Michelle Mary Kuttel

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Qualifications

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

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*

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

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)

2020 *Molecular Modeling of the Shigella flexneri Serogroup 3 and 5 O-Antigens and Conformational Relationships for a Vaccine Containing Serotypes 2a and 3a.* J. Hlozek, S. Owen, N. Ravenscroft and M. M. Kuttel*, **Vaccines** 8, 643 (2020) DOI:10.3390/vaccines8040643

\+ *Mechanistic Study of Potent Fluorinated EGFR Kinase Inhibitors with a Quinazoline Scaffold against L858R/T790M/C797S Resistance Mutation: Unveiling the Fluorine Substituents Cooperativity Effect on the Inhibitory Activity.* F. B. Akher* , A. Farrokhzadeh, N. Ravenscroft, and M. M. Kuttel, **J. Phys. Chem. B.** 124:28, 5813?5824 (2020) DOI:10.1021/acs.jpcb.0c03440.

\+ *Cryptococcus neoformans capsular GXM conformation and epitope presentation: a molecular modelling study.* M. M. Kuttel*, A. Casadevall and S. Oscarson, **Molecules** 25:11, 2651 (2020). DOI:10.3390/molecules25112651.

\+ *Effects of Glucosylation and O-Acetylation on the Conformation of Shigella flexneri Serogroup 2 O-Antigen Vaccine Targets.* J. Hlozek, N. Ravenscroft, and M. M. Kuttel*, **J. Phys. Chem. B.** 124:14, 2806-2814 (2020). DOI:10.1021/acs.jpcb.0c01595.

2019 *Modeling the conformations of Neisseria meningitidis serogroup A CPS and a carba-analogue: implications for vaccine development.* J. Hlozek, N. Ravenscroft, and M. M. Kuttel*, **Carbohyd. Res.** 486, Article 107838, (2019). DOI:10.1016/j.carres.2019.107838.

\+ *A Mechanistic Study of a Potent and Selective Epidermal Growth Factor Receptor (EGFR) Inhibitor against L858R/T790M Resistance Mutation* Farideh Akher, Abdolkarim Farrokhzadeh*, Neil Ravenscroft, Michelle Kuttel, **Biochemistry**, 58:41, 4246-4259 (2019), DOI:10.1021/acs.biochem.9b00710

\+ *O-acetylation of typhoid capsular polysaccharide confers polysaccharide rigidity and immunodominance by masking additional epitopes.* K. Hitri, M. Kuttel, G.i De Benedetto, K. Lockyer, F. Gao, P. Hansal, T. R. Rudd, E. Beamish, S. Rijpkema, N. Ravenscroft, B. Bolgiano*, **Vaccine**, 37: 3866-3875 (2019). DOI: 10.1016/j.vaccine.2019.05.050

\+ *Conformation and cross-protection in Group B Streptococcus serotype III and Streptococcus pneumoniae serotype 14: a molecular modeling study.* M. M. Kuttel*, N. Ravenscroft, **Pharmaceuticals**, 12: 28 (2019). DOI: 10.3390/ph12010028

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.

Publications

Journal Articles contd. (* **denotes corresponding author**)

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)

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).

Publications

Peer-Reviewed Conference Proceedings cont.

SAICSIT 16-18 Sept. 2019 *Skukuza* *South Africa*	*A scalable database model of RFI data for MeerKAT radio telescope,* Gerald Nathan Balekaki, Michelle Kuttel, Sarah Blyth, Anja Schroeder **SAICSIT '19 Proceedings of the 2019 Annual Research Conference on South African Institute of Computer Scientists and Information Technologists**, doi: 10.1145/3351108.3351127
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.
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**, 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 (listing 2017-2019 only)

25-31 Aug.. 2019
Milan, Italy

Abstracts: **Glyco25: XXV International Symposium on Glycoconjugates**, *Capsular polysaccharide antigens: unravelling the helical hypothesis.* M. M. Kuttel*, N. Ravenscroft, **Glycoconj J** 36:4, 253 (2019).

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
Lisbon, 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

Invited Seminars

(2016-present only)

21 August 2019
GSK, Siena, Italy

A role for molecular modelling in glycoconjugate vaccine design: case studies from meningococcus.
Invited talk for GSK Vaccines Institute for Global Health.

28 August 2018
FDA, Silver Spring MD, USA

Molecular modelling and vaccine design: case studies from pneumococcus and cryptoccoccus.
Invited talk for FDA/CBER/Laboratory of Polysaccharides.

