NITheCS

National Institute for
Theoretical and Computational Sciences

ANNUAL REPORT

2022

Celebration of achievement

The hardest problems of pure and applied science can only be solved

by the open collaboration of the

worldwide scientific community

~ Kenneth G. Wilson, winner of the 1982 Nobel Prize for Physics

CONTENT

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
NMU	Nelson Mandela University
NRF	National Research Foundation
NWU	North-West University
RU	Rhodes University
SADiLAR	South African Centre for Digital Language Resources
SASA	South African Statistical Association
SU	Stellenbosch University
UCT	University of Cape Town
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

The year 2022 has been a period of great activity. We welcomed new initiatives and collaborations that support and enable us to fulfil the vision of NITheCS.

We also continued our journey to become a fully-fledged institution, embedded in the foundations of science and technology in the theoretical and computational sciences. We are indebted to the local and international experts who support our growth and progress. In particular, we thank the NITheCS Steering Committee under the leadership of Dr Happy Sithole for support and guidance. Under the committee's guidance, we remain focused on developing the eight identified thematic areas of NITheCS. We also look forward to finalising some legal structures and completing the transition process.

NITheCS is encouraged by the support from organisations and individuals who share a single vision of excellence and make their time and expertise available to us. These include the Department of Science and Innovation (DSI) and the National Research Foundation (NRF).

This report provides further details about our activities. We remain grateful to all participants and presenters for supporting these programmes. This support enables us to continue to present events that cover all our thematic areas of specialisation. Our thanks go to the organisations and individuals who make it possible for us to continue our work.

May 2023 be a good, healthy and productive year for all!

Interim Director: NITheCS

Our people

3.1 Staff profile

The staff profile of NITheCS at 31 December 2022 is shown below:

Directorate

Position / Hours expressed as a portion of an 8-hour workday	Institution	Number of staff members	Portion of workday expressed as the number of full-day / active staff
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	Institution	Number of staff members	Portion of workday expressed as the number of full-day / active staff
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 the number of full-day / active staff	Persons
Science Writer (Lia Labuschagne)	1	0.38	0.375
Fundraising Officer (Juby Govender)	1	0.5	0.5
Website and Content Manager / IT / Graphic Design (Belinda Virét)	1	0.63	0.625
TOTAL	**3**	**2.00**	

Internship / Capacity Development Staff

Position / Hours expressed as a portion of an 8-hour workday	Number of persons	Portion of workday expressed as the number of full-day / active staff
Aluwani Guga (PhD student) (2/8)	1	0.25
Thuthukile Khumalo (PhD student) (2/8)	1	0.25
TOTAL	**2**	**0.50**

3.2 Postdoctoral fellows

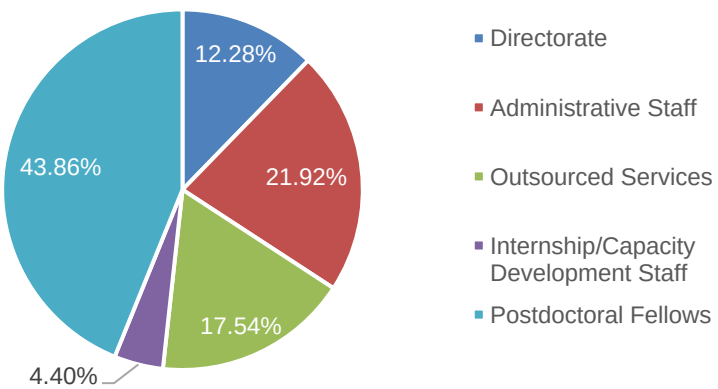
The postdoctoral fellows per node at 31 December 2022 are shown below. All positions are two-year contracts.

NITheCS node	Number of postdocs	Names of postdocs
Stellenbosch University	2	Dr Lehlonolo Mongalo (South African) Dr Danial Saadadatmand (Iranian)
University of KwaZulu-Natal	0	None at present
University of the Witwatersrand	3	Dr Atanu Bhatta (Indian) Dr Chandan Jana (Indian) Dr Teflon Rabambi (South African)
TOTAL	**5**	

3.3 Staff complement

Staff category	Number of staff per category (expressed in full-time hours)
Directorate	1.40
Administrative Staff	2.50
Outsourced Services	2.00
Internship/Capacity Development Staff	0.50
Postdoctoral Fellows	5.00
TOTAL OF NITheCS STAFF MEMBERS	**11.40**

Staff complement (categories expressed as a percentage of the total):



Associates

4.1 About our Associates

To achieve NITheCS' strategic goals, it is crucial to maintain a national network of Associates throughout South Africa. It is also important to grow our international links to ensure NITheCS can set itself on par with its counterparts across the world.

We are pleased that the number of Associates increased during the year. This was partly due to the results of the roadshows in the second half of 2021 at South African tertiary institutions. At these online events, led by Prof Francesco Petruccione, attendees were informed that the National Institute for Theoretical Physics (NITheP) was being transformed into NITheCS. Furthermore, the new institute embraced eight thematic fields of study.

Higher visibility and wider engagement within the tertiary institution community and other circles, as well as acknowledgement of the benefits of affiliation also grew the numbers of our Associates.

Associates are presented with numerous opportunities to enrich their knowledge in related fields through NITheCS colloquia, mini-schools, workshops and other events. Meeting with peers and students from other fields of study within the NITheCS themes also enables Associates to expand their network.

