NITheCS

National Institute for
Theoretical and Computational Sciences

ANNUAL REPORT 2023

'Science knows no country, because knowledge belongs to humanity, and is the torch which illuminates the world. Science is the highest personification of the nation because that nation will remain the first which carries the furthest the works of thought and intelligence.'

~ Louis Pasteur

CONTENTS

ABBREVIATIONS

AIMS	African Institute for Mathematical Sciences
CHPC	Centre for High Performance Computing
CNRS	National Centre for Scientific Research
CoE-MaSS	Centre of Excellence in Mathematical and Statistical Sciences
CSIR	Council for Scientific and Industrial Research
DSI	Department of Science and Innovation
ICTP	International Centre for Theoretical Physics
iThemba LABS	iThemba Laboratory for Accelerator Based Sciences
MUT	Mangosuthu University of Technology
NMU	Nelson Mandela University
NRF	National Research Foundation
NWU	North-West University
RU	Rhodes University
SADiLAR	South African Centre for Digital Language Resources
SANBI	South African National Biodiversity Institute
SASA	South African Statistical Association
SU	Stellenbosch University
UCT	University of Cape Town
UFS	University of the Free State
UJ	University of Johannesburg
UKZN	University of KwaZulu-Natal
UL	University of Limpopo
UNISA	University of South Africa
UNIVEN	University of Venda
UNIZULU	University of Zululand
UP	University of Pretoria
UWC	University of the Western Cape
WITS	University of the Witwatersrand

REPORT OF THE INTERIM DIRECTOR

During 2023 NITheCS continued on its path to becoming a fully-fledged legal entity. An important milestone was reached with the announcement towards the end of the year by the Department of Science and Innovation (DSI) and the National Research Foundation (NRF) that Stellenbosch University (SU) had been awarded a consortium application bid to host NITheCS.

Since its formation in 2021, NITheCS has pursued its transformative path with a small administrative staff. Despite our growing list of programmes, events and initiatives to support our eight thematic science areas, the Institute's own infrastructure remains small and focused. We lean heavily on the collaborative and distributed structure of our more than 270 Associates and other collaborators to focus on our goals and, importantly, the critical significance of diversity and equity. With the new hosting arrangement at SU, we will be able to offer our services to 26 local universities and several scientific institutions from 2024.

The level of expertise among our Associates becomes evident when one realises that each Associate holds at least a PhD in one of the eight relevant disciplines we represent. While their own contributions are vital for the local scientific community, they play a vital role in supporting and participating in the exchange and discussion of new scientific developments and in training young scientists through colloquiums, mini-schools and other NITheCS events. We are positive about the role of NITheCS in strengthening the basic sciences in South Africa and invite and appreciate input to the work related to our eight core themes.

A pipeline for students

As a key driving factor of our work, we aim to establish a student pipeline from undergraduate to postgraduate to postdoc and early career, while also addressing socio-economic development through training and research. To do this we employ different techniques. Among others, we present or support many events aimed at training and research – from mathematics training and support, to computer programming and scientific communication skills.

Our events are tailored towards collaboration and interaction between disciplines: our mini-schools and colloquiums are aimed not only at specialists, but also generalists and those interested in the work of other scientists. Importantly, many of our events take place as hybrid events. The aim of this is to be inclusive and allow access to participants in areas that are further afield. For this reason, most of our events are also available for online viewing after being presented.

Another approach is to support the work of some of our institutional Associates, such as the Carpentries, who present online training courses. We also publicise events presented by other organisations working in the science field, and particularly those of Associates' bodies.

Acknowledgements

We remain indebted to the local and international experts who have been supporting our growth and progress during 2023. In particular, we thank the NITheCS Steering Committee for its support and guidance under the leadership of Dr Happy Sithole. As of 2024, the Steering Committee has been dissolved under the new management arrangement with SU. However, we will still lean heavily on the wisdom and guidance of the Management Committee and Scientific Advisory Board, as each person's contribution to our activities takes us closer to achieving our aims.

This annual report contains details about the people who make NITheCS work as well as the related activities. We also report back among others on our research programmes, communication and outreach work.

Lastly, my appreciation goes to the hard working team of office staff and support specialists who ensure the NITheCS wheels keep turning in the direction of reaching our overall objectives.

Francesco Petruccione
Interim Director: NITheCS

SHORT BIOGRAPHY:

Prof Francesco Petruccione

Italian-born Francesco Petruccione is a physicist and academic leader, serving as both a professor at Stellenbosch University and the interim director of NITheCS.

He pursued his undergraduate studies in physics at the University of Freiburg, Germany, where he earned his first degree in the field. He continued his academic journey at the same institution, earning his doctorate in 1988 and his Habilitation degree (Dr. rer. nat. habil.) in 1994.

In 2004, he became a professor of Theoretical Physics at UKZN. A year later, he was awarded an Innovation Fund grant to establish a Centre for Quantum Technology. Prof Petruccione went on to hold the position of South African Research Chair for Quantum Information Processing and Communication Technology in 2007.

In addition to his role as interim director of NITheCS, Prof Petruccione also held an adjunct professor position at the Korean Advanced Institute for Science and Technology. In 2018, he was appointed Pro Vice-Chancellor of Big Data and Informatics at UKZN. Four years later, he moved to Stellenbosch University as a professor of Physics and Quantum Computing in the Physics Department and the School of Data Science and Computational Thinking.

Prof Petruccione is highly regarded in his field. In 2023 he was honoured with the title of *Cavaliere della Stella d'Italia*, or Order of the Star of Italy, at a function at the Italian Embassy in Cape Town for his groundbreaking work in physics and quantum computing.

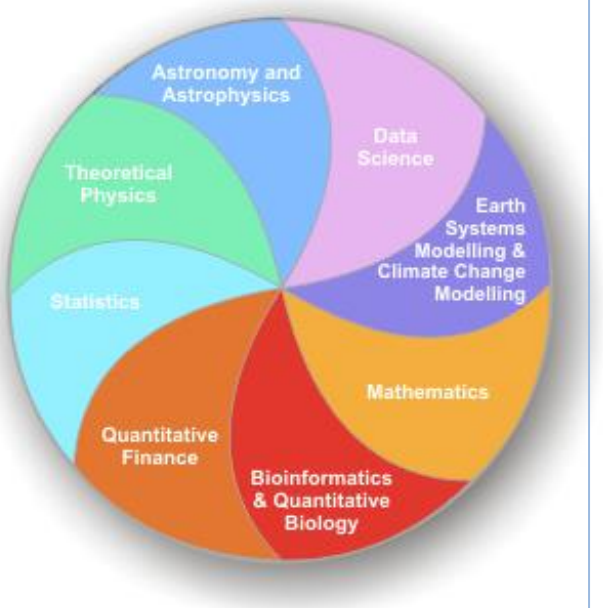
NITheCS OVERVIEW

The National Institute for Theoretical and Computational Sciences (NITheCS) is part of the South African science, technology and innovation landscape. The Institute is supported among others by the South African Institute of Physics (SAIP), the Department of Science and Innovation (DSI) and the National Research Foundation (NRF).

The Institute's activities are specific to eight thematic areas in which applied science is fostered, and its emphasis is on moving science from research to impact. The thematic areas are seen in the graphic on the right.

South Africa's research capabilities depend on supporting scientists with programmes and activities relating to underlying scientific principles and recent achievements. Sustaining the foundational role of the theoretical and computational sciences requires a collaborative effort by among others the scientific community, relevant government organisations, academia and research institutes, as well as private sector financial supporters. As such, NITheCS also has a vital role in transforming society and driving forward the scientific understanding among all societal groups.

Some of the activities through which NITheCS conducts its work include regular colloquiums and mini-schools, internships, summer schools, other presentations and networking opportunities. Among others, NITheCS also encourages visits from local and international scientists, supports bursary holders, facilitates research opportunities and encourages community service.



Thematic areas of NITheCS

Key Strategic Objectives

The key strategic objectives of NITheCS are to:

- achieve equitable participation of all SA communities in its activities,
- support the pipeline of students from undergraduate through postgraduate to postdoctoral research and their early career development,
- help strengthen basic scientific endeavour in the country,
- support historically disadvantaged institutions (HDIs),
- address socio-economic development through training and research, and
- support major science programmes.

Structure

Towards the end of 2023 the Department of Science and Innovation (DSI) and the National Research Foundation (NRF) announced that Stellenbosch University had been awarded the consortium application bid to host NITheCS.

Spearheaded by Prof Sibusiso Moyo, Deputy Vice-Chancellor: Research, Innovation and Postgraduate Studies, an SU consortium had submitted a multi-thematic application to the NRF and the DSI, which was assessed through a single-phase peer review process.

Although already formed in 2021, NITheCS is still in a transformative phase. The successful allocation to SU to host the Institute is the first and very important step to establish NITheCS as a legal entity.

Governance

The NITheCS governance system is that of a national Centre of Excellence (CoE), which is subject to the notarisation of a binding contract between the granter, the National Research Foundation (NRF), and the grantee, namely Stellenbosch University.

NITheCS operates in an independent environment, with Stellenbosch University providing administrative support.

The Institute has a management committee and a Scientific Advisory Board.

Management committee	Scientific Advisory Board
The NITheCS management committee comprises: • Interim Director: Francesco Petruccione (SU) • Deputy Director: Joao Rodrigues (Wits) • Deputy Director: Sunil Maharaj (UKZN) • Associate Representative: William Horowitz (UCT) • Associate Representative: Zurab Janelidze (SU)	• Mary-Jane Bopape (NRF–SAEON) • Sekazi Mtingwa (US Nuclear Regulatory Commission) • Adrian Mulholland (University of Bristol) • Petros Ntoahae (UL) • Daya Reddy (UCT) • Spenta Wadia (International Centre for Theoretical Sciences, India) • Scott Woodley (University College London)

Steering Committee (has since been dissolved)

The NITheCS Interim Steering Committee (STEERCOM) was dissolved in late 2023. The following people served on the committee:

Chairman		Dr Happy Sithole, Director of the CHPC at the CSIR
Interim Director of NITheCS *(ex officio)*		Prof Francesco Petruccione (SU)
Members	**Statistics**	President of SASA: Dr Warren Brettenny (NMU)
	Mathematics	Director of AIMS: Prof Barry Green Director of CoE-MaSS: Prof Fazal M Mahomed (WITS)
	Astronomy	SARAO representative: Ms Kim de Boer
	Biosciences	Professor in Computational Biology: Prof Nicola Mulder (UCT) SANBI: Dr Monica Mwale
	Quantitative Finance	Senior lecturer in the department of Statistics and Actuarial Science: Dr Mesias Alfeus (SU)
	CHPC	Director of the CHPC: Dr Happy Sithole
	Climate modelling	Professor in Climate Modelling: Prof Francois Engelbrecht (WITS)
	Theoretical Physics	Professor in Theoretical Physics: Prof Amanda Weltman (UCT) NITheCS Management: Prof João Rodrigues (WITS)
	Data Science	Director of the Stellenbosch School of Data Science and Computational Thinking: Prof Kanshukan Rajaratnam (SU) Manager: Data Intensive Research Initiative of South Africa (DIRISA)/NICIS: Dr Anwar Vahed (DIRISA)
	Industry (banking/finance sector)	Head of Advanced Analytics at First National Bank: Dr Mark Nasila
	NRF	Main member: Executive Director of the Research Chairs and Centres of Excellence, NRF: Dr Makobetsa Khati Alternate: Director of the Centres of Excellence, NRF: Mr Nathan Sassman
	DSI	Director of Basic Sciences: Dr Sagren Moodley

OUR PEOPLE

Staff profile

NITheCS has a small administrative staff. For its main activities, the Institute has a collaborative and distributed structure that focuses on, among others, the critical importance of diversity and equity.

The staff profile of NITheCS as at 31 December 2023 is as below:

Directorate

Position/Hours expressed as a portion of an 8-hour workday	Institution	Number of staff members	Portion of workday expressed as percentage of full day
Interim Director: Francesco Petruccione/ 8/8	Stellenbosch University	1	1
Deputy Director Sunil Maharaj/ 1.6/8	University of KwaZulu-Natal	1	0.2
Deputy Director João Rodrigues/ 1.6/8	University of the Witwatersrand	1	0.2
TOTAL		**3**	**1.4**

Administrative staff

Position/Portion of an 8-hour workday	Institution	Number of staff members	Portion of workday expressed as percentage of full day
Institute Manager: René Kotze/ Full day	Stellenbosch University	1	1
Operations Manager: Neli Mncube/ Full day	University of KwaZulu-Natal	1	1
Admin Officer: Farah-Naaz Moosa/ Half day	University of the Witwatersrand	1	0.5
TOTAL		**3**	**2.5**

Outsourced services

Position	Number of persons	Portion of workday expressed as percentage of full day
Science Writer: Lia Labuschagne	1	0.375
Website and Content Manager / IT / Graphic Design: Belinda Virét	1	0.625
TOTAL	**2**	**1**

Internship(s)/Capacity Development staff

Position/hours expressed as a portion of an 8-hour workday	Number of persons	Portion of workday expressed as percentage of full day
Aluwani Guga PhD student 2/8	1	0.25
Thuthukile Khumalo PhD student 2/8	1	0.25
TOTAL	**2**	**0.50**

Postdoctoral fellows

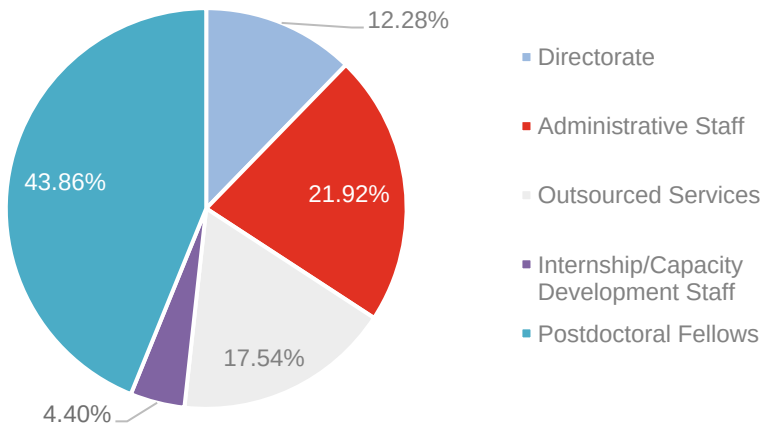
The postdoctoral fellows per node as at 31 December 2023 are shown below. All positions are two-year contracts.

NITheCS node	Number of postdocs	Names of postdocs
Stellenbosch University	3	Dr Lehlohonolo Mongalo (South African) contract ended 31 January 2023 Dr Graeme Pleasance (South African) Dr Danial Saadadatmand (Iranian)
University of KwaZulu-Natal	0	None at present
University of the Witwatersrand	3	Dr Atanu Bhatta (Indian) Dr Yannick Mvondo-she (Cameroonian) Dr Mbavhalelo Mulokwe (South African)
TOTAL	**6**	

Staff statistics

Staff category	Number of staff per category (expressed in full-time hours)
Directorate	1.40
Administrative Staff	2.50
Outsourced Services	1.00
Internship/Capacity Development staff	0.50
Postdoctoral Fellows	5.00
TOTAL STAFF MEMBERS	**11.40**

Staff category, expressed as a percentage of the total:



ASSOCIATES

Associates overview

NITheCS is indebted to its national network of Associates throughout South Africa for its vital contribution to achieving the Institute's strategic goals. The strength and growth of our Associate numbers is particularly important: this supports the NITheCS aim to maintain strong international links and guarantees cooperation with relevant global partners while ensuring the Institute remains comparable with its counterparts across the world.

Benefits to Associates

Associates of NITheCS have the advantage of affiliation with a national institute. Associates are invited to present talks at NITheCS events such as colloquiums and mini-schools. In addition to opportunities to network, NITheCS also offers Research Programmes with the aim to encourage collaboration between researchers from various institutions. There are also conferences, workshops, mobility programmes, visitor programmes and student internships under the leadership of NITheCS Associates.

Contact with peers made via NITheCS and at NITheCS events often leads to collaborative efforts.

Requirements to become an Associate

Individual Associate:

- PhD in one of the eight NITheCS thematic areas (mid to senior career level)
- List of publications
- Works at South African university or relevant industry.

Junior Associate:

- Currently enrolled for a PhD degree in one of the eight NITheCS thematic areas, or a South African postdoc
- List of publications
- Employed at a South African university or in a relevant industry

Institutional Associate:

An organisation or institution that:

- specialises in any of the NITheCS thematic areas
- has access to a wealth of knowledge, resources and infrastructure
- has expertise and commitment to scientific research and innovation advance science and technology.

Strategic Assoicate:

- Individuals who do not directly operate within the eight NITheCS themes,
- Position or influence within their fields, which allows them to act as ambassadors, advocates and catalysts for change, thereby helping to drive our mission.

By the end of 2023, NITheCS had more than 270 Individual Associates who represent all the relevant thematic areas covered by NITheCS. The names of Associates are published in this report and also appear on the NITheCS website.

Associate Representatives

An Associate is selected every four years to serve as Associate Representative to represent the body of Associates at NITheCS strategic meetings. NITheCS currently has two Associate Representatives: Prof Will Horowitz (UCT) and Prof Zurab Janelidze (SU).

Prof Will Horowitz (UCT)

Prof Zurab Janelidze (SU)

General administration and responsibilities

Although NITheCS Associates have no set responsibilities, the Institute encourages its Associates to present talks or lectures at our events and supervise interns on our internship programme. Calls are also issued for Associates to assist us in disseminating information to their communities, such as spreading the word about student training or outreach programmes.

