 Dec. 2011
Stockholm,
Sweden

CarbBuilder: an adjustable tool for building 3D molecular structures of carbohydrates for molecular simulation, Michelle Kuttel, Yue Mao, Göran Widmalm, Magnus Lundborg, **Proceedings of the 7th IEEE International Conference on e-Science**, p 395-402.

Publications

Peer-Reviewed Conference Proceedings

SAICSIT
11-13 Oct 2010
Bela-Bela
South Africa

Panopticon: A Scalable Monitoring System, Duncan Clough, Stefano Rivera, Michelle Kuttel, Vincent Geddes, Patrick Marais, **Proceedings of South African Institute for Computer Scientists and Information Technologists Conference (SAICSIT 2010)**, p 39-47.

AfriVIS
21-23 June 2010
Franshoek
South Africa

Dynamic Load Balancing of Lattice Boltzmann Free-Surface Fluid Animations, A. Reid, J. Gain, M. Kuttel, **Proceedings of Afrigraph2010: the 7th International Conference on Virtual Reality, Computer Graphics, Visualization and Interaction in Africa**, p 91-100.

\+

Visualization of Solution Sets from Automated Docking of Molecular Structures, J. Jansen van Vuuren, M. Kuttel, J. Gain **Proceedings of Afrigraph2010: the 7th International Conference on Virtual Reality, Computer Graphics, Visualization and Interaction in Africa**, p 111-120.

IEEE ICC
23-27 May 2010
Cape Town
South Africa

An Electronic Health Care Cardiac Monitoring System, Gregory Chandran, Hanh Le, Michelle Kuttel, Sena Allen, Robert Koletka **Proceedings of IEEE International Communications Conference (ICC2010)**, pages 1-5.

Conferences

Oral presentations 2012-2018

20-24 August, 2018
Boston, MA, USA

American Chemical Society Fall 2018 National Meeting and Exposition
CARB 78: Conformational modelling of fungal mannan polysaccharide antigens: Implications for the rational design of anti-fungal vaccines. Michelle M. Kuttel

17-23 July 2018
Libon, Portugal

29th International Carbohydrate Symposium (ICS2018)
Comparison of capsular polysaccharide conformations in Streptococcus *group B serotype III and* Streptococcus pneumoniae *serotype 14: implications for immunogenicity.* M. M. Kuttel*, N. Ravenscroft

20-24 August, 2017
Washington D.C. USA

American Chemical Society Fall 2017 National Meeting and Exposition
Advances in Glycan Structure & Dynamics Symposium (invited talk)
CARB 74: Investigating serotype cross-protection in carbohydrate vaccines: a molecular modelling approach. Michelle M. Kuttel, Neil Ravenscroft

July 2-7, 2017
Barcelona, Spain

19th European Carbohydrate Symposium
Conformation and dynamics of pneumococcal capsular polysaccharide antigens, Michelle M. Kuttel*, Neil Ravenscroft

15-19 Sept. 2015
Split, Croatia

Abstracts: XXIII International Symposium on Glycoconjugates, *Modelling the conformation of bacterial polysaccharide antigens*, M. M. Kuttel*, N. Ravenscroft, **Glycoconj J** 32, 240 (2015).

24-26 Nov. 2014
Cape Town

eResearch Africa 2014
Design and development of effective web and mobile applications for visualizing molecular structure.

12-17 Jan. 2014
Bangalore, India

27th International Carbohydrate Symposium (ICS)
Molecular modelling of Streptococcus Pneumoniae *capsular polysaccharide antigens*

6-10 Oct. 2013
UCT, Cape Town

eResearch Africa 2013
Enabling rapid launch of molecular simulations

22-27 July, 2012
Madrid, Spain

26th International Carbohydrate Symposium (ICS)
O124: Redesigning Carbohydrate Symbols

Seminars and Invited Talks

Invited Talk
29 August 2017
Pfizer Inc, Pearl River, NY USA

Polysaccharide Structure/Conformation: role in glycoconjugate vaccines.
Dr A. Krishna Prasad (Director, Vaccine Research and Early Development, Pfizer Inc) invited me to the Pfizer Pearl River facility to give a talk on my molecular modelling work on carbohydrate vaccine antigens.