200 Associates milestone

In early July 2022, we achieved a milestone as we welcomed the 200th individual Associate into our community.

During the year, the number of NITheCS Associates increased by almost 22% overall. This was led by a 24% increase in the number of individual Associates.

NITheCS hosted the annual Associates Workshop in November and December.

At 31 December 2022, the Associates who had successfully applied for NITheCS affiliation were as follows:

4.1.1. Individual Associates (205 Associates)

Astronomy/Astrophysics (22)

- Prof Amare Abebe (North-West University)
- Dr Geoffrey Beck (University of the Witwatersrand)
- Prof Andrew Chen (University of the Witwatersrand)
- Prof Roger Deane (University of the Witwatersrand)
- Dr Marisa Geyer (South African Radio Astronomy Observatory)
- Prof Matt Hilton (University of KwaZulu-Natal)
- Prof Deepak Kar (University of the Witwatersrand)
- Dr Michael Kosch (SANSA)
- Prof Lerothodi Leeuw (University of the Western Cape)
- Dr Michelle Lochner (University of the Western Cape & SARAO)
- Dr Stefan Lotz (South African National Space Agency)
- Prof Ilani Loubser (North-West University)
- Dr Daniel Moeketsi (North-West University)
- Dr Jack Radcliffe (University of Pretoria)
- Prof Soebur Razzaque (University of Johannesburg)
- Prof Mattia Vaccari (University of Cape Town)
- Prof Sivakumar Venkataraman (University of KwaZulu-Natal)
- Prof Christo Venter (North-West University)
- Prof Bruce Watson (Stellenbosch University)
- Prof Patricia Whitelock (University of Cape Town)
- Prof Hartmut Winkler (University of Johannesburg)
- Prof Patrick Woudt (University of Cape Town)

Bioinformatics and Quantitative Biology (15)

- Prof Matthew Adeleke (University of KwaZulu-Natal)
- Prof Tulio de Oliveira (Stellenbosch University)
- Prof Morne du Plessis (National Institute For Communicable Diseases)
- Dr Uljana Hesse (University of the Western Cape)
- Prof Cang Hui (Stellenbosch University)
- Prof Tjaart Kruger (University of Pretoria)
- Dr Sandra MacFadyen (Stellenbosch University)
- Dr Monica Mwale (South African National Biodiversity Institute)
- Prof Olugbenga Oluwagbemi (Sol Plaatje University)
- Prof Hugh-George Patterton (Stellenbosch University)
- Dr Ché Sobashkar Pillay (University of KwaZulu-Natal)
- Dr Verena Ras (University of Cape Town)
- Prof Peter Scogings (University of KwaZulu-Natal)
- Prof Özlem Taştan Bishop (Rhodes University)
- Prof Vernon Visser (University of Cape Town)

Data Science (26)

- Dr Jean Bashingwa (University of Cape Town)
- Dr Stella Bvuma (University of Johannesburg)
- Prof Kelvin Bwalya (University of Johannesburg)
- Prof Marelie Davel (North-West University)
- Dr Emmanuel Dufourq (Stellenbosch University)
- Dr Marcel Dunaiski (Stellenbosch University)
- Dr Samuel Egieyeh (University of the Western Cape)
- Dr Sydney Kasongo (Stellenbosch University)
- Prof Langa Khumalo (North-West University)
- Prof Rodney Kroon (Stellenbosch University)
- Prof Alan Matthews (University of KwaZulu-Natal)
- Prof Thomas Meyer (University of Cape Town)
- Dr Thipe Modipa (University of Limpopo)
- Prof Deshen Moodley (University of Cape Town)
- Dr Alfred Mwanza (Sol Plaatje University)
- Dr Ibidun Obagbuwa (Sol Plaatje University)
- Prof Babu Paul (University of Johannesburg)
- Dr Mpho Raborife (University of Johannesburg)
- Prof Kanshukan Rajaratnam (Stellenbosch University)
- Prof Benjamin Rosman (University of the Witwatersrand)
- Dr Makhamisa Senekane (University of Johannesburg)
- Dr Fritz Solms (S-PLANE Automation / Stellenbosch University)
- Prof Hossana Twinomurinzi (University of Johannesburg)
- Prof Menno van Zaanen (North-West University)
- Prof Serestina Viriri (University of KwaZulu-Natal)
- Prof Sahal Yacoob (University of Cape Town)

Earth Systems Modelling & Climate Change Modelling (6)

- Dr Mary-Jane Bopape (NRF-SAEON)
- Prof Francois A. Engelbrecht (University of the Witwatersrand)
- Dr Mohau Mateyisi (Council for Scientific and Industrial Research)
- Dr Shingirai Nangombe (Council for Scientific and Industrial Research)
- Prof Abel Ramoelo (University of Pretoria)
- Prof Colleen Vogel (University of the Witwatersrand)

Mathematics (38)

- Prof Dharmanand Baboolal (University of KwaZulu-Natal)
- Prof Bubacarr Bah (African Institute for Mathematical Sciences)
- Prof Jacek Banasiak (University of Pretoria)
- Prof Mapundi Banda (University of Pretoria)
- Prof Aroon Beesham (Mangosuthu University of Technology)
- Dr Ronalda Benjamin (Stellenbosch University)