Associates' details and statistics

As at 31 December 2023, the NITheCS Associates are:

Individual Associates (275)

Astronomy/Astrophysics (24)

1. Prof Amare Abebe (North-West University)
2. Dr Geoffrey Beck (University of the Witwatersrand)
3. Prof Andrew Chen (University of the Witwatersrand)
4. Prof Roger Deane (University of the Witwatersrand)
5. Dr Marisa Geyer (SKA Observatory)
6. Prof Matt Hilton (University of the Witwatersrand)
7. Prof Deepak Kar (University of the Witwatersrand)
8. Dr Michael Kosch (SANSA)
9. Prof Lerothodi Leeuw (University of the Western Cape)
10. Dr Michelle Lochner (University of the Western Cape)
11. Dr Stefan Lotz (South African National Space Agency)
12. Prof Ilani Loubser (North-West University)
13. Dr Lucia Marchetti (University of Cape Town)
14. Dr Daniel Moeketsi (Council for Scientific and Industrial Research)
15. Dr Teboho Moloi (University of Cape Town)
16. Dr Jack Radcliffe (University of Pretoria)
17. Prof Subharthi Ray (University of KwaZulu-Natal)
18. Prof Soebur Razzaque (University of Johannesburg)
19. Prof Mattia Vaccari (University of Cape Town)
20. Prof Sivakumar Venkataraman (University of KwaZulu-Natal)
21. Prof Christo Venter (North-West University)
22. Prof Patricia Whitelock (University of Cape Town)
23. Prof Hartmut Winkler (University of Johannesburg)
24. Prof Patrick Woudt (University of Cape Town)

Bioinformatics and Quantitative Biology (26)

1. Prof Matthew Adeleke (University of KwaZulu-Natal)
2. Dr Clement Agoni (University of KwaZulu-Natal)
3. Prof Tulio de Oliveira (Stellenbosch University)
4. Prof Morne du Plessis (National Institute For Communicable Diseases)
5. Prof Catharine Esterhuysen (Stellenbosch University)
6. Prof John Hargrove (Stellenbosch University)
7. Dr Uljana Hesse (University of the Western Cape)
8. Prof Cang Hui (Stellenbosch University)
9. Prof Tjaart Kruger (University of Pretoria)
10. Dr Pietro Landi (Stellenbosch University)
11. Dr Sandra MacFadyen (Stellenbosch University)
12. Prof Alen Manyevere (University of Fort Hare)
13. Dr Kim Martin (Stellenbosch University)
14. Prof Guy Midgley (Stellenbosch University)
15. Dr Monica Mwale (South African National Biodiversity Institute)
16. Prof Olugbenga Oluwagbemi (Sol Plaatje University)
17. Prof Hugh-George Patterton (Stellenbosch University)
18. Dr Ethel Phiri (Stellenbosch University)
19. Dr Ché Sobashkar Pillay (University of KwaZulu-Natal)
20. Dr Verena Ras (University of Cape Town)
21. Prof Peter Scogings (University of KwaZulu-Natal)
22. Prof Paul Sumner (University of Fort Hare)
23. Prof Özlem Taştan Bishop (Rhodes University)
24. Dr Fidele Tugizimana (University of Johannesburg)
25. Prof Cari van Schalkwyk (Stellenbosch University)
26. Prof Vernon Visser (University of Cape Town)

Data Science (40)

1. Dr Jean Bashingwa (University of Cape Town)
2. Dr Stella Bvuma (University of Johannesburg)
3. Prof Kelvin Bwalya (University of Johannesburg)
4. Prof Roelof Coetzer (North-West University)
5. Prof Marelie Davel (North-West University)
6. Prof Anton Du Plessis (Stellenbosch University)
7. Dr Emmanuel Dufourq (Stellenbosch University)
8. Dr Marcel Dunaiski (Stellenbosch University)
9. Dr Samuel Egieyeh (University of the Western Cape)
10. Prof Absalom El-Shamir Ezugwu (North-West University)
11. Prof Richard Harris (University of the Free State)
12. Dr Edgar Jembere (University of KwaZulu-Natal)
13. Dr Sydney Kasongo (Stellenbosch University)
14. Prof Langa Khumalo (North-West University)
15. Prof Rodney Kroon (Stellenbosch University)
16. Dr Adriana Marais (Stellenbosch University)
17. Prof Alan Matthews (University of KwaZulu-Natal)
18. Prof Thomas Meyer (University of Cape Town)
19. Dr Thipe Modipa (University of Limpopo)
20. Prof Deshen Moodley (University of Cape Town)
21. Dr Alfred Mwanza (Sol Plaatje University)
22. Dr Pieter Neethling (Stellenbosch University)
23. Prof Clement Nyirenda (University of the Western Cape)
24. Dr Ibidun Obagbuwa (Sol Plaatje University)
25. Dr Michael Olusanya (Sol Plaatje University)
26. Prof Babu Paul (University of Johannesburg)
27. Dr Mpho Raborife (University of Johannesburg)
28. Prof Kanshukan Rajaratnam (Stellenbosch University)
29. Prof Benjamin Rosman (University of the Witwatersrand)
30. Dr Makhamisa Senekane (University of Johannesburg)
31. Dr Fritz Solms (Stellenbosch University)
32. Prof Christine Steenkamp (Stellenbosch University)
33. Dr Lynndle Square (North West University)
34. Prof Hossana Twinomurinzi (University of Johannesburg)
35. Dr William Vambe (Walter Sisulu University)
36. Prof Darelle van Greunen (Nelson Mandela University)
37. Prof Menno van Zaanen (North-West University)
38. Prof Serestina Viriri (University of KwaZulu-Natal)
39. Prof Bruce Watson (Stellenbosch University)
40. Prof Sahal Yacoob (University of Cape Town)

Earth Systems Modelling & Climate Change Modelling (10)

1. Dr Mary-Jane Bopape (NRF-SAEON)
2. Prof Roelof Burger (North-West University)
3. Dr Thama Duba (University of the Witwatersrand)
4. Prof Francois A. Engelbrecht (University of the Witwatersrand)
5. Prof Tafadzwanashe Mabhaudhi (University of KwaZulu-Natal)
6. Dr Mohau Mateyisi (Council for Scientific and Industrial Research)
7. Prof Guy Midgley (Stellenbosch University)
8. Dr Shingirai Nangombe (Council for Scientific and Industrial Research)
9. Prof Abel Ramoelo (University of Pretoria)
10. Prof Colleen Vogel (University of the Witwatersrand)

Mathematics (54)

1. Prof Dharmanand Baboolal (University of KwaZulu-Natal)
2. Prof Bubacarr Bah (African Institute for Mathematical Sciences)
3. Dr Liam Baker (Stellenbosch University)
4. Prof Jacek Banasiak (University of Pretoria)
5. Prof Mapundi Banda (University of Pretoria)
6. Prof Aroonkumar Beesham (Mangosuthu University of Technology)
7. Dr Ronalda Benjamin (Stellenbosch University)
8. Prof Gareth Boxall (Stellenbosch University)
9. Dr Byron Brassel (Durban University of Technology)
10. Prof Willem Conradie (University of the Witwatersrand)
11. Dr Andrew Craig (University of Johannesburg)

12. Dr Patrick Djomegni (North-West University)
13. Prof Themba Dube (University of South Africa)
14. Dr Partha Pratima Ghosh (University of South Africa)
15. Dr Amartya Goswami (University of Johannesburg)
16. Dr James Gray (Stellenbosch University)
17. Dr Mandlenkosi Gwetu (University of KwaZulu-Natal)
18. Prof Yorick Hardy (University of the Witwatersrand)
19. Dr Sheldon Herbst (University of Johannesburg)
20. Dr Michael Hoefnagel (Stellenbosch University)
21. Prof David Holgate (University of the Western Cape)
22. Prof Karin-Therese Howel (Stellenbosch University)
23. Prof Zurab Janelidze (Stellenbosch University)
24. Dr Tamar Janelidze-Gray (University of Cape Town)
25. Dr Wen-Chi Kuo (University of the Witwatersrand)
26. Dr Luke Oluwaseye Joel (University of Johannesburg)
27. Dr Eder Kikianty (University of Pretoria)
28. Dr Sophie Marques (Stellenbosch University)
29. Prof Fortuné Massamba (University of KwaZulu-Natal)
30. Prof Dephney Mathebula (University of South Africa)
31. Dr Simo Mthethwa (University of KwaZulu-Natal)
32. Dr Hendrik Jacobus Michiel Messerschmidt (University of Pretoria)
33. Dr Boitumelo Moletsane (University of the Witwatersrand)
34. Dr Rendani Netshikweta (University of Venda)
35. Prof Farai Nyabadza (University of Johannesburg)
36. Dr Nelson Kyakutwika (Stellenbosch University)
37. Dr Charles Msipha (Tshwane University of Technology)
38. Prof Inderasan Naidoo (University of South Africa)
39. Prof Loyiso Nongxa (University of the Witwatersrand)
40. Prof Olivier Otafudu (North-West University)
41. Prof Paran Pillay (University of the Western Cape)
42. Prof Helmut Prodinger (Stellenbosch University)
43. Dr Cerene Rathilal (University of KwaZulu-Natal)
44. Dr Riana Roux (Stellenbosch University)
45. Prof Thekiso Seretlo (North-West University)
46. Prof Charalampos (Haris) Skokos (University of Cape Town)
47. Dr Ridhwaan Suliman (Council for Scientific and Industrial Research)
48. Prof Sanne ter Horst (North-West University)
49. Prof Brink van der Merwe (Stellenbosch University)
50. Dr Francois van Niekerk (Stellenbosch University)
51. Dr Vivien Visaya (University of Johannesburg)
52. Prof Bruce Watson (University of the Witwatersrand)
53. Dr Dawit Worku (Cape Peninsula University of Technology)
54. Dr Bertin Zinsou (University of the Witwatersrand)

Quantitative Finance (22)

1. Prof Franck Adekambi (University of Johannesburg)
2. Dr Mesias Alfeus (Stellenbosch University)
3. Prof Conrad Beyers (University of Pretoria)
4. Dr Rechelle Jacobs (University of the Western Cape)
5. Prof Riaan de Jongh (North-West University)
6. Dr Hermann Donfack (University of Johannesburg)
7. Prof Michael Graham (Stellenbosch University)
8. Dr Michael Kateregga (Exigent-Group Limited & AIMS)
9. Dr Alexis Levendis (Momentum Metropolitan)
10. Prof Eben Maré (University of Pretoria and Absa)
11. Prof Farai Mhlanga (University of Limpopo)
12. Dr Chioma Okoro (University of Johannesburg)
13. Prof Daniel Polakow (Stellenbosch University)
14. Prof Charl Pretorius (North-West University)
15. Prof Helgard Raubenheimer (North-West University)
16. Prof Ronald Richman (Old Mutual Insure)
17. Prof Willem Schutte (North-West University)
18. Dr Mondisane Seitshiro (North-West University)
19. Dr Neill Smit (North-West University)
20. Prof David Taylor (University of Cape Town)
21. Dr Corli van Zyl (North-West University)
22. Prof Tanja Verster (North-West University)

Statistics (10)

1. Prof Andriette Bekker (University of Pretoria)
2. Prof Renette Blignaut (University of the Western Cape)
3. Prof Inger Fabris-Rotelli (University of Pretoria)
4. Prof Johannes Ferreira (University of Pretoria)
5. Prof Freedom Gumedze (University of Cape Town)
6. Dr Justin Harvey (Stellenbosch University)
7. Dr Shawn Carl Liebenberg (North-West University)
8. Prof Sugnet Lubbe (Stellenbosch University)
9. Prof Delia North (University of KwaZulu-Natal)
10. Prof Lizanne Raubenheimer (Rhodes University)

Theoretical Physics (89)

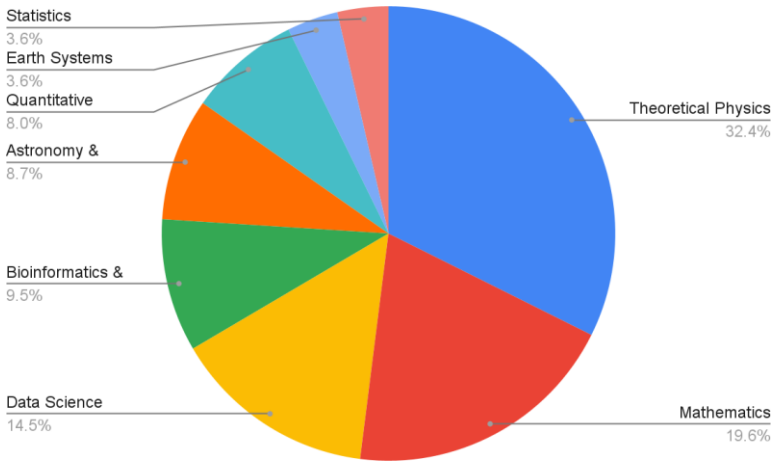
1. Prof Igor Barashenkov (University of Cape Town)
2. Dr Bruce Bartlett (Stellenbosch University)
3. Prof Bruce A Bassett (AIMS) (South African Astronomical Observatory) (University of Cape Town)
4. Prof Nigel Bishop (Rhodes University)
5. Prof Moritz Braun (University of South Africa)
6. Dr Jeandrew Brink (University of the Free State)
7. Prof Erwin Bruning (University of KwaZulu-Natal)
8. Prof Martin Bucher (University of KwaZulu-Natal)
9. Dr Hsin Cynthia Chang (University of KwaZulu-Natal)
10. Prof Hasani Chauke (University of Limpopo)
11. Prof Nithaya Chetty (University of the Witwatersrand)
12. Prof Fabio Cinti (Stellenbosch University)
13. Dr Chris Clarkson (University of Cape Town)
14. Prof Alan Cornell (University of Johannesburg)
15. Dr Alvaro de la Cruz Dombriz (University of Cape Town)
16. Prof Robert de Mello Koch (University of the Witwatersrand)
17. Prof Cesareo A Dominguez (University of Cape Town)
18. Prof Peter Dunsby (University of Cape Town)
19. Prof Rocco Duvenhage (University of Pretoria)
20. Prof Hans Eggers (Stellenbosch University)
21. Prof George Ellis (University of Cape Town)
22. Prof Stefan Ferreira (North-West University)
23. Prof Aurona Gerber (University of South Africa)
24. Prof Hendrik Geyer (Stellenbosch University)
25. Prof Irvy (Igle) Gledhill (University of the Witwatersrand)
26. Dr Kevin Goldstein (University of the Witwatersrand)
27. Dr Japie Greeff (North-West University)
28. Prof Shajid Haque (University of Cape Town)
29. Prof Dieter Heiss (Stellenbosch University)
30. Dr Shinji Hirano (University of the Witwatersrand)
31. Prof Will A. Horowitz (University of Cape Town)
32. Prof Vishnu Jejjala (University of the Witwatersrand)
33. Dr Anslyn John (Stellenbosch University)
34. Prof Daniel Joubert (University of the Witwatersrand)
35. Prof Steven Karataglidis (University of Johannesburg)
36. Dr Garreth Kemp (University of Johannesburg)
37. Prof Alex Kies (University of KwaZulu-Natal)
38. Dr Joseph Kirui (University of Venda)
39. Dr Isobel Kolbe (University of the Witwatersrand)
40. Prof Thomas Konrad (University of KwaZulu-Natal)
41. Dr Hannes Kriel (Stellenbosch University)
42. Prof Mantile Lekala (University of South Africa)
43. Dr Mawande Lushozi (University of Cape Town)
44. Prof Yin-Zhe Ma (University of KwaZulu-Natal)
45. Prof Roy Maartens (University of the Western Cape)
46. Prof Sunil Maharaj (University of KwaZulu-Natal)
47. Dr Adriana Marais (Stellenbosch University)
48. Prof Oluwole Daniel Makinde (Stellenbosch University)
49. Dr Eric Maluta (University of Venda)
50. Dr Refilwe Edwin Mapasha (University of Pretoria)
51. Prof Rapela Regina Maphanga (Council for Scientific and Industrial Research)
52. Prof Alan Joseph Michael Medved (Rhodes University)
53. Dr Peace Prince Mkhonto (University of Limpopo)

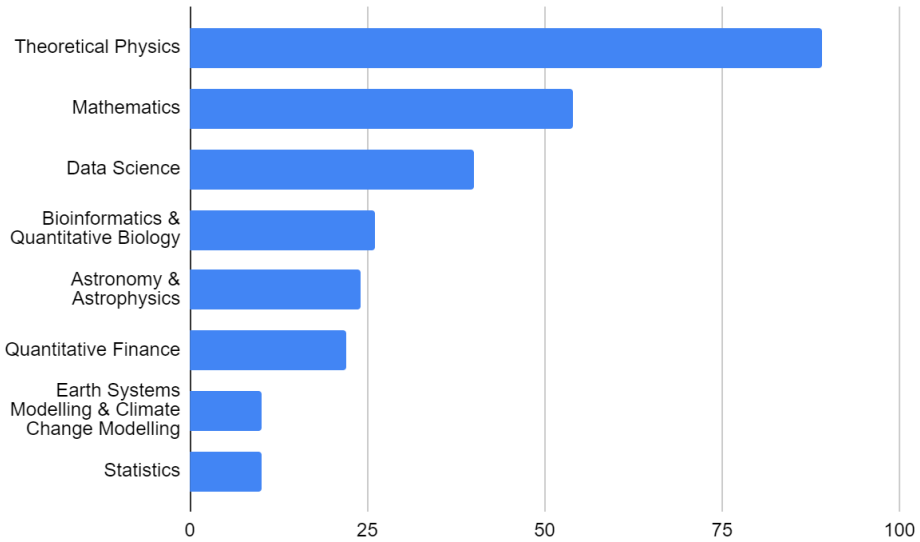
54. Dr Shazrene Mohamed (University of Cape Town/South African Astronomical Observatory)
55. Dr Bishop Mongwane (University of Cape Town)
56. Prof Kavilan Moodley (University of KwaZulu-Natal)
57. Prof Thuto Mosuang (University of Limpopo)
58. Prof Kristian Muller-Nedebock (Stellenbosch University)
59. Prof Azwinndini Muronga (Nelson Mandela University)
60. Prof Jeff Murugan (University of Cape Town)
61. Dr Kingsley Obodo (North-West University)
62. Prof Nico Orce (University of the Western Cape)
63. Dr Giuseppe Pellicane (University of KwaZulu-Natal)
64. Prof Andre Peshier (University of Cape Town)
65. Prof Denis Pollney (Rhodes University)
66. Prof Martin Porrmann (University of KwaZulu-Natal)
67. Prof Marius Potgieter (North-West University)
68. Prof Alex Quandt (University of the Witwatersrand)
69. Dr Abdulrafiu Raji (University of South Africa)
70. Prof Sergei Rakitianski (University of Pretoria)
71. Dr Stef Roux (Council for Scientific and Industrial Research)
72. Prof Frederik Scholtz (Stellenbosch University)
73. Prof Pavlo Selyshchev (University of Pretoria)
74. Dr Jonathan Shock (University of Cape Town)
75. Prof Ilya Sinayskiy (University of KwaZulu-Natal)
76. Dr Izak Snyman (University of the Witwatersrand)
77. Prof Du Toit Strauss (North-West University)
78. Prof Mark Tame (Stellenbosch University)
79. Dr Gary Tupper (University of Cape Town)
80. Dr Aniekan Magnus Ukpong (University of KwaZulu-Natal)
81. Dr Herman Uys (Stellenbosch University)
82. Prof Judy van Biljon (University of South Africa)
83. Prof Brandon van der Ventel (Stellenbosch University)
84. Dr Robert Warmbier (University of Johannesburg)
85. Prof Andre Weideman (Stellenbosch University)
86. Prof Herbert Weigel (Stellenbosch University)
87. Prof Heribert Weigert (University of Cape Town)
88. Prof Amanda Weltman (University of Cape Town)
89. Prof Konstantinos Zoubos (University of Pretoria)

NITheCS colloquium, presented by NITheCS Associate Dr Sophie Marques (SU) and Dr Leandro Boonzaaier (SU) at the Neelsie Cinema, Stellenbosch University in February 2023.