29 August 2017
Pfizer Inc, NY, USA

Polysaccharide Structure/Conformation: role in glycoconjugate vaccines.
Invited talk for Pfizer Pearl River facility.

June 2016
U. Malaga, Spain

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

Research Funding

	Grant	Collaborators
Current grants		
11/2017-11/2022 **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
grad. April 2019	Samuel Mabakane	Ph.D*	*Novel visualizations for optimization of parallel programs*
grad. April 2018	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
grad. June 2011	Ian Tunbridge	PhD*	*Course-grained Simulation of Protein Docking with Graphics Processing Units*, Co-supervisor: Dr James Gain
to grad. Dec. 2020	Alex Fourie	M.Sc$^+$	*Conformational analysis of E. Coli carbohydrate antigens*
to grad. Dec. 2020	Audrey Penz	M.Sc$^+$	*Designing useful ways to support mid-career professionals in creating better financial futures.*
grad. April 2019	Adrianna Pinska	M.Sc.	*Accelerated Coarse-Grained Molecular Dynamics Simulations of Protein-Protein Docking*, Co-supervisor: Assoc. Prof. James Gain
grad. April 2019	Edmore Tutsirayi Moyo	MSc	*Accelerated NeuroEvolution of Augmenting Topologies on a Heterogeneous System Architecture* , Co-supervisor: Dr Geoff Nitschke
grad. Dec. 2018	Kumbirai Chigudu	M.Sc$^+$	*Design of a Prototype Mobile Application Interface for Efficient Accessing of Electronic Laboratory Results by Health Clinicians*
grad. April 2017	Zaheer Timol	M.Sc.	*Chemical and conformational studies of bacterial cell surface polysaccharide repeating units.*, Principal Supervisor: Neil Ravenscoft (Chemistry)
grad. Dec 2015	Genevieve Chang	M.Sc$^+$	*Designing an effective carbohydrate-building application user interface for the Android tablet environment.*
grad. June 2015	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
grad. June 2015	Scott Badenhorst	M.Sc.	*HPC acceleration of astronomical H1 source detection.*, Co-supervisor: Dr Sarah Blyth (UCT Astronomy)
grad. Dec 2014 degree with distinction	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)
grad. Dec 2014	Andrew Potgieter	M.Sc$^+$	*Parallelization of the Weighted Histogram Analysis Method*
grad. Jun 2014 degree with distinction	Duncan Clough	M.Sc.	*Fluid Dynamics*, Principal Supervisor: Assoc. Prof. James Gain
grad. Dec 2013 degree with distinction	Neann Mathai	M.Sc.	*Molecular modelling of the* Streptococcus Pneumoniae *serogroup 6 capsular polysaccharide antigens.*, Co-supervisor: Assoc. Prof. Neil Ravenscroft (Chemistry)
grad. Dec 2013	Richard Baxter	M.Sc.	*GPU-based Acceleration of Radio Interferometry Point Source Visibility Simulations in the MeqTrees Framework*, Principal Supervisor: Patrick Marais
grad. Dec 2010	Rudolf van den Berg	M.Sc.$^+$	*Force-extension of the Amylose Polysaccharide*
grad. Dec 2010	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
grad. Dec 2009 degree with distinction	Juan-Pierre Longmore	M.Sc.	*Realistic Interactive Sand: A GPU-based Framework*, Principal Supervisor: Dr Patrick Marais
grad. Dec 2009	Ashley Reid	M.Sc.	*Practical Fluid Dynamics for the Animation Industry*, Principal Supervisor: Dr James Gain
grad. Jun 2009 degree with distinction	Peter McMahon	M.Sc.	*Accelerating Bioinformatics Applications using Reconfigurable Computers*
grad. Dec 2008	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

Leadership & Responsibility

2019 **External examiner**
External examiner for the "Big Data" Masters level module, Department of Computer Science, University of Pretoria, South Africa.

2016-2018 **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.

2012-2020 **Journal article reviewer**
Analytical Chemistry (1), Astronomy and Computing (1), Beilstein Journal of Organic Chemistry (1), Bioinformatics (5), Biopolymers (1), Carbohydrate Research (7), Cellulose (2), Computers and Geosciences (1), Frontiers in Microbiology(1), International Journal of Computational Science and Engineering (1), International Journal of Molecular Sciences (1), Journal of Chemical Theory and Computation (3), Journal of Computational Chemistry (1), Journal of Molecular Graphics and Modelling (1), The Journal of Physical Chemistry (2), MDPI Molecules (2), PLOS ONE (2), Powder Technology (2), Pure and Applied Chemistry (1), South African Computer Journal (6), South African Journal of Chemistry (1)

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**.