- Prof Gareth Boxall (Stellenbosch University)
- Prof Willem Conradie (University of the Witwatersrand)
- Dr Andrew Craig (University of Johannesburg)
- Prof Themba Dube (University of South Africa)
- Dr Partha Ghosh (University of South Africa)
- Dr Amartya Goswami (University of Johannesburg)
- Dr James Gray (Stellenbosch University)
- Dr Mandlenkosi Gwetu (University of KwaZulu-Natal)
- Prof Yorick Hardy (University of the Witwatersrand)
- Dr Rhameez Sheldon Herbst (University of Johannesburg)
- Dr Michael Hoefnagel (Stellenbosch University)
- Prof Karin-Therese Howel (Stellenbosch University)
- Prof Zurab Janelidze (Stellenbosch University)
- Dr Tamar Janelidze-Gray (University of Cape Town)
- Dr Luke Oluwaseye Joel (University of Johannesburg)
- Dr Eder Kikianty (University of Pretoria)
- Dr Sophie Marques (Stellenbosch University)
- Prof Fortuné Massamba (University of KwaZulu-Natal)
- Prof Dephney Mathebula (University of South Africa)
- Dr Hendrik Jacobus Michiel Messerschmidt (University of Pretoria)
- Dr Charles Msipha (Tshwane University of Technology)
- Prof Loyiso Nongxa (University of the Witwatersrand)
- Prof Paran Pillay (University of the Western Cape)
- Prof Helmut Prodinger (Stellenbosch University)
- Dr Cerene Rathilal (University of Johannesburg)
- Dr Riana Roux (Stellenbosch University)
- Dr Ridhwaan Suliman (Council for Scientific and Industrial Research)
- Prof Sanne ter Horst (North-West University)
- Prof Brink van der Merwe (Stellenbosch University)
- Dr Vivien Visaya (University of Johannesburg)
- Dr Dawit Worku (Cape Peninsula University of Technology)
- Dr Bertin Zinsou (University of the Witwatersrand)

Quantitative Finance (8)

- Prof Conrad Beyers (University of Pretoria)
- Prof Riaan de Jongh (North-West University)
- Dr Chioma Okoro (University of Johannesburg)
- Prof Helgard Raubenheimer (North-West University)
- Prof Ronald Richman (Old Mutual Insure)
- Prof Willem Schutte (North-West University)
- Prof David Taylor (University of Cape Town)
- Prof Tanja Verster (North-West University)

Statistics (4)

- Prof Andriette Bekker (University of Pretoria)
- Prof Renette Blignaut (University of the Western Cape)
- Prof Freedom Gumedze (University of Cape Town)
- Prof Delia North (University of KwaZulu-Natal)

Theoretical Physics (86)

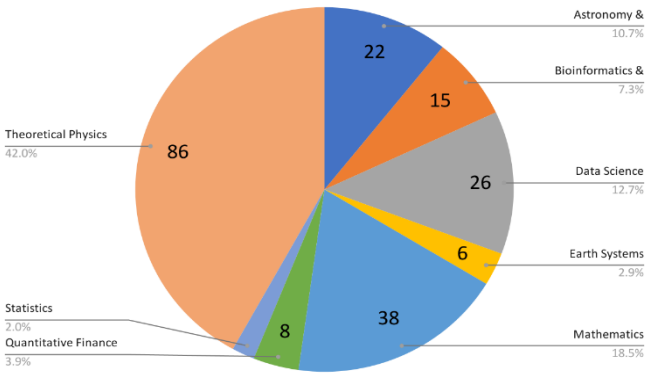
- Prof Igor Barashenkov (University of Cape Town)
- Dr Bruce Bartlett (Stellenbosch University)
- Prof Bruce A Bassett (AIMS) (South African Astronomical Observatory) (University of Cape Town)
- Prof Nigel Bishop (Rhodes University)
- Prof Moritz Braun (University of South Africa)
- Dr Jeandrew Brink (University of the Free State)
- Prof Erwin Bruning (University of KwaZulu-Natal)
- Prof Martin Bucher (University of KwaZulu-Natal)
- Dr Hsin Cynthia Chang (University of KwaZulu-Natal)
- Prof Nithaya Chetty (University of the Witwatersrand)