Individual Associates per theme

Theme	Number of Associates per theme
Astronomy and Astrophysics	24
Bioinformatics & Quantitative Biology	26
Data Science	40
Earth Systems Modelling & Climate Change Modelling	10
Mathematics	54
Quantitative Finance	22
Statistics	10
Theoretical Physics	89
TOTAL	**275**





Junior Associates (18)

Astronomy and Astrophysics (1)

1. Dr Teboho Moloi (Durban University of Technology)

Data Science (8)

1. Dr Nikita Bernier (University of the Western Cape)
2. Mr Lindani Dube (North-West University)
3. Dr Lorène Jeantet (Stellenbosch University and AIMS)
4. Mr Asad Jeewa (University of KwaZulu-Natal)
5. Dr Shane Josias (Stellenbosch University)
6. Dr Thokozani Kunene (University of Johannesburg)
7. Dr Mpho Mafata (Stellenbosch University)
8. Dr Kim Martin (Stellenbosch University)

Mathematics (2)

1. Dr Mathew Aibinu (Durban University of Technology)
2. Mr Nathan Mulaja Tshakatumba (University of South Africa)

Quantitative Finance (1)

1. Mr Pierre Mananga (ALM Consulting)

Statistics (2)

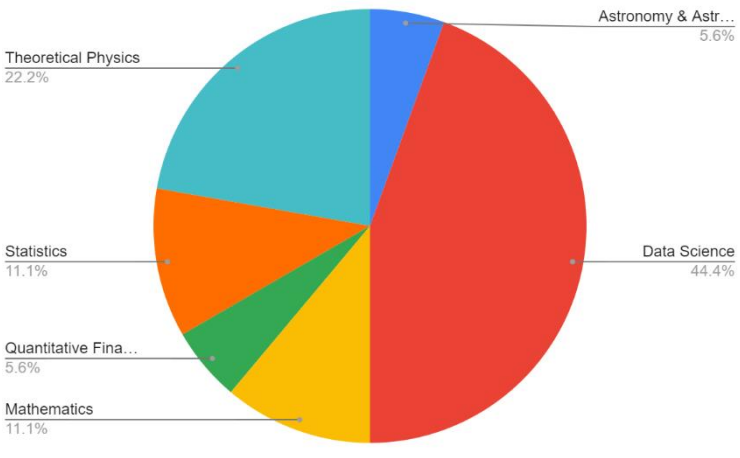
1. Dr Christine Kraamwinkel (University of Pretoria)
2. Dr Farai Mlambo (University of the Witwatersrand)

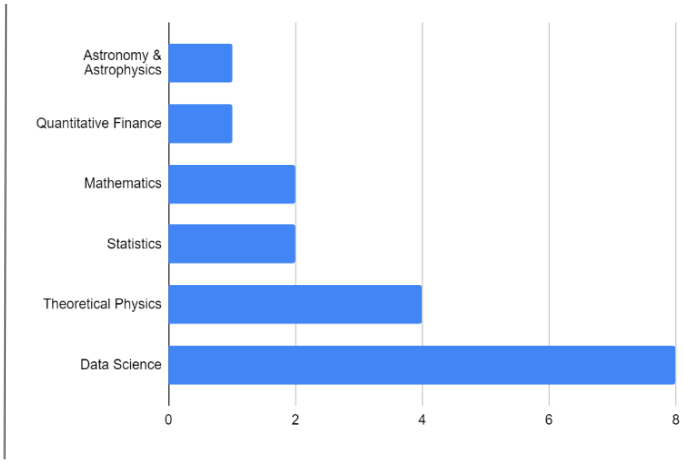
Theoretical Physics (4)

1. Dr Yannick Mvondo-She (University of Pretoria)
2. Dr Masimba Paradza (Cape Peninsula University of Technology)
3. Dr David Tshwane (Council for Scientific and Industrial Research)
4. Mr Ayanda Zungu (Sol Plaatje University)

Junior Associates per theme

Theme	Number of Associates per theme
Astronomy & Astrophysics	1
Data Science	8
Mathematics	2
Quantitative Finance	1
Statistics	2
Theoretical Physics	4
TOTAL	**18**





Institutional Associates (19)

1. African Institute for Mathematical Sciences (AIMS)
2. Centre for AI Research (CAIR)*
3. Centre for Space Research (NWU)*
4. Centre for Theoretical Physics (UCT)*
5. Cosmology Group (UCT)
6. DSI/NRF CoE in Strong Materials (WITS)
7. Hartebeesthoek Radio Astronomy Observatory
8. Institute for Intelligent Systems (UJ)
9. International Centre for Theoretical Physics (ICTP)
10. iThemba LABS
11. MIT Kavli Institute
12. School for Data Science and Computational Thinking (SU)
13. South African Astronomical Observatory
14. South African Radio Astronomy Observatory
15. South African Statistical Association
16. The Carpentries
17. The National Graduate Academy
18. The South African Centre for Digital Language Resources
19. UCT CERN Research Centre

Strategic Associates (9)

Data Science (2)

1. Dr Krishna Govender (Council for Scientific and Industrial Research)
2. Prof Kanshukan Rajaratnam (Stellenbosch University

Mathematics (1)

1. Prof Barry Green (African Institute for Mathematical Sciences)

Theoretical Physics (6)

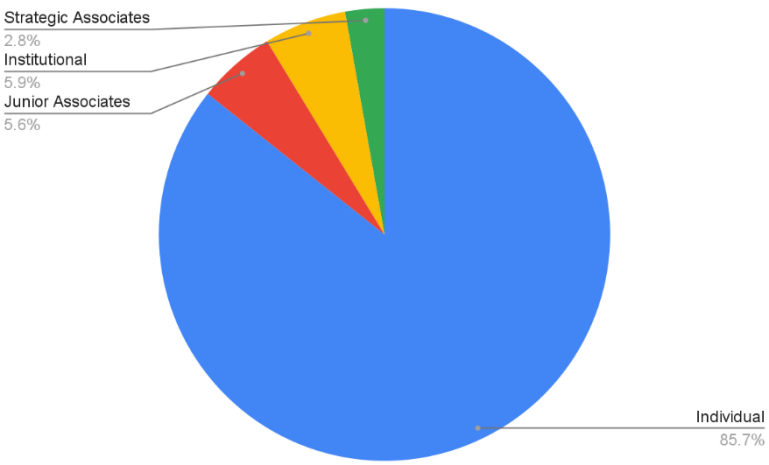
1. Dr Faïçal Azaiez (iThemba LABS)
2. Prof Ludwig Combrinck (Hartebeesthoek Radio Astronomy Observatory)
3. Prof Lesley Cornish (DST-NRF Centre of Excellence in Strong Materials)
4. Dr Laure Gouba (Abdus Salam International Centre for Theoretical Physics)
5. Dr Joseph Kirui (University of Venda)
6. Dr Sreekanth Rallapalli (Botho University)

Summary of Associates per category

Number of Associates per category

Category	Number of Associates
Individual Associates	275
Junior Associates	18
Institutional Associates	19
Strategic Associates	9
TOTAL	**321**

Percentage of Associates per category



Individual Associates per province and theme

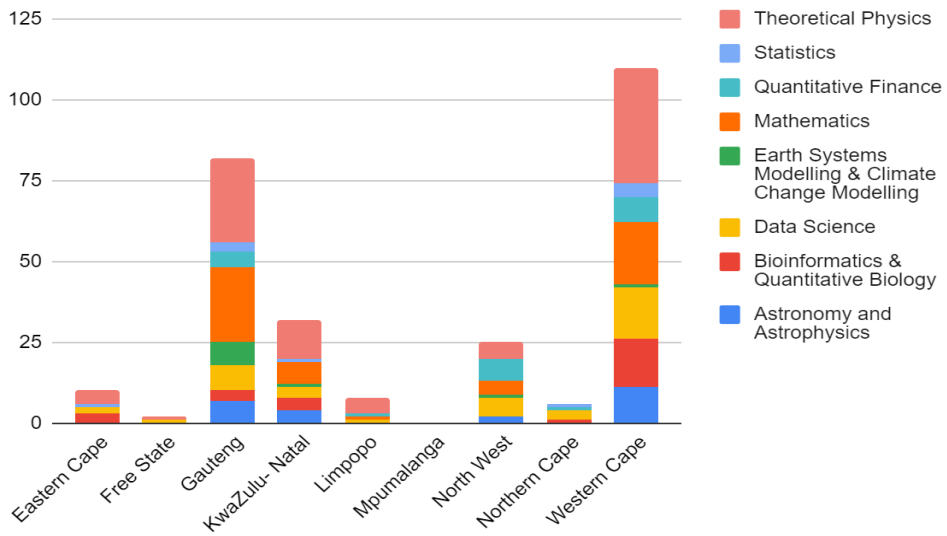
Individual Associates form the largest component of the NITheCS Associates group.

Almost 82% of the individual NITheCS Associates are affiliated with tertiary institutions in the Western Cape (107 Associates), Gauteng (86 Associates) and KwaZulu-Natal (32 Associates).

Around 32% of individual Associates work in the theoretical physics field. Mathematics is the next biggest field for individual Associates (19,6%), while 14,5% work in the field of data science.

Individual Associates per province and theme as at 31 December 2023

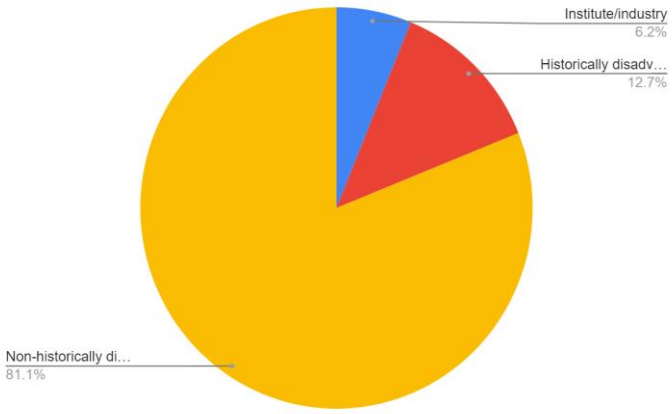
Theme	Eastern Cape	Free State	Gauteng	KwaZulu-Natal	Limpopo	Mpuma-langa	North West	Northern Cape	Western Cape	TOTAL
Astronomy and Astrophysics			8	3			2		11	24
Bioinformatics & Quantitative Biology	3		3	4				1	15	26
Data Science	2	1	8	3	1		6	3	16	40
Earth Systems Modelling & Climate Change Modelling			7	1			1		1	10
Mathematics			23	7	1		4		19	54
Quantitative Finance			5		1		7	1	8	22
Statistics	1		3	1				1	4	10
Theoretical Physics	4	1	26	12	5		5		36	89
TOTAL	**10**	**2**	**83**	**31**	**8**	**0**	**25**	**6**	**110**	**275**



Associates' affiliation

Affiliation	Number of individual Associates
Institute/industry	17
Historically disadvantaged institution*	35
Non-historically disadvantaged institution	223
TOTAL	**275**

* FH, UWC, UZ, UL, WSU, UNIVEN, UNISA, CPUT, MUT, CUT, TUT, VUT and DUT



Individual Associates per race

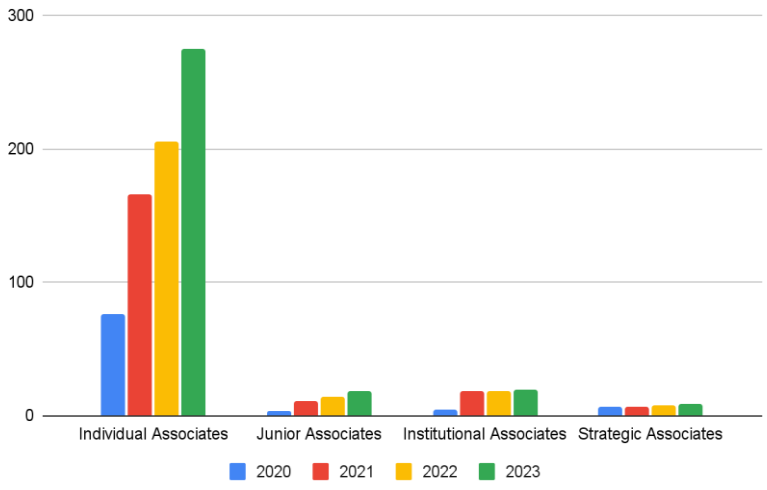
Individual Associates per race (%)	
Black (African, Coloured, Indian)	90%
White	10%
TOTAL	**100%**

Individual Associates per gender

Individual Associates per gender (%)	
Female	
Male	
TOTAL	**100%**

Annual growth in Associate numbers

Category	2020	2021	2022	2023
Individual Associates	76	166	205	275
Junior Associates	3	11	14	18
Institutional Associates	4	18	18	19
Strategic Associates	6	6	8	9
TOTAL	**89**	**201**	**245**	**321**



BURSARIES

Overview

NITheCS bursaries are administered via the National Research Foundation (NRF). Applications for NITheCS bursaries are made directly on the online NRF portable application system.

NITheCS held an information session for students on 31 May 2023 about the bursary application process for NRF-DSI Postgraduate Student Funding. A total of 11 MSc and 9 PhD bursaries were awarded.

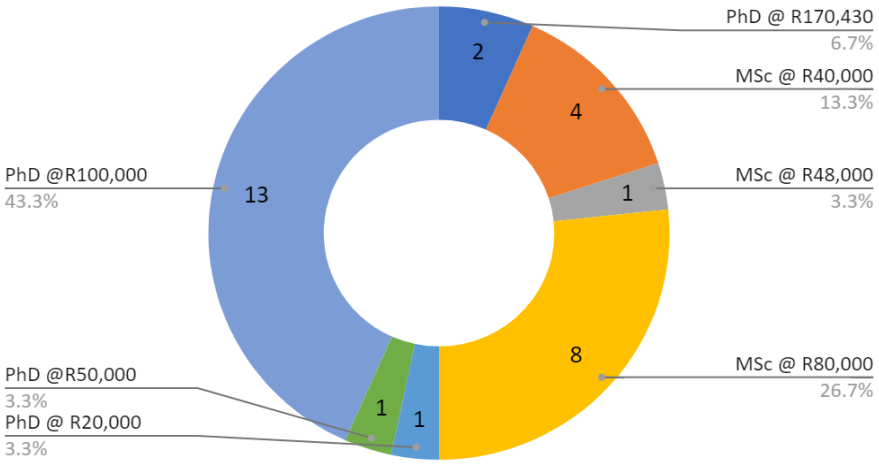
Workshops with bursary holders serve as opportunities to interact with one another and, importantly, as checkpoints relating to bursary holders' progress. The annual workshop for bursary holders was held online on 1 December 2023 and led by NITheCS Interim Director Prof Francesco Petruccione. Bursary holders made brief, but high-standard presentations to inform all workshop participants about the direction and progress of their research. Prizes were awarded to the best Masters and Doctorate presentations.

Bursaries: numbers and values

Summary of bursaries paid out in 2023:

Bursary level	Number of bursaries	Bursary value (Rand)	Bursaries paid (Rand)
MSc	11		1 746 738,00
PhD	9		1 461 371,00
TOTAL	20		3 208 109,00

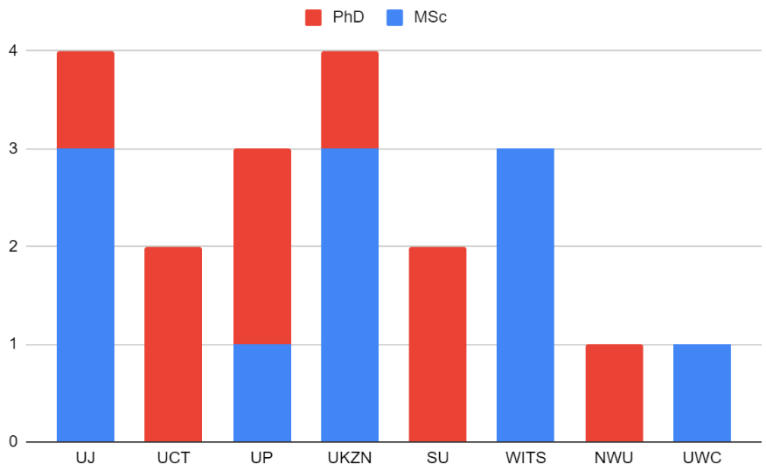
Bursaries paid out in 2023



Distribution of bursary holders per academic level

MSc & PhD Bursaries per University

University	MSc	PhD	Total
UJ	3	1	4
UCT		2	2
UP	1	2	3
UKZN	3	1	4
SU		2	2
WITS	3		3
NWU		1	1
UWC	1		1
TOTAL	**11**	**9**	**20**



Bursary holders' demographics

NITheCS aims at the following DSI-NRF Postgraduate Student Funding balances:

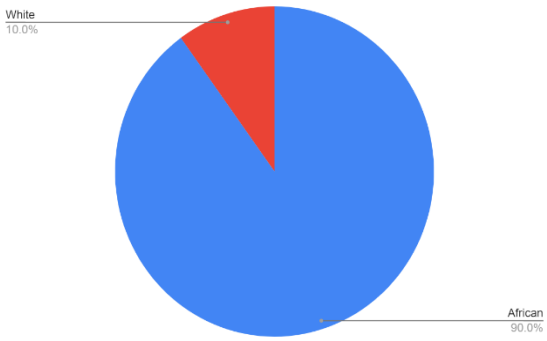
- 95% to South African citizens and permanent residents
- 5% to students from the SADC countries and the rest of the world
- 55% to women

South African citizens and permanent residents' targets are further disaggregated in terms of race and disability as follows:

- 90% African (Black, Coloured and Indian)
- 10% White
- 1% Students who are persons living with a disability

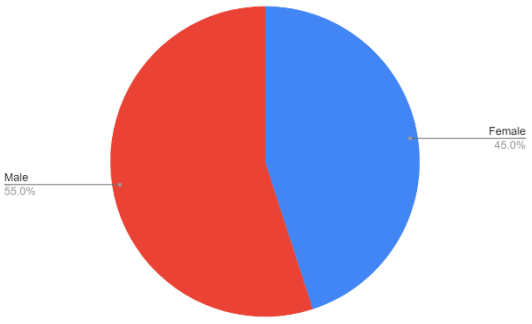
Bursary holders per race

Race	Bursary holders	
	Number	Percentage
Black (African, Coloured, Indian)	18	90%
White	2	10%
TOTAL	**20**	**100%**



Bursary holders per gender

Gender	Bursary holders	
	Number	Percentage
Female	9	45%
Male	11	55%
TOTAL	**20**	**100%**



PROGRAMMES AND EVENTS

Overview

NITheCS' programmes and activities are arranged and managed by a small administrative staff. These activities include research programmes, internships, NITheCS events, outreach work and vigorous communication using numerous media. Importantly, NITheCS also actively supports events presented by associate bodies.