PhD short course
June 2016
U. Malaga, Spain

Visual Thinking and Visualization
Dept. of Computer Science PhD programme course on how visual thinking theory can help with design of effective interactive multidimensional data displays.

Winter Schools
July 2012,2011,2009

Parallel Programming with OpenMP
One-day lectures for Centre for High Performance Computing (CHPC) Winter Schools in Parallel Computing in Bloemfontein (2012), Johannesburg (2011) and Cape Town (2009).

16 July, 2008

Introduction to High Performance Computing
School on Electronic Structure Methods, African Institute of Mathematical Sciences, Muizenberg, Cape Town, South Africa

16 March, 2010

Developing software for visualizing, analyzing and simulating chemical structures
Department of Chemistry, University of Cape Town, South Africa

2 July, 2008

Visualization and modelling of exopolysaccharides from Inquilinus limosus
Department of Life Sciences, University of Trieste, Trieste, Italy

30 March, 2005

Modelling carbohydrates: methods for carbohydrate simulation and visualization
John Innes Centre, Norwich Research Park, Colney, Norwich, UK

Awards

2014

Finalist (Second runner-up) in "Distinguished Young Woman Scientist, Physical and Engineering Sciences" category of the South African Department of Science and Technology's **Women in Science Awards**.

2016-2020

NRF C2 Rating
I was rated as a C2 researcher by the National Research Foundation (NRF) of South Africa for research work done up to the **end of 2014**. This rating is valid from 01 January 2016 to 31 December 2020.
The C category is defined by the NRF as: *"Established researchers with a sustained recent record of productivity in the field."*

2010-2015

NRF Y Rating
I was rated as a Y researcher by the National Research Foundation (NRF) of South Africa for research work done up to the **end of 2008**. This rating was valid from 01 January 2010 to 31 December 2015.

2007

Apple Research and Technology Support (ARTS) Programme Laureate
Project Title: *Computer Simulation and Visualization of Saccharide Gels and Glasses*
$30 000 of Apple solutions and technical support
http://www.apple.com/uk/education/hed/arts/winners.html

2002

U.C.T. University Scholarships Committee Award

2000-2002

University of Cape Town Research Associateship
Awarded in recognition of research excellence at the doctoral level.