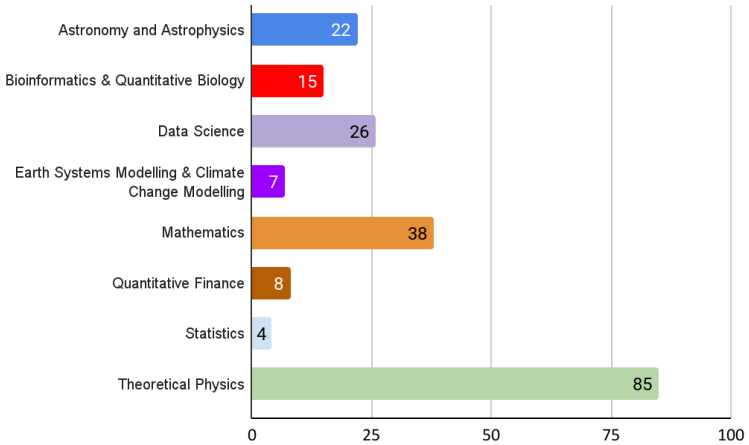
- Prof Fabio Cinti (Stellenbosch University)
- Dr Chris Clarkson (University of Cape Town)
- Prof Alan Cornell (University of Johannesburg)
- Dr Alvaro de la Cruz Dombriz (University of Cape Town)
- Prof Robert de Mello Koch (University of the Witwatersrand)
- Prof Cesareo A Dominguez (University of Cape Town)
- Prof Peter Dunsby (University of Cape Town)
- Prof Rocco Duvenhage (University of Pretoria)
- Prof Hans Eggers (Stellenbosch University)
- Prof George Ellis (University of Cape Town)
- Prof Stefan Ferreira (North-West University)
- Prof Aurona Gerber (University of South Africa)
- Prof Hendrik Geyer (Stellenbosch University)
- Prof Irvy (Igle) Gledhill (CSIR/University of the Witwatersrand)
- Dr Kevin Goldstein (University of the Witwatersrand)
- Dr Japie Greeff (North-West University)
- Prof Shajid Haque (University of Cape Town)
- Prof Dieter Heiss (Stellenbosch University)
- Prof Manfred Hellberg (University of KwaZulu-Natal)
- Dr Shinji Hirano (University of the Witwatersrand)
- Prof Will A. Horowitz (University of Cape Town)
- Prof Vishnu Jejjala (University of the Witwatersrand)
- Dr Anslyn John (Stellenbosch University)
- Prof Daniel Joubert (University of the Witwatersrand)
- Prof Steven Karataglidis (University of Johannesburg)
- Prof Alex Kies (University of KwaZulu-Natal)
- Dr Joseph Kirui (University of Venda)
- Prof Thomas Konrad (University of KwaZulu-Natal)
- Dr Hannes Kriel (Stellenbosch University)
- Prof Mantile Lekala (University of South Africa)
- Dr Mawande Lushozi (University of Cape Town)
- Prof Yin-Zhe Ma (University of KwaZulu-Natal)
- Prof Roy Maartens (University of the Western Cape)
- Prof Sunil Maharaj (University of KwaZulu-Natal)
- Prof Oluwole Daniel Makinde (Stellenbosch University)
- Dr Eric Maluta (University of Venda)
- Prof Rapela Regina Maphanga (Council for Scientific and Industrial Research)
- Dr Refilwe Edwin Maphasha (University of Pretoria)
- Prof Alan Joseph Michael Medved (Rhodes University)
- Dr Peace Prince Mkhonto (University of Limpopo)
- Dr Shazrene Mohamed (University of Cape Town/South African Astronomical Observatory)
- Dr Bishop Mongwane (University of Cape Town)
- Prof Kavilan Moodley (University of KwaZulu-Natal)
- Prof Thuto Mosuang (University of Limpopo)
- Prof Kristian Muller-Nedebock (Stellenbosch University)
- Prof Azwinndini Muronga (Nelson Mandela University)
- Prof Jeff Murugan (University of Cape Town)
- Dr Kingsley Obodo (North-West University)
- Prof Nico Orce (University of the Western Cape)
- Dr Giuseppe Pellicane (University of KwaZulu-Natal)
- Prof Andre Peshier (University of Cape Town)
- Prof Denis Pollney (Rhodes University)
- Prof Marius Potgieter (North-West University)
- Prof Alex Quandt (University of the Witwatersrand)
- Dr Abdulrafiu Raji (University of South Africa)
- Prof Sergei Rakitianski (University of Pretoria)
- Dr Stef Roux (Council for Scientific and Industrial Research)
- Prof Frederik Scholtz (Stellenbosch University)
- Prof Pavlo Selyshchev (University of Pretoria)
- Dr Alessandro Sergi (University of KwaZulu-Natal)

- Dr Jonathan Shock (University of Cape Town)
- Prof Jonathan Sievers (University of KwaZulu-Natal)
- Prof Ilya Sinayskiy (University of KwaZulu-Natal)
- Dr Izak Snyman (University of the Witwatersrand)
- Prof Du Toit Strauss (North-West University)
- Prof Mark Tame (Stellenbosch University)
- Dr Gary Tupper (University of Cape Town)
- Dr Aniekan Magnus Ukpong (University of KwaZulu-Natal)
- Dr Herman Uys (Stellenbosch University)
- Prof Judy van Biljon (University of South Africa)
- Prof Andre Weideman (Stellenbosch University)
- Prof Herbert Weigel (Stellenbosch University)
- Prof Heribert Weigert (University of Cape Town)
- Prof Amanda Weltman (University of Cape Town)
- Prof Konstantinos Zoubos (University of Pretoria)
- Prof Hasani Chauke (University of Limpopo)

Individual Associates per theme

Theme	Number of Associates per theme
Astronomy and Astrophysics	22
Bioinformatics & Quantitative Biology	15
Data Science	26
Earth Systems Modelling & Climate Change Modelling	6
Mathematics	38
Quantitative Finance	8
Statistics	4
Theoretical Physics	86
TOTAL	**205**





4.1.2 Junior Associates (14 Associates)

Astronomy and Astrophysics (1)
- Dr Teboho Moloi (University of Cape Town)

Bioinformatics & Quantitative Biology (1)
- Dr Kim Martin (Stellenbosch University)

Data Science (5)
- Dr Mathew Aibinu (Durban University of Technology)
- Dr Nikita Bernier (University of the Western Cape)
- Dr Shane Josias (University of Stellenbosch)
- Dr Thokozani Kunene (University of Johannesburg)
- Dr Mpho Mafata (University of Stellenbosch)