In practice, the Institute could not function efficiently without the support of relevant specialist bodies to further the goals of collaboration and support the basic and computational sciences included in the eight relevant thematic areas. This support allows for a rich and far-reaching programme with opportunities for many individuals and organisations.

In short, this enables the Institute to continue focusing among others on the critical importance of diversity and equity. NITheCS understands how important it is to reach out to the wider community of scientists and further multidisciplinary cooperation.

NITheCS Colloquium in the Neelsie Cinema, Stellenbosch University

Event accessibility
Many events are in a hybrid (in-person as well as online) format to allow for the attendance of people in many different geographical locations. This becomes increasingly important as the Institute grows with more members and collaborators who reside in different parts of the country and all over the world. In addition, many of our colloquiums, mini-schools and other events are recorded and uploaded (with permission of the presenters) to the NITheCS YouTube channel. This further broadens the reach of our events.

Local universities and NITheCS Associates
Especially important for the NITheCS programme of activities is the unstinting support of local universities that allows the Institute to meet the goal to support the local scientific community. In particular, we are grateful to the individual academics who have led our colloquiums and workshops. Our Associates play a vital role in these events and among others their contributions are vital for the local scientific community. As mentioned elsewhere, our Associates support and participate in training young scientists through colloquiums, mini-schools, internships, courses, workshops and other NITheCS events.

Special programmes, events and outreach
As part of the NITheCS growth and development focus, the Institute has continued to present and support among others the events below. More details about these programmes and events appear further on in this report.

The International Year of Basic Sciences for Sustainable Development (IYBSSD) that started in 2022 ended on 30 June 2023. NITheCS hosted two events in 2023 that highlighted the importance of the basic sciences in local society and aimed to inspire dialogue on key issues that lead to sustainable development.

The *13th CHPC Coding Summer School and the 5th NITheCS Summer School on the Foundations of Theoretical and Computational Science* was held at various university campuses from 30 January until 10 February. It introduces postgraduate students to programming, as well as the theoretical and computational sciences.

The *Scientific Seminar Series* of talks are co-hosted by NITheCS and the Department of Physics at Stellenbosch University.

NITheCS was a main supporter at the *Spring School on Theoretical and Computational Foundations of Quantum Technologies* held in the Northern Drakensberg in October. The School is aimed at postgraduate students in physics, mathematics, applied mathematics, and computer science

Students learn coding skills at the 13th CHPC Coding Summer School and the 5th NITheCS Summer School on the Foundations of Theoretical and Computational Science

who are interested in both theoretical and computational aspects of quantum technologies.

The *STEM MentHER* programme, launched in 2022 to guide and streamline aspiring female Grade 12 learners into the STEM fields of tertiary study, continued during 2023. NITheCS is an enthusiastic supporter of this programme, which was introduced to the Western Cape and KwaZulu-Natal in 2023.

The *Modern African Nuclear DEtector LAboratories (Mandelab)* programme at the universities of the Western Cape (UWC) and Zululand (UniZulu) is sponsored by the UK Science and Technology Facilities Council (STFC), the two universities and NITheCS.

NITheCS was again one of the main supporters at the 2023 *Southern African Conference for Artificial Intelligence Research* (SACAIR) with its focus on growing a formidable network of talented students working in AI from across Africa.

The International Centre for Theoretical Physics (ICTP), NITheCS and the Centre for High Performance Computing (CHPC) collaborated to present the High Performance Computing for Sustainable Development programme in April in Stellenbosch, with prominent speakers from Italy and South Africa.

International Day of Mathematics (March): Special events for high school learners and undergraduates were arranged to celebrate this day.

NITheCS again sponsored one of the local heats of the international science competition FameLab, which is managed locally by the South African Agency for Science and Technology Advancement and science communication agency Jive Media Africa.

NITheCS sponsored some of the prizes at the Eskom Expo for Young Scientists, which gives learners an opportunity to showcase their own science projects. The winners were Rinae Mudau (Physics), Witness Itumeleng Nkge (Mathematics), Ciara Mlange (Climate) and Andiswa Mabuza (Physics).

Various workshops were held and included among others the online software training courses/workshops presented by The Carpentries that seek to strengthen local data science and programming skills. Other workshops included a day-long workshop at SACAIR2023, titled 'Machine Learning in Support of Computational and Theoretical Sciences Knowledge Discovery in Time Series Data'. There were also workshops for our Associates and bursary holders. More details about workshops appear in this report.

Attendance at expos and other platforms for collaboration: NITheCS participated in person at various events, including AI Expo Africa, Science Forum South Africa, the CHPC National Conference, Table Mountain Delta, the Southern Africa Mathematical Sciences Association Annual Conference, Optics and Photonics Africa Congress (OPA2023), Spring School in Stellenbosch and the 3rd African Conference on Fundamental and Applied Physics.

Further details:
Additional details about some of the events mentioned above are also provided in this report.

The STEM MentHER organisers at the launch of the programme at the University of KwaZulu-Natal

Finalists in FameLab 2023. Winner of the NITheCS heat, Goratileone Oepeng (UP), is on the far right.

South Africa's top 15 high school mathletes attended a training camp sponsored by NITheCS and led by Dr Liam Baker (SU), with the aid of undergraduates from the Massachusetts Institute of Technology

Witness Itumeleng Nkge, one of the NITheCS prize winners at the Eskom Expo for Young Scientists

The launch of National Science Week 2023

Summary of activities

Type of activity	Number of activities / events
NITheCS colloquiums	49
Schools	3
Mini-schools	9
Mathematics revision lessons	5
Scientific Seminar Series	2
Seminars co-hosted with Quantum@SUN and SAQuTI	13
Africa-Europe CoRE-AI Masterclasses	3
Workshops	10
Sponsorships and/or events in which NITheCS has participated	15
Other events	3

Event details

NITheCS Colloquiums

NITheCS colloquiums in 2023 mostly took place in a regular Monday time slot. The presenters were generally academic lecturers and postdoctoral researchers, but speakers with international affiliation, people from the private sector and recommended doctoral students were also invited to share their insights and present their research on relevant topics.

Our colloquiums on 14 March and 19 June were specifically aligned to topics of the International Year of Basic Sciences for Sustainable Development (IYBSSD). This brings the total number of events aligned to IYBSSD topics to nine during the year of celebration which ended in June 2023. A full report on all the NITheCS events related to the IYBSSD is available at https://nithecs.ac.za/international-year-of-basic-sciences/.

The table below sets out details relating to the colloquiums that were hosted or co-hosted by NITheCS during 2023.

Details of NITheCS colloquiums 2023

Date	Speaker	Affiliation	Title	Registrants to attend in person / online	YouTube views to date
3 Feb	Prof Uwe Jaekel	Koblenz University of Applied Sciences, Germany	Solving nonlinear classification problems with a complex valued almost linear perceptron	40	59
6 Feb	Prof Tommie Meyer	University of Cape Town	Knowledge Representation and Reasoning (in the age of Machine Learning)	157	93
13 Feb	Dr Leandro Boonzaaier (SU) Dr Sophie Marques (SU)		What are the possible near field structures one can define over the multiplicative group of a near field?	43	30

20 Feb	Ulrich Paquet	AIMS	AI and Chess: A Retrospective and Future Story	155	89
24 Feb	Prof Dario Rosa	Institute for Basic Science; University of Science & Technology, South Korea	Moving Towards Quantum Technologies: The Case of Quantum Batteries	59	65
27 Feb	Prof Menno van Zaanen	South African Centre for Digital Language Resources	Describing language: formal and empirical approaches	57	33
3 Mar	Emma King	University of Saarland, Germany	Universal cooling dynamics toward a quantum critical point		32
6 Mar	Dr Mesias Alfeus	Stellenbosch University	A Gentle Quantitative Modelling Approach for Rough Crude Oil Prices	36	48
13 Mar	Prof John Hargrove	South African Centre for Epidemiological Modelling and Analysis	Tsetse, trypanosomiasis and climate change: Lessons from Field Data collected in the Zambezi Valley of Zimbabwe	37	32
14 Mar	Prof Zurab Janelidze	Stellenbosch University	The Mind, Mathematics and Sustainable Development	76	72
17 Mar	Dr Adrian Budini	Centro Atómico Bariloche, Argentina	Minimal operational approach to quantum non-Markovianity		30
20 Mar	Prof Marino Gran	Université catholique de Louvain, Belgium	Categories, groups, and non-abelian algebraic structures	38	103
24 Mar	Prof Marco Merkli	Memorial University of Newfoundland, Canada	Open Quantum Systems		97
27 Mar	Dr Pietro Landi	Stellenbosch University	The mathematics of love	92	90
24 Apr	Dr Wolfgang Huber	European Molecular Biology Laboratory, Germany	Multi-Omics and Spatial Single Cell Methods for Precision Medicine of Blood Cancers	36	32
8 May	Dr Tshiamo Motshegwa	African Open Science Platform	African Open Science Platform – Towards a Continental Open Science Vision	67	27
15 May	Dr Cerene Rathilal	University of KwaZulu-Natal	On Sublocales: Metric Sublocales and Property S	48	34
22 May	Prof Nigel Bishop	Rhodes University	Observations and the Damping of Gravitational Waves by Matter	48	68
29 May	Prof Olugbenga Oluwagbemi	Middlesex University, UK	Towards Resolving Challenges Associated with Climate Change Modelling in the African Continent	66	56
5 Jun	Dr Fidele Tugizimana	University of Johannesburg	Big data and computational strategies in metabolomics studies	57	46
12 Jun	Prof Loyiso Nongxa	University of the Witwatersrand	South African Mathematical Sciences Research Landscape in 2050	58	78
19 Jun	Mesias Alfeus (Stellenbosch University) MJ (Thinus) Booysen (Stellenbosch University) David Holgate (University of the Western Cape) Guy Midgley (Stellenbosch University) Hugh Patterton (Stellenbosch University) Ethel Phiri (Stellenbosch University)		Panel discussion: 'Building a Sustainable Future: The Power of Basic Sciences	46	Not recorded

26 Jun	Prof Alan Cornell	University of Johannesburg	Black holes and nilmanifolds: quasinormal modes as the fingerprints of extra dimensions?	30	67
3 Jul	Prof Alessandra Di Pierro	University of Verona, Italy	Quantum Kernels: Challenges and Solutions		95
14 Jul	Prof Erik Schlögl	University of Technology, Sydney, Australia	SOFR Term Structure Dynamics – Discontinuous Short Rates and Stochastic Volatility Forward Rates *(joint work with Alan Brace and Karol Gellert)*	44	37
21 Jul	Prof Sam Cohen	University of Oxford, UK	Approximating PDEs with wide neural networks	70	119
24 Jul	Prof Joseph Indekeu	KU Leuven, Belgium	Wetting and Nonwetting of Fluids	9	63
31 Jul	Prof Zurab Janelidze	Stellenbosch University	A New Horizon for Teaching and Learning of Mathematics	69	82
7 Aug	Dr Japie Greeff	North-West University	Advantages and challenges of artificial intelligence for universities	51	106
10 Aug	Prof Robert Faff	Bond Business School, Australia	Academic research in science	50	76
14 Aug	Prof Inger Fabris-Rotelli	University of Pretoria	Spatial Epidemiology	40	78
21 Aug	Dr Anwar Vahed	Data Intensive Research Initiative of South Africa	Big data: the South African strategy and implementation	78	93
30 Aug	Prof Estate Khmaladze	Victoria University of Wellington, New Zealand	On what Probability Theory and Mathematical Statistics do	62	210
31 Aug	Prof Martin Bucher	Laboratoire APC, Université Paris Cité/CNRS	Cosmology and Computation: Challenges for Mapping the Early Universe		Not recorded
4 Sep	Prof Absalom Ezugwu	North-West University	Machine Learning Research Initiatives and Contributions from Africa: A Three-Decade Retrospective	34	253
11 Sep	Prof Fabio Dercole	Politecnico di Milano, Italy	Should we do applied Complex Systems Dynamics in primary school?	39	72
18 Sep	Dr Ryan Sweke	IBM Research	Quantum machine learning with parameterized quantum circuits	34	117
18 Sep	Prof Refilwe Nancy Phaswana-Mafuya	University of Johannesburg	Winning Mentors: Tips on building a successful mentorship relationship	210	49
2 Oct	Dr Christine Darve	European Spallation Source, Sweden	Engaging in a digital educated world with large scale-projects		71
9 Oct	Prof Emmanuel Adetiba	Durban University of Technology & Covenant University, Nigeria	FEDGEN: A FEDerated GENeral 'Omics' Cloud Computing Infrastructure for Precision Medicine and Artificial Intelligence Research in Africa		152
16 Oct	Dr Guo-Jian Wang	University of KwaZulu-Natal	The Future: Machine Learning in Cosmology and Astrophysics	39	42
20 Oct	Prof Andrea Macrina	University College London & University of Cape Town	The Financial Impact of Carbon Emissions on Power Utilities Under Climate Scenarios	24	Not recorded

23 Oct	Dr Sandra MacFadyen	Vrije Universiteit Amsterdam & Stellenbosch University	Simple Threads, Chaotic Weaves: Unravelling the Complex Tapestry of Nature	26	62
30 Oct	Prof Nico Orce	University of the Western Cape	Universality of the Elemental Abundances	62	70
6 Nov	Prof Lyudmila Moskaleva	University of the Free State	What Makes Nanoporous Gold a Unique Catalyst? Insights from Modelling Studies of its Surface Chemistry		Not recorded
13 Nov	Dr Aniekan Magnus Ukpong	University of KwaZulu-Natal	Probing the nature of many-body entanglement in quantum spin liquids: insights from lattice field theories	25	64
20 Nov	Dr Adriana Marais	Stellenbosch University	A Century of Biophotons	24	76
27 Nov	Dr Lungile Sitole	University of Johannesburg	The Role of Science Centres in STEAM Education	40	17
4 Dec	Prof Tanja Verster	North-West University	The Changing Landscape of Financial Predictive Models	102	45
TOTAL				2 118	3133

Schools

NITheCS hosts, co-hosts and sponsors several schools. During 2023, these were:

Date	School
30 Jan-10 Feb	The 13th CHPC Coding Summer School and The 5th NITheCS Summer School on the Foundations of Theoretical and Computational Science
24-28 Oct	Spring School: 'Theoretical and Computational Foundations of Quantum Technologies'
25-27 Oct	Spring School – Stellenbosch: 'On Symmetries of Differential & Difference Equations and Their Applications'

Mini-Schools

NITheCS hosted nine mini-schools during 2023. Each mini-school comprises a series of lectures that mostly extend over four weeks and the topics change monthly. Our community is invited to attend these lectures to expand their knowledge.

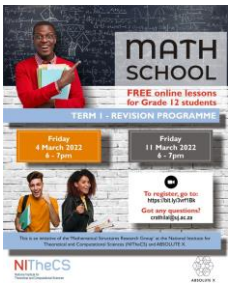
Details relating to mini-schools

Date	Speaker and affiliation	Topic	No. of registrants	YouTube views to date
Mar	Prof Boris Malomed (Tel Aviv University), Prof Sergey Dmitriev (Russian Academy of Sciences), Prof Herbert Weigel (Stellenbosch University) and Dr Danial Saadatmand (Stellenbosch University)	An Introduction to Solitons and Solitary Waves in Physics and Mathematics	87	L1: 273 L2: 80 L3: 80 L4: 100
Apr	Binjamin Barsch (Centre for High Performance Computing)	Mastering Pandas: An in-depth Guide in Data Science Techniques for Researchers	345	L1: 173 L2: 68 L3: 60 L4: 45
May	Prof Jonathan Shock (UCT), Dr Pallab Basu (WITS), Prof Vishnu Jejjala (WITS) and Mr Cameron Beetar (UCT)	From Physics to Machine Learning and back again: Applications of Machine Learning to Theoretical	160	L1: 155 L2: 90 L3: 81 L4: 88

		Physics, and Physics inspired Machine Learning		
Jun	Dr Sunandan Gangopadhyay (S.N. Bose National Centre for Basic Sciences, India)	A short introduction to path integral approach to quantum mechanics and quantum field theory	77	L1: 165 L2: 85 L3: 43 L4: 61
Jul	Dr Mesias Alfeus (Stellenbosch University)	Introduction to Quantitative Finance	240	L1: 292 L2: 105 L3 & L4: 76
Aug	Prof Joseph Indekeu (KU Leuven, Belgium)	Phase transitions and critical phenomena at surfaces and interfaces	12	L1: 65 L2: 35 L3: 31 L4: 31
Sept	Filippos Sytilidis (Oxford University, UK)	Cerf theory and pseudo-isotopy	18	L1: 87 L2: 25 L3: 27 L4: 42 L5: 45 L6: 27
Oct	Jeremy Cohen (Imperial College London), Dr Kim Martin (SU), Dr Martin O'Reilly (Alan Turing Institute), Michelle Barker (Research Software Alliance)	Research Software Engineering as an exciting career and a critical component of the research ecosystem	96	L1: 86 L2: 56 L3: 51 L4: 38
Nov	Prof Georgies Alene (Addis Ababa University, Ethiopia), Prof Yedilfana Setarge Mekonnen (Addis Ababa University, Ethiopia), Dr Kingsley Obodo (North-West University), Prof Tjaart Krüger (University of Pretoria)	Energy Materials	73	L1: 69 L2: 70 L3: 20 L4: 94
TOTAL			1 108	3 019

Mathematics revision lessons

To help ensure school learners achieve sufficient competence and the appropriate grades in mathematics to study in the science fields, we co-sponsored 'Math School: Math School: revision lessons for grade 12s.'