Research Funding

	Grant	Collaborators
Current grants		
11/2017-11/2020 **570 000 USD**	Pfizer Inc., Pearl River, NY, USA *Investigating the molecular and conformational basis of cross-protection in conjugate vaccines.*	Assoc. Prof. Neil Ravenscroft
2018-2021 **210 000 ZAR**	National Research Foundation (NRF) Competitive Support for Rated Researchers (CSRR) Grant *Carbohydrate anti-fungal vaccines: correlating structure with activity*	Assoc. Prof. Neil Ravenscroft
Previous grants		
2014-2016 **390 000 ZAR**	The South African Medical Research Council *Modelling of carbohydrate antigen structures to improve conjugate vaccine development*	Assoc. Prof. Neil Ravenscroft
2011-2014 & *2015-2018* **2 900 000 ZAR**	The South African Square Kilometre Array Project: The MeerKAT High Performance Computing (HPC) for Radio Astronomy Research Programme *Developing Efficient Software for Large-Scale Radio Interferometry*	Assoc. Prof. Patrick Marais Assoc. Prof. James Gain Dr Sarah Blythe Dr Kurt van der Heyden Dr Catherine Cress (UWC)
2011-2013 **300 000 ZAR**	UCT Vice-Chancellor's Strategic Fund Grant *Summer Undergraduate Research Experience (SURE)*	Assoc. Prof. Hussein Suleman Assoc. Prof. James Gain
2010-2012 **408 200 ZAR**	National Research Foundation (NRF) Competitive Support for Unrated Researchers (CSUR) Grant *Software for protein-protein binding*	Dr Patrick Marais, Dr James Gain Dr Alexander Zawaira Dr Robert Best (Cambridge U., UK) John Stone (U. Illinois, USA)
2008/2009 **600 000 ZAR**	National Bioinformatics Network *Visualization for molecular modelling and optimization*	Dr James Gain Dr Patrick Marais
2008/2009 **200 000 ZAR**	National Research Foundation (NRF) Grant *Massively Parallel Computing for Simulation*	Dr James Gain Dr Patrick Marais
2008/2009 **94 500 ZAR**	South Africa/Italy Cooperation Agreement National Research Foundation (NRF) Grant *Bacterial polysaccharides: from structure to vaccines*	Assoc. Prof. Neil Ravenscroft Prof. Roberto Rizzo (U. Trieste, IT), Dr Paula Cescutti (U. Trieste, IT)
2008 **15 850 ZAR**	UCT University Research Council Conference Travel Grant *Congress of the World Association of Theoretical and Computational Chemists 2008*	
2006/2007 **23 000 ZAR**	University Emerging Researcher Grant *Design of parallel software for molecular simulation*	
2006/2005 **162 000 ZAR**	National Bioinformatics Network *Docking Atomic Structures into Low-Resolution Maps*	Prof. Trevor Sewell Dr James Gain
2006 **116 000 ZAR**	University Research Council Stimulation Grant *Developing physicochemical methods for the structural profiling of Inulin*	Dr Neil Ravenscoft Assoc. Prof. Susan Bourne

Postgraduate Graduation

Student	Degree	Thesis Title
Kumbirai Chigudu	M.Sc$^+$	*Design of a Prototype Mobile Application Interface for Efficient Accessing of Electronic Laboratory Results by Health Clinicians*
Nathan Geffen	Ph.D	*Design and implementation of programming tools for the microsimulation of infectious disease epidemics with a focus on HIV and TB* Co-supervisor: Andrew Boulle
Zaheer Timol	M.Sc.	*Chemical and conformational studies of bacterial cell surface polysaccharide repeating units.* Principal Supervisor: Neil Ravenscoft (Chemistry)
Genevieve Chang	M.Sc$^+$	*Designing an effective carbohydrate-building application user interface for the Android tablet environment.*
Christopher Schollar	M.Sc.	*Handling Radio Frequency Interference for the KAT7 Radio Telescope* Principal supervisor: Dr Sarah Blyth (UCT Astronomy); Co-supervisor: Dr Anja Schroeder
Scott Badenhorst	M.Sc.	*HPC acceleration of astronomical H1 source detection.* Co-supervisor: Dr Sarah Blyth (UCT Astronomy)
Marc Gordon	M.Sc$^+$	*Force Field Comparison through Computational Analysis of Capsular Polysaccharides of Streptococcus pneumoniae Serotypes 19A and F.* Co-supervisor: Assoc. Prof. Neil Ravenscroft (Chemistry)
Andrew Potgieter	M.Sc$^+$	*Parallelization of the Weighted Histogram Analysis Method*
Duncan Clough	M.Sc.	*Fluid Dynamics* Principal Supervisor: Assoc. Prof. James Gain
Neann Mathai	M.Sc.	*Molecular modelling of the* Streptococcus Pneumoniae *serogroup 6 capsular polysaccharide antigens.* Co-supervisor: Assoc. Prof. Neil Ravenscroft (Chemistry)
Richard Baxter	M.Sc.	*GPU-based Acceleration of Radio Interferometry Point Source Visibility Simulations in the MeqTrees Framework* Principal Supervisor: Patrick Marais
Ian Tunbridge	PhD*	*Course-grained Simulation of Protein Docking with Graphics Processing Units* Co-supervisor: Dr James Gain
Rudolf van den Berg	M.Sc.$^+$	*Force-extension of the Amylose Polysaccharide*
Johannes Jansen van Vuuren	M.Sc.	*Visualization of high-dimensional solution sets for docking of molecular structures into EM micrographs* Co-supervisor: Dr James Gain
Juan-Pierre Longmore	M.Sc.	*Realistic Interactive Sand: A GPU-based Framework* Principal Supervisor: Dr Patrick Marais
Ashley Reid	M.Sc.	*Practical Fluid Dynamics for the Animation Industry* Principal Supervisor: Dr James Gain
Peter McMahon	M.Sc.	*Accelerating Bioinformatics Applications using Reconfigurable Computers*
John Kyeyune	M.Sc.	*Parallel Monte Carlo Simulations in LIBOR market models* Principal supervisor: Dr Peter Ouwehand