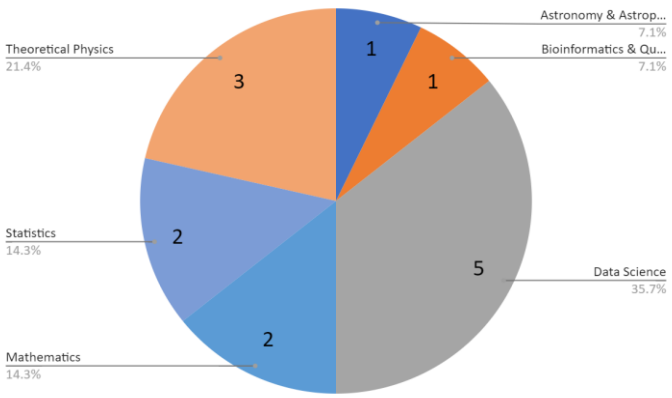
Mathematics (2)
- Dr Mathew Aibinu (Durban University of Technology)
- Mr Nathan Mulaja Tshakatumba (University of South Africa)

Statistics (2)
- Dr Christine Kraamwinkel (University of Pretoria)
- Dr Farai Mlambo (University of the Witwatersrand)

Theoretical Physics (3)
- Dr Masimba Paradza (Cape Peninsula University of Technology)
- Dr David Tshwane (CSIR)
- Mr Ayanda Zungu (North-West University)

Junior Associates per theme

Theme	Number of Associates per theme
Astronomy & Astrophysics	1
Bioinformatics & Quantitative Biology	1
Data Science	5
Earth Systems Modelling & Climate Change Modelling	0
Mathematics	2
Quantitative Finance	0
Statistics	2
Theoretical Physics	3
TOTAL	**14**



4.1.3 Institutional Associates (18)

- African Institute for Mathematical Sciences (AIMS)
- Cosmology Group (UCT)
- Centre for AI Research (CAIR)
- Centre for Space Research (NWU)
- Centre for Theoretical Physics (UCT)
- DSI/NRF CoE in Strong Materials at WITS
- Hartebeesthoek RAO, HartRAO
- Institute for Intelligent Systems (UJ)
- International Centre for Theoretical Physics (ICTP)
- iThemba LABS
- School for Data Science and Computational Thinking (SU)
- South African Astronomical Observatory (SAAO)
- South African Radio Astronomy Observatory (SARAO)
- South African Statistical Association (SASA)
- The Carpentries
- The National Graduate Academy of Mathematical and Statistical Sciences
- The South African Centre for Digital Language Resources (SADiLaR)
- UCT CERN Research Centre

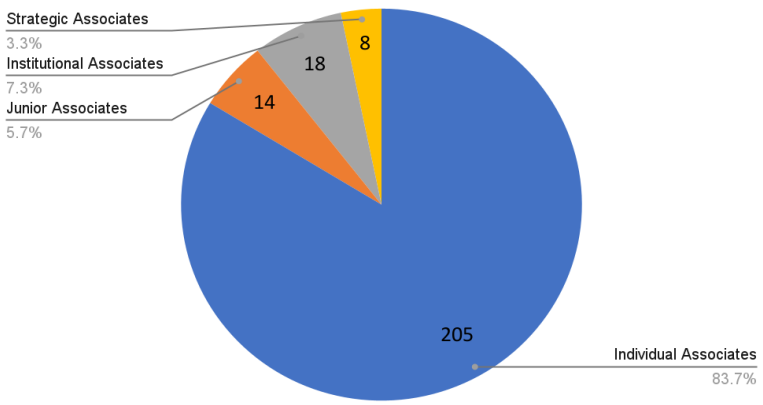
4.1.4 Strategic Associates (8)

- Dr Faïçal Azaiez (CEO of IThemba LABS)
- Prof Ludwig Combrinck (HartRAO)
- Prof Lesley Cornish (DSR/NRF CoE in Strong Materials)
- Dr Krishna Govender (CSIR)
- Prof Barry Green (AIMS)
- Dr Joseph Kirui (HoD Physics Department UNIVEN)
- Prof Kanshukan Rajaratnam (Director: School for Data Science and Computational Thinking at Stellenbosch University)
- Dr Sreekanth Rallapalli (Botho University)

4.2 Summary of Associates per category

Category	Number of Associates
Individual Associates	205
Junior Associates	14
Institutional Associates	18
Strategic Associates	8
TOTAL	**245**