This initiative, driven by Dr Cerene Rathilal (UJ), provides online mathematics revision lessons to grade 12 students, covering terms 1, 2 and 3. Recordings of the online lessons are accessible via the NITheCS YouTube channel.

Summary of the math revision lessons in 2023

Date	Topic	No. of registrants to watch online	YouTube views to date
3 Mar	Term 1 revision	806	97
10 Mar			52
18 Aug	Term 3 revision	386	95
25 Aug			78
1 Sep			86
TOTAL		**1 192**	**408**

Scientific Seminar Series

These talks are co-hosted by NITheCS and the Department of Physics at Stellenbosch University.

Date	Speaker	Affiliation	Title
25 Jan	Prof James R. Carey	University of California, Berkeley, USA	Insect biodemography: A 21st century guided tour of concepts, empirical results and novel applications
31 May	Prof Frank Tanser	CERI, Stellenbosch University	The rise (and fall?) of South Africa's HIV epidemic: Population insights from rural KwaZulu-Natal

Seminars co-hosted with Quantum@SUN and SAQuTI

Date	Speaker	Affiliation	Title	YouTube views
9 Jun	Dr Ahsan Nazir	University of Manchester, UK	Quantum work statistics at strong reservoir coupling	93
15 Jun	Bruce Liu	SpinQ	SpinQ Desktop Quantum Computer for Education and Research	187
23 Jun	Alan Kahan	National University of Córdoba, Argentina	Structural crossovers in trapped ions dispersively coupled to optical cavities	31
7 Jul	Dr Garry Kemp	University of Johannesburg	A generalized dominance ordering for 1/2-BPS states	64
14 Jul	Dr Latévi M. Lawson	AIMS, Ghana	Path integral in position deformed Heisenberg algebra	48
21 Jul	Abhishek Agarwal	National Physical Laboratory, UK	Modelling non-Markovian noise in driven superconducting qubits	93
28 Jul	Taliesin Beynon	Deep Learning Indaba	Transformers, graphs, and hypergraphs	Not available
11 Aug	Rivan Rughubar	University of Cape Town	Approximating classical kernels on NISQ computers	83
22 Sep	Prof Nana Liu	Shanghai Jiao Tong University, China	Analog quantum simulation of partial differential equations	79
6 Oct	Mingyu Kang	Duke University, US	Trapped-ion quantum simulations for condensed-phase chemical dynamics: seeking a quantum advantage	117
20 Oct	Prof Nadja Bernardes	Federal University of Pernambuco, Brazil	Approximating Invertible Maps by Recovery Channels: Optimality and an Analysis of Qudit Channels	29

Africa-Europe CoRE-AI Masterclasses

We held 3 Masterclasses during 2023, focused on topics relating to artificial intelligence. Here are the details:

Date	Speaker	Affiliation	Title	YouTube views to date
1 Nov	Prof David Sumpter	Uppsala University, Sweden	Data science and modelling of football	62
17 Nov	Dr Joyce Nakatumba-Nabende and Dr Andrew Katumba	Makerere University, Uganda	Responsible AI, bias and fairness	32
29 Nov	Prof Onime Clement (ICTP, Italy) and Dr Solomon Gizaw (Addis Ababa University, Ethiopia)		High-performance Computing Architecture and Parallel Computing	77
TOTAL				171

Workshops

Carpentry workshops

NITheCS hosted five Carpentry workshops in 2023 with the aim to provide graduate students and other researchers with opportunities to learn valuable computing skills to enable them 'to do more in less time and with less pain'. The hands-on workshops covered basic concepts and tools, including programme skills and design, version control, data management and task automation. Participants were encouraged to help one another and apply their learnings to their own research problems.

Date	Workshop	Number of attendees
20-24 Nov	Software Carpentries Workshop: 'Unix Shell, Python, Git and R'	25
30 Oct-3 Nov	Data Carpentry (Genomics) Workshop	32
26-29 Sep	Shell, Git, Plotting and Programming in Python	53
28 Aug-1 Sep	Shell, Git and programming with R	22
24-28 Jul	Software Carpentry Workshop	65
TOTAL		197

South African Conference for Artificial Intelligence Research

NITheCS was a sponsor at the Conference for Artificial Intelligence Research (SACAIR2023) and hosted a day-long workshop titled 'Machine Learning in Support of Computational and Theoretical Sciences Knowledge Discovery in Time Series Data'. Led by the principal investigators, NITheCS Associates Marelie Davel (NWU) and Stefan Lotz (SANSA), the event provided a forum for discussion and brainstorming ideas related to knowledge discovery in time series data. Submissions were invited from researchers on the topic prior to the event, which was held at STIAS in Stellenbosch.

Bursary-related workshops

Information Session Workshop: NITheCS hosted a workshop at a National Research Foundation event in July before issuing a call for NITheCS bursary applications. The aim was to help stakeholders understand the implementation of the NRF-DSI Postgraduate Student Funding Policy.

Bursary holders' Workshop: the annual workshop for NITheCS bursary holders was held on 1 December. The 30 bursary holders were given an opportunity to provide short presentations and insight into their research. Three guest speakers recounted their achievements to motivate the bursary holders.

Other workshops

Here is a summary of other workshops that NITheCS hosted, co-hosted or sponsored in 2023:

Date	Details	Title
1-2 Mar	An online workshop organised by the Institute of Theoretical Physics, Jagiellonian University, Kraków, Faculty of Physics, Astronomy and Informatics, Nicolaus Copernicus University, Toruń and NITheCS	Celebrating the Choi-Jamiołkowski Isomorphism
3-4 July & 6-7 Jul	QBronze 109: Quantum Programming Workshop	Quantum Computing and Programming
18-19 Sep	6th ATMRESET Workshop	Numerical methods and machine learning on Atmospheric Science
21 Nov	A Century of Biophotons Workshop	'Biophotonics and artificial intelligence for improved diagnostics' by Patience Mthunzi-Kufa
29 Nov-1 Dec	Regional – Global Modelling Workshop	Jointly hosted by Stellenbosch University School for Climate Studies and NITheCS
11 Dec	NITheCS Mini-workshop presented by Prof Nikolai Antonenko (BLTP, JINR, Russia), Dr Gurgen Adamian (BLTP, JINR, Russia) & Prof Sergei Rakitianski (University of Pretoria)	Exploring Theoretical Work at the Joint Institute for Nuclear Research (JINR)
8-10 & 15-17 Dec	QNickel9 - a free workshop organised by QCousins of QTurkey, QIran, QSouthAfrica and QUAE	Quantum Computing and Programming Workshop

Other engagement: Skills and knowledge development

NITheCS sponsored or co-sponsored several initiatives during 2023 that focused on skills and knowledge development. Engagement is primarily via events that encourage learners to consider careers in the fields of science covered by NITheCS. Below are details relating to programmes and events mentioned briefly earlier.

International Day of Mathematics: High school learners were again made more aware of mathematics through an online celebration of the International Day of Mathematics in March. We also celebrated the International Day of Mathematics (IDM) on 14 March with a special hybrid programme aligned to a topic of the International Year of Basic Sciences for Sustainable Development. For high school learners and undergraduates, an online programme was presented on 11 March by Dr Cerene Rathilal (UKZN). A total of 632 participants registered to attend this event.

UKZN Mathematics Club: Students from grade 8 - 12 who have a passion for Math were invited to attend this online event, which aimed to sharpen their number-sense skills through an explorative mathematics and problem-solving session. In total, 266 students registered to attend.

Abstract Algebra - Holiday Programme for Aspiring Mathematicians: Two events were arranged and hosted online for high school students during the year. The first was held on 5 April, with an audience of 151 students, while the second took place in July for 236 students.

FameLab: NITheCS heat: The search was on for the next 'Science Pop Idol' in the NITheCS-sponsored heat of the FameLab contest in May. Scientists aged 18 to 35 years in the NITheCS fields of science could further develop their communication skills as they were challenged to explain a science concept in three minutes. The heat winner, who went on to compete in the national finals, was Goratileone Oepeng (UP). The runner-up was Adeshina Odugbemi (UWC). FameLab is managed locally by the South African Agency for Science and Technology Advancement and science communication agency Jive Media Africa.

STEM MentHER: The STEM MentHER programme launched in 2022 to guide and streamline aspiring female Grade 12 learners, continued and expanded in 2023. It is hoped that successful candidates will become role models for other girls. A total of 36 girls from Gauteng, the Western Cape and KwaZulu-Natal could participate in the programme, led by Dr Cerene Rathilal (UKZN) and Dr Lungile Sitole (Soweto Science Centre). NITheCS provided branded materials for the programme, as well as marketing materials to advertise the programme.

SAIP Conference: The Department of Physics at UZ hosted the 67th Annual Conference of the South African Institute of Physics, SAIP2023, from 3 to 7 July. The theme of the conference was 'Transforming lives of our communities through Physics.' NITheCS sponsored one of the tracks at the conference, provided funding to students to attend the conference and donated prizes, which were awarded to learners in various categories. The proceedings of the conference are available electronically on the SAIP website: www.saip.org.za.

Eskom Expo for Young Scientists: NITheCS helps to encourage young minds to grow their interest in science by participating in the Eskom Expo for Young Scientists. School learners can showcase their own scientific projects at this annual event held in July. NITheCS attended the exhibition in person and welcomed visitors to the NITheCS stand. We also sponsored some of the prizes: learners are given an opportunity to showcase their own science projects. The winners of the NITheCS prizes were Nkangala's Rinae Mudau (Physics), Bojanala's Witness Itumeleng Nkge (Mathematics), Ehlanzeni's Ciara Mlange (Climate) and Nkangala's Andiswa Mabuza (Physics).

Teacher Development Programme: The UJ Soweto Science Centre, in partnership with NITheCS, the UJ Faculty of Education, Africa Teen Geeks and UKZN, presented an online teacher training event focused on the topic 'Teaching strategies for inclusivity.' The programme sought to promote the professional development of teachers on a broad scale. Hosted by Dr Cerene Rathilal (UKZN), it reached some 500 teacher attendees.

Fundamano: The theatrical production Fundamano 2 was produced by students at Stellenbosch University on 1 December and presented mathematics concepts in an entertaining show that 'takes you on a journey of appreciating the complexity of mathematics as something arising naturally by a need for a better solution to a real-life problem. The show gained much positive feedback.

NITheCS Women's Month Writing Retreat: Female NITheCS Associates could apply for a grant of R10 000 to fund a self-run retreat, as an opportunity to focus on a piece of work without interruption.

Sponsorships and/or events in which NITheCS has participated

NITheCS sponsored or co-sponsored several events throughout the year and participated in some of the accompanying expos. These include:

Date	Details	Title
22-24 Mar	Hybrid event at UWC	'XI Tastes of Nuclear Physics: A New Era of Medical Applications through Simulations, Big Data & Machine Learning
23 Mar	Science Café Stellenbosch talk by Prof Willie Brink (Stellenbosch University)	Demystifying the Science behind ChatGPT
29 Mar	Colloquium at the Mathematics Division of Stellenbosch University presented by Dr Bruce Bartlett (Stellenbosch University)	Coherent loop states and their applications
12-14 Jul	Deep Learning IndabaX South Africa	Machine learning and artificial intelligence conference
27 Jul	Lunch hour presentation	Music Meets Abstract Mathematics
25-29 Sep	Conference	The 3rd African Conference on Fundamental and Applied Physics
5 Oct	Music Meets Abstract Mathematics II - a free concert presented by a NITheCS project team led by Zurab Janelidze and Hans Roosenschoon	Piano improvisations of mathematical structures
2 Nov	8th Annual Public Lecture, hosted by the Departments of Physics, Physiological Sciences, and Chemistry and Polymer Science	The Science behind the 2023 Nobel Prizes in Physics, Chemistry, and Medicine
2-3 Nov	AI Expo Africa	
6-11 Nov	Optics and Photonics Africa Congress (OPA2023)	
21-24 Nov	Southern Africa Mathematical Sciences Association Annual Conference	
26 Nov-1 Dec	Table Mountain Delta 2023	14th Southern Hemisphere Conference on the Teaching and Learning of Undergraduate Mathematics and Statistics
27 Nov-1 Dec	South African Statistical Association (SASA) conference	The 64th Annual Conference of the South African Statistical Association
4-7 Dec	2023 CHPC National Conference	Machine Learning, Cloud and Quantum Computing: The Changing Landscape of HPC
5 Dec	NITheCS Workshop at the Southern African Conference for Artificial Intelligence Research (SACAIR)	Machine Learning in Support of Computational and Theoretical Sciences Knowledge Discovery in Time Series Data
6-8 Dec	Science Forum South Africa 2023	Igniting Conversations About Science – People, Partnerships, Priorities for the Decadal Plan

Other events

Date	Details	Title	YouTube views
14 Apr	NITheCS Public Lecture by Dr Yaseera Ismail (UKZN)	Developments towards a Quantum Internet	49
17-21 Apr	Synergy Summit by the ICTP, NITheCS and CHPC School	High Performance Computing for Sustainable Development in Government, Academia and Industry	Not available
27 Oct	NITheCS Seminar by Prof Sergey V. Meleshko (Suranaree University of Technology, Thailand)	Symmetries of equations with nonlocal terms	Not available

Prof Francesco Petruccione with some of the attendees at the NITheCS stand at AI Expo Africa 2023. This event took place at the Sandton Convention Centre, Johannesburg, from 2-3 November.

RESEARCH PROGRAMMES

Overview:

NITheCS launched its research programmes in 2020/2021. These involve the entire network of Associates affiliated to South African universities, as well as several international collaboration partners. The duration of each programme is at least 12 months. An additional programme, Quantitative Finance, was added in 2023.

Research programmes and principal investigators (PIs)

The 2023 research programmes are listed below and full reports are available on our website at https://nithecs.ac.za/research-2/research/

Investigators/proposers	Topic	Highlights
Prof Amare Abebe (NWU) **Prof Aroon Beesham (MUT)** **Dr Shajid Haque (UCT)** **Prof Yin-Zhe Ma (UKZN)** **Prof Soebur Razzaque (UJ)** **Prof Bruce Watson (SU)**	New insights into astrophysics and cosmology with theoretical models confronting observational data	39 Papers published 37 Conference participation 4 Students supervised
Prof Marelie Davel (NWU) **Dr Stefan Lotz (SANSA)**	Machine learning in support of theoretical and computational science	8 Collaborators 11 Research workshops 3 Papers published
Prof Martin Bucher (UKZN) **Dr Japie Greeff (NWU)**	Genomics, bioinformatics, and advanced medicine	4 Students supervised 7 Collaborators 14 Papers published
Dr Shajid Haque (UCT) **Prof Thomas Konrad (UKZN)** **Prof Stef Roux (NMISA,UKZN)** **Prof Jeff Murugan (UCT)** **Prof Ilya Sinayskiy (UKZN)**	Quantum technologies for sustainable development	8 Students supervised 6 Collaborators 11 Papers published
Prof Tjaart Kruger (UP) **Dr Aniekan Ukpong (UKZN)** **Dr Kingsley Obodo (NWU)** **Professor Catharine Esterhuysen (SU)**	Advanced computational modelling of materials	17 Collaborators 3 Research workshop 7 students supervised
Dr Vernon Visser (SANBI) **Prof Cang Hui (SU)** **Dr Sandra MacFadyen (SU)** **Dr Emmanuel Dufourq (SU)** **Prof John Measey (SU)**	Advancing biodiversity informatics and ecological modelling	7 Collaborators 1 Research workshop 3 students supervised
Prof Zurab Janelidze (SU) **Dr Yorick Hardy (WITS)** **Dr Partha Ghosh (UNISA)**	Space-like mathematical structures and related topics in algebra, logic and computation	4 Research workshops 28 Papers published or in process of going to press 36 Papers submitted for publication 42 Papers in progress
Dr Mesias Alfeus (SU)	Quantitative Finance	8 Papers published 1 Research workshop

Summaries of research reports

Mathematics

Principal Investigators:

The research programme is led by its Principal Investigators, currently: Prof Zurab Janelidze (SU), Dr Cerene Rathilal (UKZN) and Prof Bruce Watson (WITS).

Aims and Objectives of the programme in 2023:

The Mathematics Structures and Modelling research programme in 2023 made advances in the study of mathematical structures in logic, categories, deductive constructs (applications to mathematics education), groups, combinatorial structures (including applications of those in music), structures in algebra, geometry and topology, and analytic structures.

The aim of this research programme is to take a unified view in the study of mathematical structures across various disciplines (within and beyond mathematics), by forging collaborations that cross the traditional disciplinary boundaries. In some cases, further disciplinary research is required before inter-disciplinary research can be carried out. The results are reported in 28 papers either published or in press in the areas that have emanated from this research programme, as well as 36 papers which are submitted for publication. The rest of the results are reported in 42 papers in progress and 16 paper embryos.