*UCT does not award *cum laude* Ph.D degrees.
+ M.Sc. by Coursework and Dissertation

Postgraduate Supervision

Current students

	Student	Degree	Thesis Title
Ph.D	Christopher Laidler	Ph.D	*GPU accelerated blind searches for weak binary pulsars, using Dynamic Power Spectra and Hough Transformations.*
	Samuel Mabakane	Ph.D (part-time)	*Novel visualizations for optimization of parallel programs*
	Gerald Balekaki	Ph.D	*Automated detection and characterization of radio frequency interference for the Square Kilometer Array.* Co-supervisors: Sarah Blyth and Anja Schroeder
	Zaheer Timol	Ph.D	*Conformational studies of pneumococcal capsular polysaccharides.* Co-supervisor: Neil Ravenscoft (Chemistry)
co-supervised	Jason Hlozek	Ph.D	*Conjugate vaccine polysaccharide structural study by NMR and computational modelling techniques.* Principal Supervisor: Neil Ravenscoft (Chemistry)
M.Sc.	Adrianna Pinska	M.Sc.	*Accelerated Coarse-Grained Molecular Dynamics Simulations of Protein-Protein Docking* Co-supervisor: Assoc. Prof. James Gain
	Edmore Tutsirayi Moyo	MSc (part-time)	*Accelerated NeuroEvolution of Augmenting Topologies on a Heterogeneous System Architecture* Co-supervisor: Dr Geoff Nitschke
	Laurisha Rampersad	M.Sc$^+$	*Automated detection and characterization of radio frequency interference for the Square Kilometer Array.*
	Sidney Tirivavi	M.Sc$^+$	*Developing a mobile application to increase enthusiam for mathematics in middle school students.*

Leadership & Responsibility

2016-2019 **External examiner**
Three-year appointment as external examiner for the entire Rhodes Computer Science Department, Rhodes University, Grahamstown, South Africa.

2016 - **Inter-University Institute for Data Intensive Astronomy (IDIA)**
Member of the management Committee.

1 August 2017 - **Editor,** *Astronomy and Computing*
Astronomy and Computing is a peer-reviewed Elsevier journal that focuses on the broad area between astronomy, computer science and information technology. Current impact factor: 2.0. https://www.journals.elsevier.com/astronomy-and-computing

2018 - **Chair of the Faculty of Science Physical Planning Committee**
This committee's role is to provide advice to the Dean on space allocation and refurbishment matters in the Faculty, and to advise the Dean on budget requirements.

2017 - **UCT Science Faculty IT Committee Chair**
The Information Technology Committee's role is to formulate and periodically review Science Faculty IT policy and assist the Dean's Advisory Committee and Faculty Equipment Committee in budgetary matters relevant to Information Technology.

Administration

Faculty level

2011 - present **Faculty Physical Planning Committee member**
This committee is concerned with the renewal and maintenance of university buildings. The committee makes recommendations in respect of Departmental requests for minor works, and renewal of space and liases with Properties and Services with regard to planned and reactive maintenance procedures in the Faculty.

2011 - 2013, 2016 **Faculty IT Committee Member member**

Jan 2006 - Dec 2014 **Faculty Exam Committee member**
As a student advisor, I have been involved in the pre-FEC and FEC meetings for a number of years.