Percentage of Associates per category



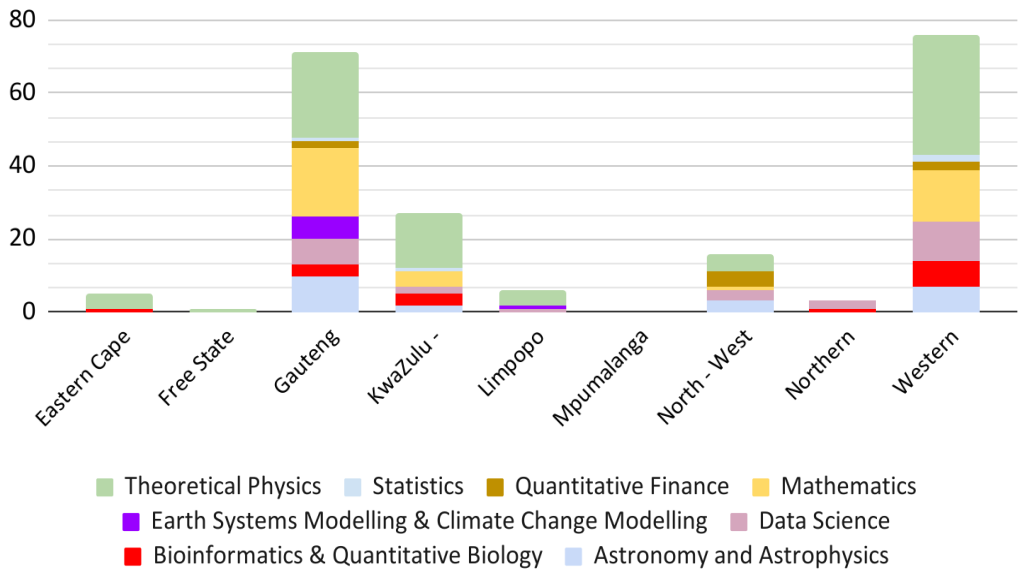
4.3 Associates per province and theme

Individual Associates are the biggest component of our Associates. Almost 72% of individual Associates are affiliated with tertiary institutions in the Western Cape (77 Associates) and Gauteng (71 Associates). The third biggest number of Individual Associates, 13%, is affiliated with universities in KwaZulu-Natal (27 Associates).

Almost 42% of individual Associates are in theoretical physics fields. Mathematics is the next biggest field for individual Associates (18%), while almost 13% are in the field of Data Science.

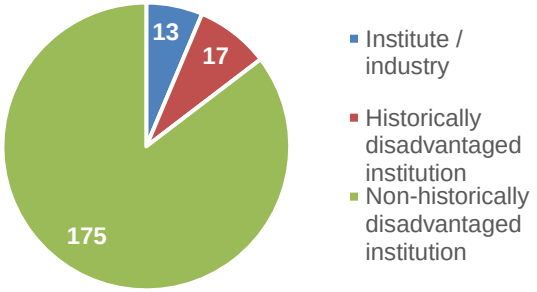
Individual Associates per province and theme as at 31 December 2022

Theme	Eastern Cape	Free State	Gauteng	KwaZulu-Natal	Limpopo	Mpuma-langa	North West	Northern Cape	Western Cape	TOTAL
Astronomy and Astrophysics			10	2			3		7	22
Bioinformatics & Quantitative Biology	1		3	3				1	7	15
Data Science			7	2	1		3	2	11	26
Earth Systems Modelling & Climate Change Modelling			6		1					7
Mathematics			19	4			1		14	38
Quantitative Finance			2				4		2	8
Statistics			1	1					2	4
Theoretical Physics	4	1	23	15	4		5		33	85
TOTAL	**5**	**1**	**71**	**27**	**6**	**0**	**16**	**3**	**76**	**205**



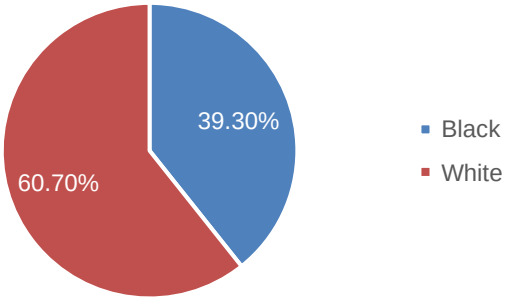
4.4 Associates' affiliation

Affiliation	Number of individual Associates
Institute / industry	13
Historically disadvantaged institution	17
Non-historically disadvantaged institution	175
TOTAL	**205**



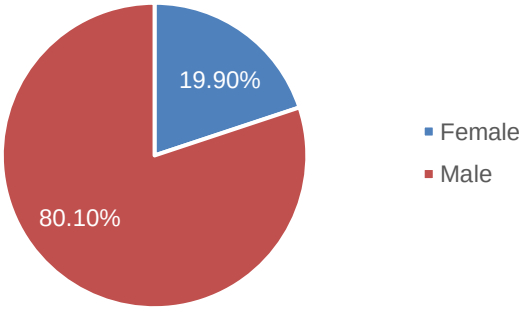
4.5 Associates per race

Individual Associates per race (%)	
Black (African, Coloured, Indian)	39.30%
White	60.70%
TOTAL	**100.00%**



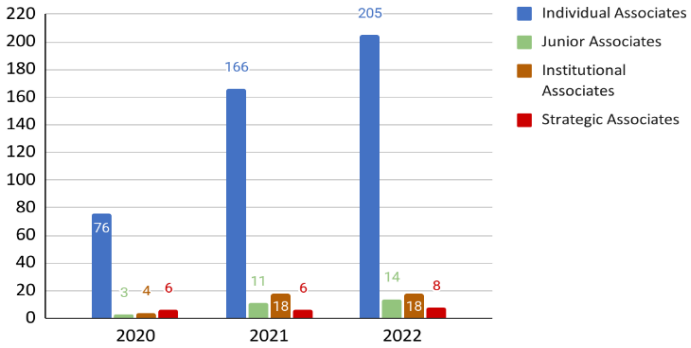
4.6 Associates per gender

Individual Associates per gender (%)	
Female	19.90%
Male	80.10%
TOTAL	**100.00%**



4.7 Annual growth in Associate numbers

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



Bursaries

5.1 Overview

Administration and procedure of application

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

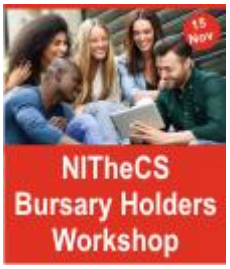
Bursary information session

In 2022, NITheCS held a bursary information session on 3 June 2022 to enhance stakeholders' understanding and implementation of the NRF-DSI Postgraduate Student Funding Policy and associated Call Implementation. A bursary application call was then issued and students had until 22 July to apply.