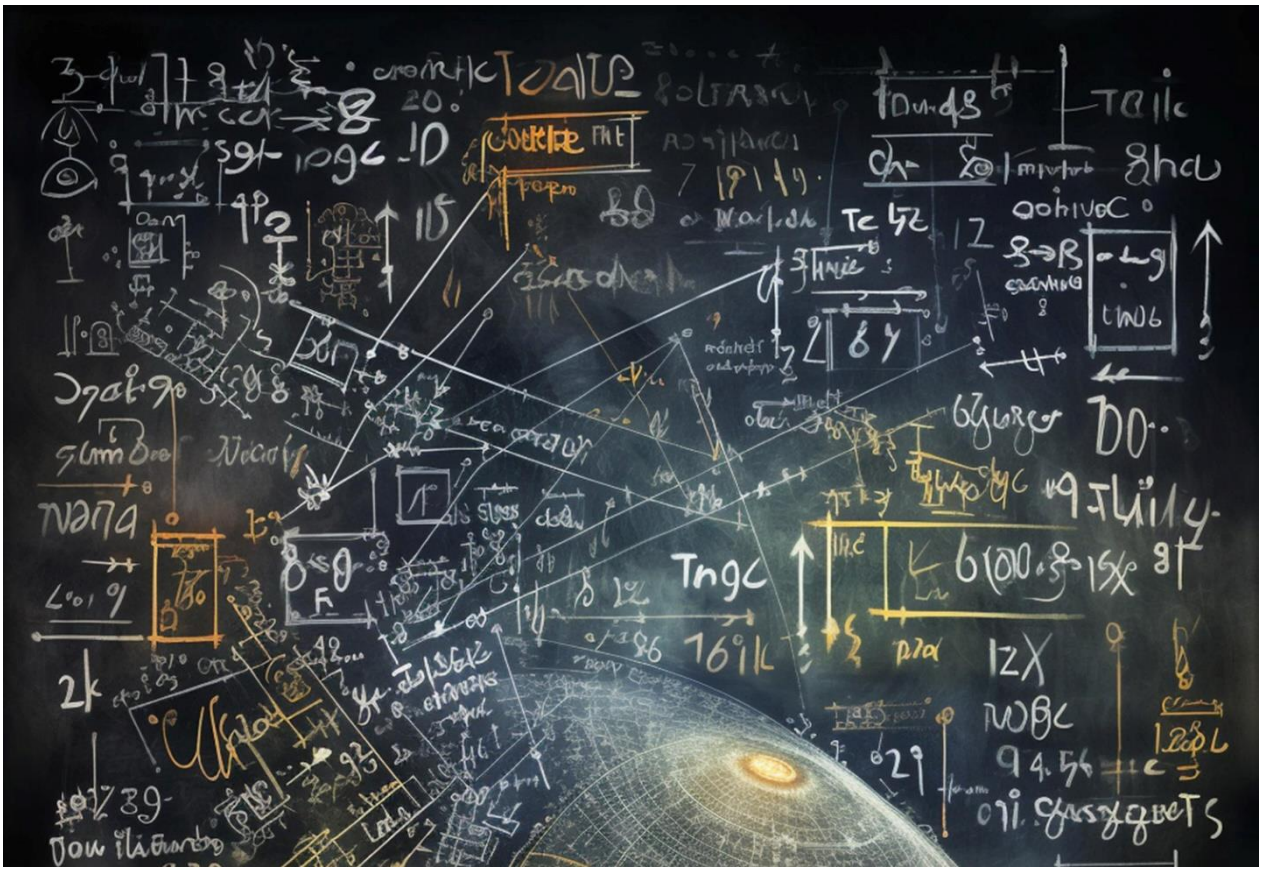
Highlights:

The Mathematical Structures and Modelling research programme focuses on blue skies research, with no predetermined research direction other than a very broad one: exploration and application of mathematical structures.

Among highlights in 2023 in terms of uncovering new and unexpected areas of application are insights gained in the area of deductive constructs in mathematics education and new combinatorial structures in music. In particular, various mathematical exploration sessions held with school learners and teachers suggest that (a) school teachers do not have a rigorous grasp of deductive reasoning; (b) school learners are capable of engaging in deductive reasoning, after they are introduced to it, even at as early as primary school level.

Challenges:

The Mathematical Structures and Modelling research group currently brings together 31 mathematicians and their students. It has been a challenge to have everyone involved equally in the research programme, and particularly to have everyone contribute equally to the interdisciplinary goals of the research programme.



Advancing biodiversity informatics and ecological modelling

Principal Investigators:

Dr Vernon Visser (SANBI), Prof Cang Hui (SU), Dr Sandra MacFadyen (SU), Dr Emmanuel Dufourq (SU), and Prof John Measey (SU).

Aims and objectives:

During the reporting period, the Advancing Biodiversity Informatics and Ecological Modelling (ABIEM) programme has made significant strides towards its objectives. The ongoing projects reflect a commitment to integrating data analysis and ecological understanding to address biodiversity challenges in South Africa and beyond.

In terms of long-term vision, the 5, 10, and 15-year goals of ABIEM are well-aligned with national and global biodiversity challenges. The programme's emphasis on interdisciplinary research, capacity building in ecological modelling, and the development of a Biodiversity Informatics Hub demonstrates a forward-thinking approach.

Strategically, ABIEM's initiatives align well with South Africa's national development goals and global biodiversity conservation efforts. The focus on data synthesis and analysis to inform decisions reflects a deep understanding of the role of informatics in addressing ecological challenges.

The expected knowledge and societal impacts of ABIEM are substantial. By enhancing data accessibility and promoting interdisciplinary research, ABIEM is poised to influence biodiversity conservation strategies significantly, both within South Africa and in the global context. The programme's emphasis on training and curriculum development is particularly noteworthy for its potential to shape future leaders in biodiversity informatics and ecological modelling.

Highlights:

During the reporting period, the Advancing Biodiversity Informatics and Ecological Modelling (ABIEM) programme achieved several notable milestones, though there were deviations from the original proposal timelines and focuses. The milestones achieved reflect a strong commitment to advancing biodiversity informatics and ecological modelling, with each project contributing valuable insights and tools for conservation efforts:

- An Ecologist's Data Pipeline Toolkit: The development of this toolkit, aimed at enhancing biodiversity data management, has progressed, albeit at a slower pace than anticipated.
- Ecology Hackathon: Initially planned for November 2023, the hackathon has been postponed to 2024 to align with the B3 Hackathon. This strategic decision, while deviating from the original timeline, opens opportunities for broader collaboration and impact in the field of biodiversity data analysis.
- Adaptive Dynamics Workshop: Hosted successfully within the proposed timeframe, this workshop marked a significant milestone. It brought together a diverse group of experts, leading to the development of new research topics in ecological modelling. This achievement aligns well with the project's aims and has fostered valuable interdisciplinary collaboration.
- Carbon Sequestration in Savanna Ecosystems: The focus on carbon accounting in savannas is progressing as planned, with significant theoretical and practical applications being developed. This research is crucial for understanding the role of savannas in global carbon dynamics.
- Behavioural Analysis of the endangered African Penguin: The project is on track, with substantial budget allocation remaining for comprehensive research. The use of innovative machine learning techniques for behavioural analysis signifies a significant milestone in understanding this endangered species.

Challenges:

Ethical clearance from the University and the governmental department of forestry fisheries and the environment took a lot of time to obtain.

Genomics, Bioinformatics and Advanced Medicine: Artificial Intelligence Interventions in Wellness and Mental Healthcare.

Principal investigators: Prof Martin Bucher (UKZN) and Dr Japie Greeff (NWU).

Aims and objectives:

The two main project goals were to create two artefacts applying artificial intelligence in the medical space. The two projects explored were the use of conversational AI in the pharmaceutical setting as well as artificial intelligence approaches to detecting state change in people with bipolar disorder. The pharmaceutical work is being done by Ms Vanessa Rufo in an MSc study under the supervision of Prof Japie Greeff and Prof JT Janse van Rensburg while the bipolar disorder work is predominantly being carried out by Prof Japie Greeff.

Research highlights:

Artificial intelligence in the pharmaceutical space

This project has progressed well, and the artefact in question is being developed as part of the MSc study of Ms Vanessa Rufo. A web interface has been created, and an Alan AI voice interface has been created for specific requests. The final part of the project is to integrate a Large Language Model back end that can deal with more complex requests than the Alan AI system that is more restrictive. The initial goal was to use BERT, but the emergence of much more advanced LLMs has caused us to move beyond BERT and instead use GPT-3.5. The current goal is to have the first full prototype ready with all components in the first semester of 2024.

Artificial intelligence in the mental health space

Two prototypes were developed between 2022 and the start of 2023 to explore classification using LLMs in both the server environment as well as on-device inference. Server classification on sentiment operated as expected, and although the capabilities of the edge-device inference were not at the same level, we did manage to get it to work. With the rapid development of LLMs however in 2023 we have switched direction away from MentalBERT and MobileBERT to LLaMA derived ALPACA models which will be used to create dedicated classifiers for specific mental health markers of distress.

Initially the idea was to create a diary-based application that would allow people to capture their thoughts and then use active learning to create on-device classifiers that would identify early markers of manic or depressive episodes in bipolar disorder diagnosed patients, but this has been moved a little further down the line so that the underlying classification models can be explored in more depth. There will still be a mobile application developed, but as there are a huge number of applications developed at the moment, it does not seem to be sensible to try and compete in the commercial space and instead focus on getting the classifiers as effective as possible in a server environment that can then be leveraged later by a mobile app as well as offer an API for use in other people's environments. The classification training will be done on synthetic data due to some problems experienced on ethical the front in terms of being able to use real world data to train the classifiers.

In exploring the use of real-world data, we have managed to build a relationship with the South African Depression and Anxiety Group as well as the Foundation for Professional Development. Additionally, in trying to understand the legal and ethical hurdles related to the nature of the project we have had great interactions with Prof Saskia Kelders from UTwente, Prof Katherine Sorsdahl from UCT, Prof Darelle van Greunen from NMU, Prof Minrie Greeff and Prof Wayne Towers from NWU.

The three classifiers that would be most impactful that have been identified are around anxiety, depression and suicidal ideation, and the synthetic data development system is in the process of being developed by Prof Japie Greeff and Mr Ian Masaga as part of his MSc in Computer Science.

Challenges:

The biggest challenges that have hit us this year have been on the ethical front in getting access to real-world data for the creation of the classifiers. We have made contact with SADAG and they are willing to share their data, but from the legal perspective and the perspective of the NWU health ethics research committee it is not possible to use data that was collected without informed consent. This however creates a huge problem in the data collection process. We are still exploring the ethical situation, but the pivot we are making for now is to create simulated data using LLMs to create the workflow for training such a theoretical classifier, so that once one exists, we can test it against a group of councilors to discover whether the technical approach will work, and then open sourcing this approach so that an organization like SADAG could take the work further, as if they approach it like an operational project it would not fall in the realms of research, and they may still gain the benefits that were envisioned.

Another challenge that is not directly related to the projects, but rather the conceptualization of the research thematic area, is that our current approach is very niche and not inclusive enough to attract researchers that are working in adjacent areas into our theme, and also requires us to identify students with specific interests in this area. As such, it is proposed that the thematic area adopt a framework like the capability approach which has as its focus creation of opportunities for people to gain more capabilities in their lives and become more capable than they were before intervention.

Advanced computational modelling of materials

Principal Investigators: Prof Tjaart Kruger (UP); Dr Aniekan Ukpong (UKZN); Dr Kingsley Obodo (NWU); Professor Catharine Esterhuysen (SU)

Aims and objectives.

Substantial progress has been made in achieving the aims and objectives of our projects in 2023:

- Theoretical models have now been developed to describe the thermoelectric properties of materials. Also, these theoretical models have been implemented computationally to simulate the behaviour of materials under different thermoelectric conditions. Computational experiments have been carried out on the CHPC's Lengau Cluster to identify the factors that limit the efficiency of thermoelectric interconversion and to explore strategies to overcome these limitations. Insights from these calculations have been used to propose experimentally feasible guidelines have been developed for the design of new materials with improved thermoelectric properties.
- A computational study was performed on a benzodithiophene-isoindigo copolymer to determine the main aggregation types. Additional computational studies of organic solar cells are ongoing.
- A theoretical-computational study was completed to determine the accuracy of approximate methods for calculating fluorescence-type spectra of photosynthetic light-harvesting complexes. A neural network model was developed for rapidly and accurately calculating spectra from molecular parameters, and *vice versa*. Multiscale QM/MM calculations were performed to calculate the exciton interactions and energy transfer dynamics in the main light-harvesting complexes of cyanobacteria for the first time. New insights were obtained about the photoprotective mechanisms of the photosynthetic light-harvesting complexes of plants and cyanobacteria.
- A quantum plasmonics model of refractive index sensing using photon correlations was developed.
- In order to undertake rational design of new catalytic materials based on catalyst species we have attempted to understand the nature of individual metal atoms interacting with the liquid organic carrier (LOHC) octahydroindole to gain further insight into the mechanism of its dehydrogenation on catalytic surfaces in collaboration with Dr Kingsley Obodo. In this way we will be able to identify what the crucial components of the interaction between metal and substrate are through energy decomposition analysis (EDA) in order to then determine which metal species could potentially be involved in forming the best mixed-metal catalytic surface. In this process we have successfully determined a suitable method and basis set for the study, and have determined that the lowest energy reactant complex with Pt is the same as that identified by Dr Obodo in his previous study, thus confirming that the computational method yields sensible results. We have also identified a similar reactant complex with Pd, as well as found corresponding transition states. A second study applying metal-organic frameworks in the catalytic conversion of CO2 has identified the nature of the interactions between the CO2 and the host-framework as well as guest-guest interactions.
- Novel materials suitable for high-capacity energy storage and energy conversion using density functional theory (DFT) calculations particularly 2D materials were discovered. The properties and characteristics of sorbent-based technologies in pollutant mitigation and environmental remediation were reviewed and discussed considering the cost and other implications.
- We designed new low platinum group metal (PGM) suitable for catalytic dehydrogenation of liquid organic hydrogen carriers (LOHC). LOHC materials are potential and promising candidates for energy storage and conversion.

Research highlights:

Dr Aniekan Ukpong

- The work has been completed on literature survey, model development and experiment design and data collection for the three focus areas:
- First principles investigation of quantum transport properties of the Kondo state in an energy material. This will involve finalising current research results on modelling of the many-body interactions involved in the spontaneous formation of Kondo effects in topological materials in the presence of a temperature gradient. Will publish the results in accredited journals.
- Computational experiments to understand the many-body interaction that are present in thermoelectric materials. This understanding will be used to create the peaks expected in the zero-bias conductivity as a unique signature of the presence of the broken-symmetry state in an energy conversion material. The responses of the zero-bias conductivity signature to applied symmetry breaking fields will be investigated explicitly to characterise the effect of phonons.
- Calculation of the mesoscopic transport signatures for describing electrons at the Kondo state will be performed on nanojunction models of thermoelectric materials.
- Data collection on our model Kondo system has been expanded to include a generalized many-body system where there is strong electron-electron correlation and many-body quantum entanglement effects. This is

important for providing a general framework for us to understand the nature of the entanglement between quantum objects (e.g. localised spins, atoms, etc. in a macroscopic condensed matter system) employed in our model. Different types of computational experiments have been performed to estimate the quantum entanglement by collecting and recording the data from computational experiments for analysis. These serve as the basis to measure the thermoelectric properties of Kondo systems under various entanglement conditions.

- Our data analyses continue. Statistical methods and machine learning techniques are used to analyse the generated computational data in comparison with reported experiments. using statistical methods. Comparisons of the experimental results with the theoretical model has been done to identify areas of agreement and discrepancies. The summary of the report has been written and dissemination of our findings have been carried out in four different indexed journals. Dissemination of the results of the study through conference presentations, seminars, and social media platforms has been done as planned.

Prof Tjaart Kruger

The focus of my project is twofold: (i) spectroscopic characterisation of the thermal and photostability of bioinspired polymer solar cells to be used as a benchmark to predict organic solar cells with improved performance in terms of both power conversion efficiency and thermal stability, and (ii) detailed investigation of photosynthetic light-harvesting complexes to extract design principles for organic solar cells.

Research highlights pertaining to focus (i) include the publication of two journal articles and the completion of a review article that is ready for submission. Research highlights of focus (ii) include:

- 1 manuscript accepted for publication; 4 manuscripts ready for submission
- 1 PhD student graduated during the past year; 1 PhD thesis submitted for examination; 2 PhD theses are in preparation.
- 1 MSc dissertation submitted for examination.
- 1 third-year student project was awarded 88%.
- Development of an open-source analysis suite for single molecule spectroscopy data: The software‘s beta version is available on GitHub (https://github.com/BioPhysicsUP/Full_SMS) and 1 journal manuscript and two PhD theses are in preparation.

Additional highlights:

- NRF‘s Research Excellence Award For Next Generation Researchers awarded to one of the PhD students
- The PI received an NRF C1 rating and was promoted to a Senior Editor of the Journal of Physics Chemistry Letters
- 1 conference was organised; 7 invited international conference presentations and 1 invited national conference presentation; 16 international conference presentations and 4 national conference presentations; oral presentation, student awards at two conferences
- 1 public lecture for primary school children on biomimicry
- Several research and training visits: Ugandan collaborator visit, Ethiopian PhD student visit, one of our PhD students visited Temple University (USA) and another PhD student visited University of Erlangen-Nuremberg in Germany.

Professor Catharine Esterhuysen

Since I only joined NITheCS in March this year the project on catalytic dehydrogenation of LOHCs was only initiated in the middle of the year and we have not yet been able to complete the study. Similarly, since I came into the project late, the study of CO2 conversion by the metal-organic framework was not in the original proposal but has shown great promise. Neither has yet yielded outputs, but the CO2 project has successfully identified the nature of the CO2 interactions which is being written up for publication.

Dr Kingsley Obodo

The research project is focused on three distinct areas: (i) Hydrogen economy via catalysis with emphasis on development of low-PGM based catalytic materials for the dehydrogenation reaction (ii) 2D materials for photocatalysis and photovoltaic application. (iii) Sorbent based technologies for environmental remediation. Research highlights on focus (i) resulted in two manuscripts published, one USA patent and 1 PhD thesis in preparation.

Research highlights on focus (ii) resulted in one manuscript accepted for publication, one 1 PhD thesis in preparation and 1 MSc graduated during the past year.

Research highlights on focus (iii) resulted in five book chapters published.