2014-2016 **Faculty Communication and Marketting Committee**

Faculty Selection Committees

2016 Lecturer/Senior Lecturer/Associate Professor, Department of Computer Science
+ Lecturer, Department of Physics
2015 Lecturer, Department of Computer Science
2014 Professor, Department of Computer Science
2012 Senior Secretary, Department of Computer Science
2011 Senior Lecturer, Department of Computer Science
Lecturer, Astronomy Department
2007 System Administrator, Department of Computer Science
Lecturer, Department of Chemistry

Administration

Departmental Level

Jan 2015 - present **Convenor: CS Honours**
I convene the following three courses, which are broadly included under the title *Honours in Computer Science*: CSC4000W, CSC4016W and CSC4003W.

Jan 2006 - Dec 2014 **Undergraduate Student Advisor:**
provided guidance on curriculum choice and study methods to undergraduates and on the Faculty exam committee.

Dec 2015 - present **Colloquium organiser:** Managing and booking departmental seminars and colloquia.

Dec 2010 - present **Departmental Fire Marshall**

Reviewing

Journal articles

- *2012-2018*: Analytical Chemistry (1), Astronomy and Computing (1), Bioinformatics (5), Biopolymers (1), Carbohydrate Research (4), Cellulose (2), Computers and Geosciences (1), Frontiers in Microbiology(1), International Journal of Computational Science and Engineering (1), Journal of Chemical Theory and Computation (2), Journal of Computational Chemistry (1), The Journal of Physical Chemistry (1), PLOS ONE (1), Powder Technology(2), South African Computer Journal (5), South African Journal of Chemistry (1)

Peer-Reviewed Conferences

ISC WOIV *2016*: Program Committee member for the ISC Workshop on In-Situ Visualization.

SACLA *2014-2016*: Program Committee member for the Annual Conference of the South African Computer Lecturers' Association Conference.

SAICSIT *2011, 2012, 2015-2017*: Program Committee member for the Annual Conference of the South African Institute of Computer Scientists and Information Technologists

Review Panels

- **BBSRC** *2012*: Biotechnology and Biological Sciences Research Council of the UK Peer Reviewer.

NRF *2011, 2014, 2015*: Member of an adjudication panel for National Research Foundation research funding applications. Application reviewer for applications.

Thesis examination

- *2011-2018*: University of the Witwatersrand (2 M.Sc), Rhodes University (1 Ph.D, 2 MSc), Stellenbosch University (1 M.Sc.), University of South Africa (1 M.Sc.), Internal UCT examiner (7 M.Sc)

Workshops

GPGPU *2013, 2014 & 2015*: Organiser of three workshops (GPGPU, GPGPU2, GPGPU2015) on general purpose programming of graphics processing units (GPGPU): http://gpu.cs.uct.ac.za.

SCAW *2004, 2006, 2007*: **Scientific Clustering Applications Workshops co-organiser.** This series of workshops aimed to stimulate discussion and interaction within the fledgling parallel computing community in South Africa.

WATOC2005 *2002-2005*: Treasurer for the 7th Congress of the World Association of Theoretically Oriented Chemists, Cape Town International Convention Center, 16-21 January 2005.

Outreach

- **Computer Club** *2012-2015*: Taught a free club at Greenfield Girls Primary teaching girls to program in Scratch (scratch.mit.edu).

Olympiad *2007-2011*: Trustee and member of the Scientific Board of the South African Computer Olympiad, a programming competition for school children.

Societies

Professional Society Membership

2006 - present: American Chemical Society - Divisions of Computers in Chemistry (COMP) and Carbohydrate Chemistry (CARB)

2011 - present: IEEE and IEEE Computer Society.

2012 - present: South African Institute of Computer Scientists and Information Technologists (SAICSIT)

2014 - present: British Computer Society (BCS), The Chartered Institute for IT. Educational Affiliate Employee Member