A total of 30 bursary holders were selected, of which 13 were completing their Masters degree and 17 were working towards their doctoral degree.

Bursary holders' workshop

The annual workshop for bursary holders, led by NITheCS Interim Director Prof Francesco Petruccione, was held online on 15 November 2022. This serves as a checkpoint to establish bursary holders' progress.



Bursary holders were asked to present briefly at the workshop to inform all participants of the direction of their research. The bursary holders' presentations were all on a very high standard.

Guest speakers were invited to give inspirational and motivational talks at the workshop:

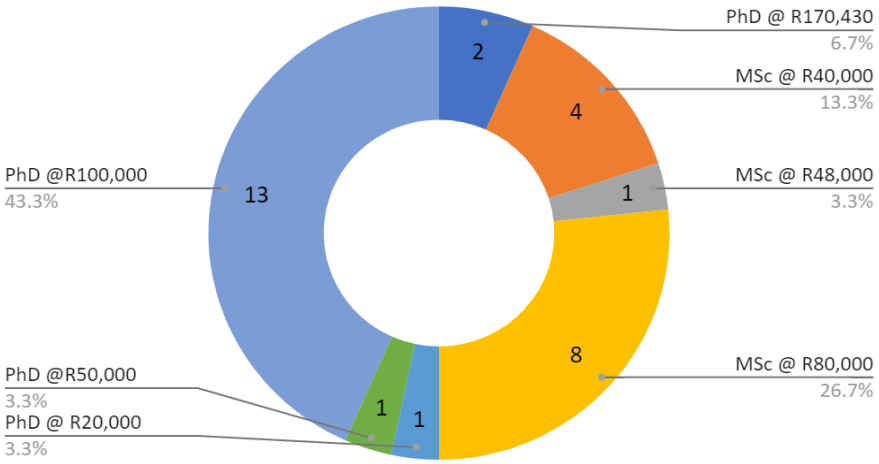
- The South African and international winner of FameLab 2022, Postdoctoral Research Fellow Dr Nehemiah Latolla (NMU)
- Winner of the NITheCS heat of FameLab 2022, Onesimo Mtintsilana (WITS and CERN)

5.2 Bursaries paid out

Summary of bursaries paid out in 2022:

Bursary level	Number of bursaries	Bursary value (Rand)	Bursaries paid (Rand)
PhD @ R170,430	2	170,430	340,860
MSc @ R40,000	4	40,000	160,000
MSc @ R48,000	1	48,000	48,000
MSc @ R80,000	8	80,000	640,000
PhD @ R20,000	1	20,000	20,000
PhD @ R50,000	1	50,000	50,000
PhD @ R100,000	13	100,000	1,300,000
TOTAL	**30**		**2,558,860**

Bursaries paid out in 2022:

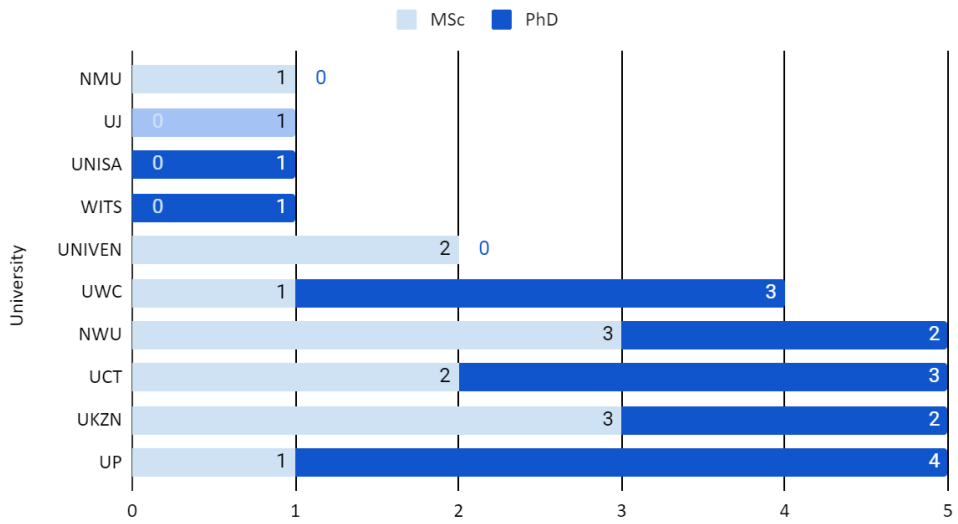


5.3 Distribution of bursary holders

MSc & PhD Bursaries per University

University	MSc	PhD	Total
NMU	1	0	1
UJ	0	1	1
UNISA	0	1	1
WITS	0	1	1
UNIVEN	2	0	2
UWC	1	3	4
NWU	3	2	5
UCT	2	3	5
UKZN	3	2	5
UP	1	4	5
TOTAL	**13**	**17**	**30**