Additional highlights:

- The PI received an NRF C2 rating
- 1 NITHeCs school was organised
- 1 mini-school organised at the CHPC national conference
- 2 invited international conference presentations
- Research and training visit at the University of Nigeria

Challenges in 2023:

Dr Aniekan Ukpong

- The CHPC's Lengau Cluster, where all my computational experiments are done, has been suffering severely from frequent downtimes due to the on-going load-shedding. This has led to several periods during which the CHPC's Supercomputer is simply unavailable to support scientific computing, and leads to a crisis of an unnecessarily long queue of submitted albeit unfinished calculations.
- It is extremely challenging to find suitable candidates who are appointable as *ad hoc* research assistants in both statistical field theory and quantum field theory, even amongst postgraduate students. It is for the reason of this challenge that I have deliberately implemented the NITheCS Research Internship in 2023 to develop local capacity and grow technical capability in my research area. When I advertised vacancies for research assistants at the UKZN, there were no applications were received. This is an inherent/apparent issue in physics, which severely affects my area/discipline in theoretical and condensed matter physics research.
- My employer (the UKZN) did not allow me to buy out my teaching time to enable me focus on research
- Due to teaching duties, I could not attend the annual meeting of the American Physical Society (APS) to discuss the results of this work. However, part of the research work has been published already in 2023 - including in the *Physical Review B*, a DHET-accredited APS Journal.

Prof Tjaart Kruger

- Due to the high levels and extended periods of load-shedding during the past year, the CHPC was frequently down and we had to wait for the continuation of projects requiring intensive calculations.
- Collaboration with the project partners at Univen turned out to be very challenging due to infrequent communication and lack of progress on their side. In addition, the main core member from Univen retired a few months ago.
- Only half of the originally planned teaching time was bought out due to a lack of suitably qualified and available people in the department. However, the Head of Department decided to replace that bought-out teaching module with one of a much heavier weight. The result was that my teaching load significantly increased this year and limited my time for research even further.

Professor Catharine Esterhuysen

As I joined the project fairly late, I was not able to complete as much as I would have liked. In addition, 2023 was a difficult year for me and my students, with the knock-on effect of the COVID-19 period affecting all of us in terms of high stress levels. Also, due to time constraints I was unable to undertake any research visits, such as to Dr Obodo for a face-to-face discussion of our results as we were working together on this project. I hope to be able to do this next year.

Dr Kingsley Obodo

- The CHPC's Lengau Cluster, where all my computational experiments are done has been suffering severely from frequent downtimes due to the on-going load-shedding and electricity crisis. This has led to several periods wherein the CHPC's Supercomputer is simply unavailable to support scientific computing, and the ensuing crisis of unnecessarily long queue of submitted but unfinished calculations.
- I would also like to see an in-person meeting with Prof Esterhuysen and a writing workshop with her.
- Visiting other research collaborators was particularly challenging due to getting the research funds late last year.

Machine learning in support of computational and theoretical sciences

Principal Investigators: Prof Marelie Davel (NWU); Dr Stefan Lotz (SANSA)

Aims and objectives:

The overarching long-term objective of this programme is to facilitate machine learning (ML) research which can support multidisciplinary research efforts at NITheCS.

This objective has three elements:

- ML research: The development of new, specialised ML techniques.
- ML as tool: Applying ML for scientific modelling applications.
- ML forum: Growing a collaborative ML community and environment within NITheCS.

The ML research programme was initiated in 2022, and a first collaborative research project was defined around a single theme. The project, 'Knowledge Discovery in Time Series Data', also referred to as 'KnowIt', aims to bring together researchers working on algorithm and technique development, and researchers whose application domains include time series data.

Research highlights and progress made during the year:

- Development of the envisaged toolkit (KnowIT v1.0). The original toolkit was developed using a forecasting library, which made the extension to alternative application tasks (classification, regression, detection) cumbersome. For this reason, the new toolkit (KnowIt v1.0) was re-developed using a more general machine learning framework (PyTorch Lightning). KnowIt is flexible enough to handle a variety of tasks while being modular enough to easily add additional features as the need arises. Its capabilities currently include configuring and importing data, model configuration and training, and extracting explanations. This toolkit facilitates the fast development and interpretation of deep neural network (DNN)-based time series models.
- The development of a new technique to analyse the accuracy of explanations against a known ground truth. This has been formalised as an MEng study, currently in progress.
- Ongoing progress in specific application areas:
    - Schoombie: Penguin prey capture event identification. Ongoing collaboration. Application under development. Initial models developed.
    - Lotz: Geomagnetic index prediction and feature attribution. Ongoing collaboration. Development of solar wind-based prediction models for geomagnetic disturbances with interpretation capability.
    - Watson & Conacher: Microbial biology time series analysis. Ongoing collaboration. A synthetic yeast-like dataset was developed using agent-based modelling. This produced data with a known ground truth that is being utilised to develop and explain spatio-temporal models of yeast interactions.
    - MacFadyen: Inter-species dynamics in ecological environment. The current KnowIT platform models time series data rather than spatio-temporal data. We therefore started with a pre-study of spatio-temporal models in a controlled environment. This collaboration is on hold until the pre-study has been concluded.
    - Modipa & Ramalepa: Natural language processing. Text generation for indigenous languages (Sepedi). Exploring the use of interpretable ML methods.
- Definition of three new postgraduate studies directly supporting this project.
- Presentations at four international events.
- A number of national and international conference presentations, proceedings and publications produced by researchers affiliated with this programme.
- Sharing findings and results at the in-person year-end workshop held 5 December in Muldersdrift, co-located with SACAIR.

Additional funding opportunities:

The NITheCS project has allowed the pursuit of additional funding opportunities. Two are promising:

- A collaboration agreement has been signed between NWU and ExploreAI. This agreement is also directly linked to the topic and visibility of the current NITheCS project.
- A co-funded SARChI chair is in the process of being established. The NRF has accepted the concept note and an MOA has been signed, pending approval of the final proposal.) This chair is linked to the NITheCS RP topic and one of the PIs of this programme.

Challenges/constraints:

There were no challenges that could not be managed. Two constraints to mention:

- The project is still gaining momentum, with stronger outputs directly linked to the project expected with the foundational phase completed (end 2023).
- More certainty with regard to the future of the research programmes now that the new NITheCS Directorate is in place will facilitate easier planning.

New insights into astrophysics and cosmology with theoretical models confronting observational data

Principal Investigators: Prof Amare Abebe (NWU); Prof Aroon Beesham (MUT); Dr Shajid Haque (UCT) Prof Soebur Razzaque (UJ) Prof Bruce Watson (SU)

Aims and Objectives:

One of the goals of our proposal was to understand astrophysical events by using tools such as the quantum complexity of quantum information theory. Quantum complexity serves as a proxy for various physical quantities and can be useful in providing new insights into astrophysical events. Toward this goal, we have already submitted a paper where we studied certain aspects of neutrino oscillations using quantum complexity. This novel approach has proven to be extremely useful and has opened a new direction for various future projects. Currently, we are working on a couple of follow-up projects based on this technique. On top of this we published some papers separately with our collaborators.

We made substantial progress in achieving the research aims this year. We have achieved the first detection of the integrated Sachs-Wolfe effect with thermal Sunyaev-Zeldovich effect, which indicates the gas is correlated in very large scales. This correlation can be used to constrain primordial non-Gaussianity.

In addition, we have proposed a new method to examine the broken-power law of the cosmic ray electrons, which spectrum may indicate the existence of dark matter annihilation. We have studied dark energy/acceleration of the universe in several cosmological models in modified gravity theories. These models can explain the current accelerated expansion of the universe, and the transition from deceleration to acceleration. The models have been subjected to observational constraints. One PhD and one MSc student are both engaged in the project. The main focus of research was constraining different alternative cosmological and gravitational models with observational data. In this context, we have studied the observational constraints of Chaplygin gas and Bianchi cosmological models as well as the alternative theories of f(R,T) and f(Q) gravity.

Research highlights:

- *Quantum Spread Complexity in Neutrino Oscillations*, Dixit, Haque, Razzaque. Explores quantum complexity's application in studying neutrino oscillations. Presented at a conference in Banff, Canada, in June 2023.
- *Very high-energy gamma rays from GRB 180720B and GRB 190829A,* Barnard, Razzaque, Joshi. Investigates emission mechanism for gamma-ray bursts (GRBs). Finds different fits for two different GRBs.
- *Decoherence, entanglement negativity, and circuit complexity for an open quantum system*, Bhattacharyya, Hanif, Haque, Paul. Compares saturation timescales in two different open quantum systems. Finds complexity saturates for a completely mixed state.
- *Solar gamma ray probe of local cosmic ray electrons,* Yang, Gao, Ma, Crocker. Shows an excess in the TeV range can induce a characteristic solar gamma ray signal. Suggests experimental verification of CREs.
- *Implications for primordial black holes from cosmological constraints on scalar-induced gravitational wave*, Cang, Ma, Gao. Provides constraints on primordial black holes created from scalar perturbations in the early universe.
- *Cross-correlation of cosmic voids with thermal Sunyaev-Zel'dovich data*, Li, Ma, Tramonte, Li. Measures the deficit in the Sunyaev-Zel'dovich Compton-y signal towards cosmic voids. Confirms voids are under-pressured regions compared to their surroundings.
- Other contributions include creating cosmological models in modified gravity theories and publishing joint papers with PhD. and MSc students.

Additional publications and highlights:

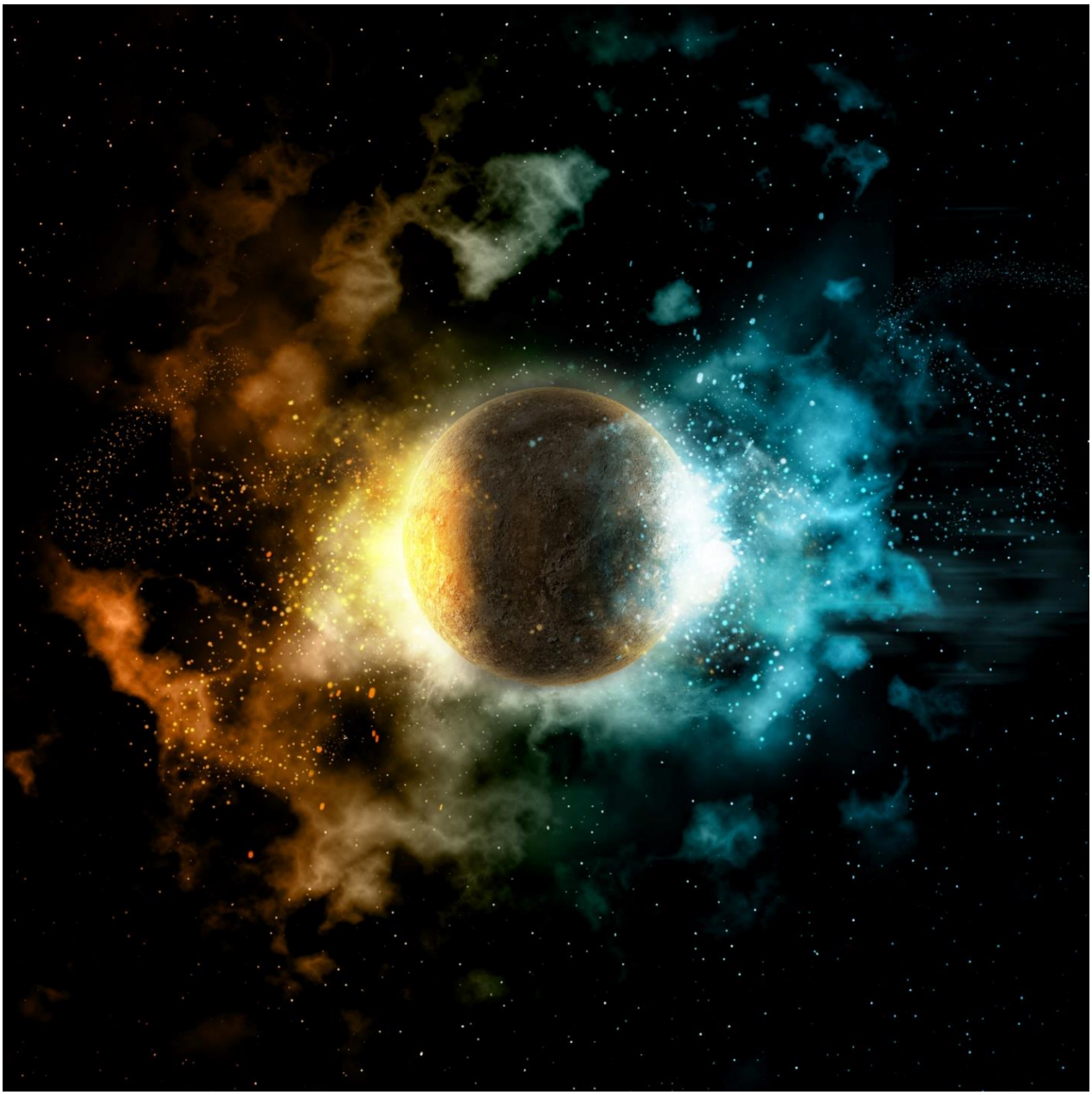
- Ayodeji Ibitoyei, Wei-Ming Dai, Yin-Zhe Ma, , Patricio Vielva, Denis Tramonte, Amare Abebe, and Aroonkumar Beesham, *Cross-correlation between the thermal Sunayev-Zeldovich effect and the Integrated Sachs-Wolfe effect*, Astrophys. J., Suppl. Ser. (arXiv:2310.18478)
- Mouhssine Koussour, Nurgissa Myrzakulov, Alnadhief HA Alfedeel, and Amare Abebe, *Constraining the cosmological model of modified f(Q) gravity: Phantom dark energy and observational insights*, Prog. Theor. Exp. Phys 113E01 (2023)
- Renier Hough, Shambel Sahlu, Heba Sami, Maye Elmardi, Anna-Mia Swart, and Amare Abebe, *Confronting the Chaplygin gas with data: background and perturbed cosmic dynamics*, Int. J. Mod. Phys. D 32 (13) 2350090 (2023)
- Nurgissa Myrzakulov, Mouhssine Koussour, Alnadhief HA Alfedeel, and Amare Abebe, *Constrained evolution of effective equation of state parameter in non-linear f(R,Lm) dark energy model: Insights from Bayesian analysis of cosmic chronometers and Pantheon samples*, Eur. Phys. J. Plus 13 (9) 852 (2023)
- Guo-JianWang, Cheng Cheng, Yin-Zhe Ma, Jun-Qing Xia, Amare Abebe, and Aroonkumar Beesham, CoLFI: *Cosmological Likelihood-free Inference with Neural Density Estimators*, Astrophys. J., Suppl. Ser. 268:7 (2023)
- Değer Sofuoğlu, Alnadhief H. A. Alfedeeli, and Amare Abebe, *Cosmographic implications of f(R, T) gravitation*, Eur. Phys. J. Plus 138:696 (2023)

- Amare Abebe, Alnadhief H. A. Alfedeel, Değer Sofuoğlu, Eltegani I. Hassan, and Rishi K. Tiwari, *Perturbations in Bianchi - V spacetimes with varying Λ, G and viscous fluids*, Universe 9(2) 61 (2023)
- Adams Duniya, Amare Abebe, Alvaro de la Cruz-Dombriz, Peter Dunsby, *Imprint of f(R) gravity in the cosmic magnification*, Mon. Not. R. Astron. Soc 518(4) 6102 (2023)
- Academic highlights: Student graduation: 2 Masters Graduation (2023), 1 Masters (estimated 2024), 1 Doctoral student (Estimated 2024)
- Papers published: 39 published, 3 under review
- Conference presentations: 37

Challenges:

- Our proposal spans multiple disciplines within physics, bringing together entirely disconnected branches. Consequently, finding a common ground for uniform contributions has been a challenge. It took us some time to establish the problem, but we are now making smooth progress.

- A challenge is the number of cosmological models apart from the standard LambdaCDM model in general relativity which satisfy observational constraints, and how to choose the best model (S).



Quantum technologies for sustainable development

Principal Investigators: Dr Shajid Haque (UCT); Prof Thomas Konrad (UKZN); Prof Stef Roux (NMISA,UKZN); Prof Jeff Murugan (UCT); Prof Ilya Sinayskiy (UKZN).

Aims and Objectives:

- The goal of this section of the proposal was to investigate the complexity of quantum many-body systems, aiming to comprehend quantum chaos and phase transitions. We have published several papers in pursuit of this objective. (Haque, Murugan)
- We aimed at designing new tools that increase the bandwidth of quantum communication. Two articles are published, one is accepted for publication, two more are in preparation. (Konrad, Roux)
- This section focuses on using universal fault-tolerant and NISQ devices for quantum computation and quantum machine learning, focusing on open quantum systems. (Sinayskiy)

Research highlights and progress made during the year

Below are summaries of work done and articles/presentations based on the work:

- *Spread Complexity and Topological Transitions in the Kitaev Chain* (Pawel Caputa, Nitin Gupta, S. Shajidul Haque, Sinong Liu, Jeff Murugan, Hendrik J. R. Van Zyl): Several recent studies contend that quantum complexity, a well-established concept in quantum information theory, could serve as an effective probe for quantum phase transitions. This work was presented in August 2023 in Korea.
- *Krylov Complexity and Spectral Form Factor for Noisy Random Matrix Models* (Arpan Bhattacharyya, S. Shajidul Haque, Ghadir Jafari, Jeff Murugan, Dimakatso Rapotu): We examine the spectral properties of two random matrix models: non-Gaussian RMT with quartic and sextic potentials, and RMT with Gaussian noise. Analyzing the quantum Krylov complexity and spectral form factor, we observe short-term suppression in both models due to decoherence, with divergent long-term behaviours. Notably, the Krylov complexity in non-Gaussian RMT and RMT with noise deviates from Gaussian RMT. Our findings highlight distinct sensitivities of spectral form factor and complexity to non-Gaussianity and noise, impacting various time domains in quantum chaos and information within open quantum systems.
- *Krylov Complexity for Jacobi Coherent States* (S. Shajidul Haque, Jeff Murugan, Mpho Tladi, Hendrik J. R. Van Zyl): We developed computational tools to extend Krylov complexity beyond conventional Hamiltonian systems. We enhanced the Lanczos algorithm to handle coherent states associated with the Jacobi group - a semi-direct product of the 3-dimensional real Heisenberg-Weyl group and the symplectic group. These coherent states, realized as squeezed states in quantum optics, serve as the basis for the Krylov basis. This enables benchmarking a scheme for numerically computing Lanczos coefficients, potentially generalizing to the broader Jacobi group. This work was presented in August 2023 in Korea.
- *Stimulated teleportation of high-dimensional information with a nonlinear spatial mode detector* (Bereneice Sephton, Adam Valles, Isaac Nape, Mitchell A. Cox, Fabian Steinlechner, Thomas Konrad, Juan P. Torres, Filippus S. Roux, Andrew Forbes.) Article under review at *Nature Communication.* We show in theory but with experimental proof that quantum teleportation based on non-linear optics to project onto entangled states (as part of a so-called Bell measurement) bears the possibility to teleport superpositions of spatial modes from a coherent state carrier to remote single photon. This leads to an increase of the bandwidth of quantum teleportation, which before was limited to low dimensional states. This is made possible because the non-linear optical effect of three-wave mixing realised in non-linear crystals does not require the preparation of multiple single photons as necessary when using linear optics to implement Bell measurements. We develop the theory of quantum teleportation of spatial modes and introduce the space bandwidth product to characterise the information capacity of the teleportation channel.
- *Teleporting a 15-dimensional state with a nonlinear spatial detector* (A. Vallés, B. Sephton, I. Nape, M. A. Cox, F. Steinlechner, T. Konrad, J. P. Torres, F. S. Roux, and A. Forbes. Article in *Optica Nonlinear Optics Topical Meeting 2023*, Technical Digest Series). New state-of-the-art for quantum teleportation with single entangled photon pair.
- *Bell inequalities for Helical Mathieu-Gauss vector modes* (Edgar Medina-Segura, Francisco I. Mecillas-Hernández, Thomas Konrad, Carmelo Rosales-Guzmán and Benjamin Perez-Garcia). Article accepted for publication by *Journal of Optics*. We analyse entanglement between polarisation and spatial modes as for particular light fields carried by single photons but also in classical states of light in terms of the violation of Bell inequalities (CHSH) and show that the violation depends on the ellipticity parameter of the considered Mathieu-Gauss modes. These light fields show “local entanglement”, i.e. variations of the polarisation on small areas of the transversal plane that might be used to quantify how many polarisation qubits the light fields can carry for quantum information processing and communication tasks.
- *Four-wave mixing in all degrees of freedom*. The Wigner functional approach is a new formalism that describes the spatio-temporal as well as the photon number degrees of freedom. This approach is here employed to derive an evolution equation for a photonic state propagating through a Kerr medium that can be used for a thorough analysis of all experimental parameters in physical quantum information systems applying a Kerr non-linearity. One student has submitted a MSc dissertation (under review) on the Wigner functional formalism.
- *Quantum optical formulation of Difference Frequency Generation and Optimal Cloning of spatial modes* (Tanita Permaul and Thomas Konrad - article in preparation). We have developed a quantum optical formulation of difference-frequency generation (DFG) that incorporates the spatial modes of light. It reproduces the well-established result for classical light beams and establishes the relation of DFG to stimulated and spontaneous parametric down conversion. These relations determine that stimulated parametric down-conversion can realise N → M d-dimensional optimal quantum cloning.

- *Hierarchical quantum circuit representations for neural architecture search* (M Lourens, I Sinayskiy, D.K. Park, C. Blank, F. Petruccione). Quantum circuit algorithms often require architectural design choices analogous to those in constructing neural and tensor networks. These tend to be hierarchical modular and exhibit repeating patterns. Neural Architecture Search (NAS) attempts to automate neural network design through learning network architecture and achieves state-of-the-art performance. We propose a framework for representing quantum circuit architectures using techniques from NAS, which enables search space design and architecture search. We use this framework to justify the importance of circuit architecture in quantum machine learning by generating a family of Quantum Convolutional Neural Networks (QCNNs) and evaluating them on a music genre classification dataset, GTZAN. Furthermore, we employ a genetic algorithm to perform Quantum Phase Recognition (QPR) as an example of architecture search with our representation. Finally, we implement the framework as an open-source Python package to enable dynamic circuit creation and facilitate circuit search space design for NAS. This work was presented in November 2023 at CERN (Switzerland)
- *Near-term algorithms for linear systems of equations* (A Pellow-Jarman, I Sinayskiy, A Pillay and F Petruccione). Finding solutions to systems of linear equations is a common problem in many areas of science and engineering, with much potential for a speed-up on quantum devices. While the Harrow–Hassidim–Lloyd (HHL) quantum algorithm yields up to an exponential speed-up over classical algorithms in some cases, it requires a fault-tolerant quantum computer, which is unlikely to be available in the near term. Thus, attention has turned to investigating quantum algorithms for noisy intermediate-scale quantum (NISQ) devices, where several near-term approaches to solving systems of linear equations have been proposed. The team's paper focuses on the Variational Quantum Linear Solvers (VQLS), and other closely related methods and adaptions. Several contributions in this paper include: the first application of the Evolutionary Ansatz to the VQLS (EAVQLS), the first implementation of the Logical Ansatz VQLS (LAVQLS), based on the Classical Combination of Quantum States (CQS) method, a proof of principle demonstration of the CQS method on real quantum hardware and a method for the implementation of the Adiabatic Ansatz on the VQLS (AAVQLS). These approaches are implemented and contrasted. The CQS method is run with moderate success on a real quantum device. The EAVQLS and AAVQLS show promise as possible improvements to the standard VQLS algorithm once refined.
- *Digital Simulation of Single Qubit Markovian Open Quantum Systems: A Tutorial* (IJ David, I Sinayskiy, F Petruccione). One of the first proposals for using quantum computers was the simulation of quantum systems. Over the past three decades, great strides have been made in developing algorithms for simulating closed quantum systems and the more complex open quantum systems. We introduce the methods used to simulate single-qubit Markovian open quantum systems. It combines existing notations into a common framework that can be extended to more complex open-system simulation problems. The only currently available algorithm for the digital simulation of single-qubit open quantum systems is discussed in detail. A modification to implementing the simpler channels removes the need for classical random sampling, thus making the modified algorithm a strictly quantum algorithm. The modified algorithm uses quantum forking to implement the simpler channels that approximate the total channel. This circumvents the need for quantum circuits with many CNOT gates.
- *QAOA Performance in Noisy Devices: The Effect of Classical Optimizers and Ansatz Depth* (A Pellow-Jarman, S McFarthing, I Sinayskiy, A Pillay, F Petruccione). The Quantum Approximate Optimization Algorithm (QAOA) is a variational quantum algorithm for Near-term Intermediate-Scale Quantum computers (NISQ) providing approximate solutions for combinatorial optimization problems. The QAOA utilizes a quantum-classical loop, consisting of a quantum ansatz and a classical optimizer, to minimize some cost functions computed on the quantum device. Here we present an investigation into the impact of realistic noise on the classical optimizer and the determination of optimal circuit depth for the Quantum Approximate Optimization Algorithm (QAOA) in the presence of noise. We find that, while there is no significant difference in the performance of classical optimizers in a state vector simulation, the Adam and AMSGrad optimizers perform best in the presence of shot noise. Under the conditions of real noise, the SPSA optimizer, along with ADAM and AMSGrad, emerge as the top performers. The study also reveals that the quality of solutions to some five-qubit minimum vertex cover problems increases for up to around six layers in the QAOA circuit, after which it begins to decline. This analysis shows that increasing the number of layers in the QAOA in an attempt to increase accuracy may not work well in a noisy device.
- *A Multi-Class SWAP-Test Classifier* (S M Pillay, I Sinayskiy, E Jembere, F Petruccione). Multi-class classification problems are fundamental in many varied domains in research and industry. To solve multi-class classification problems, heuristic strategies such as One-vs-One or One-vs-All can be employed. However, these strategies require the number of binary classification models developed to grow with the number of classes. Recent work in quantum machine learning has seen the development of multi-class quantum classifiers that circumvent this growth by learning a mapping between the data and a set of label states. Here we present the first multi-class SWAP-Test classifier inspired by its binary predecessor and the use of label states in recent work. With this classifier, the cost of developing multiple models is avoided. In contrast to previous work, the number of qubits required, the measurement strategy, and the topology of the circuits used is invariant to the number of classes. In addition, unlike other architectures for multi-class quantum classifiers, the state reconstruction of a single qubit yields sufficient information for multi-class classification tasks. Both analytical results and numerical simulations show that this classifier is not only effective when applied to diverse classification problems but also robust to certain conditions of noise. This work was presented in November 2023 at CERN (Switzerland). Four MSc and one PhD students graduated; three papers published during the reporting period) and five under review.

Challenges and constraints impacting negatively on this project for the reporting period:
We had to wait for eight months to employ a research assistant because of visa and admin waiting periods. (Konrad)

Quantitative finance

Principal Investigator: Dr Mesias Alfeus (SU)

Aims and objectives:

- Facilitate Industry-Academic Collaboration: Our primary goal is to foster robust partnerships between industry and academia by actively soliciting research problems from industry stakeholders.
- Promote High-Quality Research Outputs: We are committed to supporting and incentivising the production of high-quality research in quantitative finance.
- Provide Funding Support for Students: We endeavour to nurture the next generation of quantitative finance experts by providing partial funding opportunities for Masters and higher degree by research (HDR) students in mathematical finance. By investing in local talent, we aim to cultivate a pool of skilled professionals who can contribute to the advancement of quantitative finance both locally and globally.
- Facilitate Knowledge Sharing and Collaboration: We organise conferences and workshops where researchers can showcase their findings, exchange ideas, and collaborate on future projects.

Research Highlights for QFRP in 2023:

- International Conference Participation: Attended the prestigious International Conference on Quantitative Finance and Risk Analysis in Greece (July 22-24), indicating global engagement in the field.
- Colloquium organisation: Five colloquiums were successfully organised, providing platforms for intellectual exchange and collaboration among researchers and practitioners in quantitative finance.
- Publication success: Eight papers from QFRP were accepted and published in reputable international journals, reflecting the high quality and impactful research conducted by the team.
- Academia-Industry Collaboration: QFRP undertook four academia-industry projects, including a groundbreaking collaboration with wine cellar fine wine merchants to develop the first South African fine wine index.
- Network expansion: QFRP expanded its network, with more than 16 associates now spread across ten South African institutes. This fosters broader collaboration and knowledge sharing.
- Support for postgraduate students: QFRP awarded 21 partial funding grants to postgraduate students from over six participating South African universities.
- Summer School on Quantitative Finance: In July 2023, QFRP organized a successful summer school focused on quantitative finance. This providing valuable education and training opportunities for students and professionals.
- Collaboration with InSPiR2eS Centre: QFRP forged a collaboration with the InSPiR2eS Centre for Responsible Science (IC4RS), led by Prof. Robert Faff of Bond University, Australia. This is aimed at promoting high-quality research and responsible practices in quantitative finance.
- Workshop on NITheCS-QFW2024: QFRP organized the inaugural Workshop on NITheCS - Quantitative Finance (NITheCS-QFW2024). This served as a dynamic platform for academia and industry professionals to discuss and exchange insights on the theoretical foundations and practical applications in quantitative finance.

Challenges:

The QFRP encountered several challenges in engaging industry participation.

Despite concerted efforts by Dr Mesias Alfeus to connect with key industry players, these attempts did not materialize into collaborations or involvement in the research programme.

Similarly, Professor Francesco Petruccione faced challenges in engaging executives from FirstRand, hindering the programme's ability to establish meaningful partnerships or collaboration with industry entities.

The difficulty in securing industry involvement poses a significant obstacle to the programme's goals and potential impact and limits opportunities for practical application and real-world validation of research outcomes.

TEACHING PROGRAMME

Overview

The NITheCS South African Theory and Computational School (SATACS) is a decentralised, semi-virtual, national teaching programme in theoretical physics and the computational sciences.

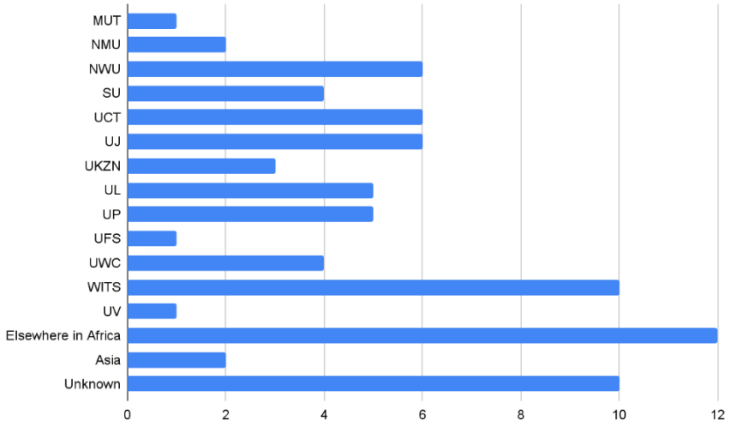
Under the directorship of Prof Will Horowitz, the SATACS goal is to provide teaching of the highest quality, pitched at Honours or Masters levels. The intention is for the programme to equal elite postgraduate programmes around the world. Courses are presented online and/or or in person, depending on the needs of relevant presenters.

In 2023 SATACS expanded its range with two additional courses. A total of 78 applications were received, which represented 21 universities. The majority of participants were Masters students (42%), followed by Doctorate students (27%) and Honours students (18%). Almost a quarter of these participants were female.

Details of SATACS courses

Presenter(s)	Topic	Duration
Prof Jeff Murugan (UCT)	Differential Geometry	1 semester
Dr Makhamisa Senekane	Trustworthy Machine Learning	1 semester
Dr Fritz Solms	Software Architecture	1 semester
Prof Tommie Meyer	Logics for Artificial Intelligence	1 semester
Dr Jaco van Zyl	Symmetries in Physics - An Introduction to Group Theory	1 semester
Prof Zurab Janelidze	Special Topics in Category Theory	1 semester
Prof Amare Abebe	Cosmology	1 semester
Prof Konstantinos Zoubos	Integrable Systems	1 semester
Prof Will Horowitz	Quantum Field Theory I	1 semester
Dr Makhamisa Senekane	Adversarial Artificial Intelligence	1 semester
Prof Jonathan Shock	Machine Learning: from Linear Regression to Deep Learning	2 semesters
Prof Laure Gouba	Ordinary Differential Equations	1 semester
Prof Will Horowitz	Quantum Field Theory II	1 semester

Applicants' institutions



INTERNSHIPS

NITheCS Internship Programme

This flagship NITheCS programme offers students a training opportunity through internship under the supervision of NITheCS Associates and their appointed tutors at a South African university. Interns are also invited to present their research reports at the annual SAIP conference the following year.

The internship programme takes place in two phases:
First phase: November / December 2023
Second phase: mid-January to mid-April 2024

2023/2024 programme:
In July 2023 NITheCS Associates were invited to suggest topics for the 2023/2024 NITheCS Internship Programme. Two virtual Information Sessions about the programme, led by Prof Francesco Petruccione, were held to inform Associates about the programme and answer questions.

A total of 138 students then applied to participate in the programme, from which 29 were selected for the 2022/2023 cohort. The internship programme took place at five institutions as follows:

- CSIR (Dr David Tshwane): 6 interns
- Nelson Mandela University (Prof A. Muronga): 19 interns
- Stellenbosch University (Prof Y. Ma): 1 intern
- University of Johannesburg (Prof A. Goswami): 1 intern
- University of KwaZulu-Natal (Dr A. Ukpong): 2 interns

Participants in the NITheCS Internship programme

Student affiliation	Female	Male	Total
Nelson Mandela University	2	1	3
Stellenbosch University	1	2	3
Sol Plaatje University		1	1
University of Limpopo	2	4	6
University of Cape Town		3	3
University of Johannesburg		1	1
University of KwaZulu-Natal		1	1
University of South Africa	1		1
University of the Witwatersrand		1	1
University of Venda	3	4	7
University of Zululand	2		2
TOTAL	**11**	**18**	**29**

SCIENTIFIC PUBLICATIONS

Publications: NITheCS affiliation

NITheCS affiliation in publications appear with the following reference: 'National Institute for Theoretical and Computational Sciences (NITheCS) South Africa'. NITheCS does not claim any funds from the Department of Higher Education and Training (DHET) for references in publications. The statistics are solely used for reporting purposes in our annual reporting to the DSI and NRF.

Number of publications per year: 2018-2023

	2018	2019	2020	2021	2022	2023
Core*	18	16	30	11	8	9
Associates	35	30	19	27	94	88
TOTAL	53	46	49	38	102	97

* Publications by NITheCS Directorate and Postdocs

List of publications

The following publications have been written or co-written by NITheCS Associates who included their NITheCS affiliation. The sources are *Web of Science* and *Scopus*.

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COMMUNICATION

Overview

NITheCS communicates widely with all its stakeholder groups to inform them about news, invite them to attend events and share information about relevant opportunities via NITheCS and associated bodies. Among others, the media and methods include:

- Direct e-mail is used for most communication with individuals.
- NITheCS Associates are entitled to have a NITheCS e-mail address on request.
- A monthly newsletter is distributed among all our Associates, interns, bursary holders and other interested parties.
- E-mailed notices about events and other matters of importance are distributed via a fast-growing e-mail list. We encourage all interested groups and individuals to join the mailing list and subscribe to the newsletter.
- A well-maintained website, https://nithecs.ac.za/, contains information about the Institute, its people and events.
- Social media: we have several social media accounts (Linked-In, X, Facebook, YouTube and Instagram) to cover different audiences and communication needs. Our X-feed (previously Twitter) also appears on the website. Social media is utilised to publish news about events, as well as notes of general information to the scientific community. Interaction on social media helps to spread awareness of NITheCS and its activities, while utilising the preferred communication preferences of the groups within the NITheCS community.
- Most colloquiums, mini-school lectures and other presentations are recorded. Pending approval of the presenters that we may do so, the recordings are uploaded and feature on our YouTube channel after the event. There are some examples at https://www.youtube.com/@nithecs. These video recordings of talks are useful resources for people who could not attend a particular event or who simply want to review the presentations. For a wider audience, they also act as examples of the work that NITheCS does.
- Media releases.
- Annual reports.

Featured scientists

We draw attention on a monthly basis to one of our Associates as Scientist of the Month. The profile is featured on the website as well as in the newsletter, and showcases the wide-ranging scientific work of our Associates, while inspiring others to follow careers in science. During 2023 the following profiles were published (speakers featured below from top left):

Dr Sandra MacFadyen – January/February; Prof Roy Maartens – March; Prof Tommie Meyer – April; Dr Lungile Sitole – June; Dr Mesias Alfeus – July; Dr Ethel E. Phiri – August; Assoc Prof Freedom Gumedze – September; Assoc Prof Inger Fabris-Rotelli – October; Prof Loyiso Nongxa – November; Dr Liam Baker – December