Bursaries per university: MSc: 13 | PhD: 17 | Total: 30



5.4 Bursary holders' demographics

NITheCS aims to achieve the DSI-NRF Postgraduate Student Funding as follows:

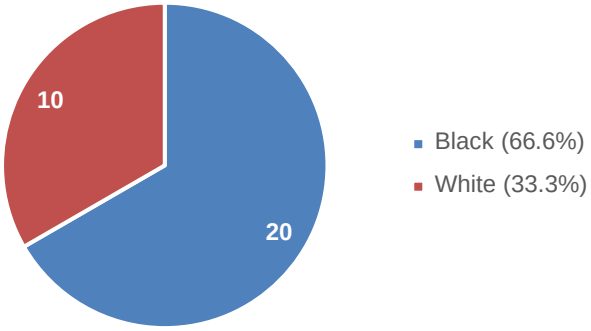
- 95% to South African citizens and permanent residents
- 5% to students from the SADC countries and the rest of the world
- 55% to women

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 living with a disability

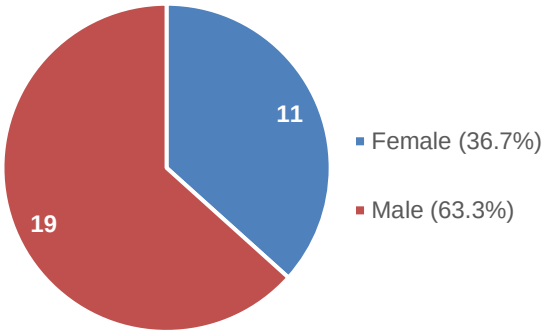
5.4.1 Bursary holders per race

Race	Bursary holders	
	Number	Percentage
Black (African, Coloured, Indian)	20	66.6%
White	10	33.3%
TOTAL	**30**	**100%**



5.4.2 Bursary holders per gender

Gender	Bursary holders	
	Number	Percentage
Female	11	36.7%
Male	19	63.3%
TOTAL	**30**	**100%**



Activities in 2022

6.1 Overview

As COVID-19 restrictions eased, many 'in person' / physical activities resumed in 2022. Many of our events now take place in both formats and allow for the attendance of people in many different locations.

Collaboration

To sustain our activities, the small NITheCS administrative staff depends on its collaborative and distributed structure that focuses among others on the critical importance of diversity and equity. In practice, we could not function efficiently without the support of relevant specialist bodies to further our goals of collaboration and support the basic and computational sciences.

Especially important for our daily work is the unstinting support of local universities. Without their support, we could not be successful in performing our duties and meeting our goal to support the local scientific community. In particular, we are grateful to the academics who have led our colloquia and workshops.

Many local universities are interested in becoming NITheCS nodes in future. This process is already underway and will increase our footprint.

We are particularly proud of our 249 Associates. With Associates holding at least a PhD in one of the eight relevant disciplines, their contributions are vital for the local scientific community. Our Associates also support and participate in training young scientists through colloquia, mini-schools, internships, courses, workshops and other NITheCS events. These events remain important in our efforts to reach out to the wider community of scientists and further multidisciplinary cooperation.

Special events and outreach

In addition to our regular events, we have hosted, co-hosted or participated in some important events together with other experts in the fields we support. Most notable in 2022 was the International Year of Basic Science for Sustainable Development (IYBSSD). Several NITheCS presentations during the year related to themes of the IYBSSD.

NITheCS was involved in organising one of the symposia that forms part of Nobel in Africa. This is a Stellenbosch Institute for Advanced Study (STIAS) initiative in partnership with Stellenbosch University, under the auspices of the Nobel Foundation and the Royal Swedish Academy of Sciences (KVA), with funding from the Knut & Alice Wallenberg Foundation.

NITheCS also organised and sponsored the outreach programme of public lectures that formed part of the Nobel in Africa initiative. More information about the public lectures is provided in this report, and we thank all the participants in this effort for their valued contributions.

Mandelab

Among the other events presented or actively supported was the commissioning of the Modern African Nuclear DEtector LAboratories (Mandelab) at the universities of the Western Cape (UWC) and Zululand (UniZulu). NITheCS Associate Prof Nico Orce was instrumental in acquiring the Mandelab facilities.

There was also the First International Congress on Advanced Computational Modelling of Materials (CAMOM), the 2022 Southern African Conference for Artificial Intelligence Research, the 7th Biennial African School of Fundamental Physics and Applications, the Symposium on Biodiversity Informatics in South Africa, and the Spring School on Theoretical and Computational Foundations of Quantum Technologies.

We have also continued to support among others the online training courses presented by The Carpentries. These online software workshops form part of our work to strengthen local data science and programming skills.

Programmes for school learners

The STEM MentHER programme was launched in 2022 to guide and streamline aspiring female Grade 12 learners in Gauteng into the STEM fields. Based on its success, there are plans to offer the programme in other regions in South Africa.

High school learners were made aware of mathematics in everyday life through an online celebration of the International Day of Mathematics and a photo challenge, while Grade 12 learners were offered online math revision at the end of the first, second and third terms.

Our Career Fest was open to high school learners and aimed to inform them of various career opportunities.

Further, NITheCS sponsored one of the local heats of 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. The winner of the NITheCS heat, Onesimo Mtintsilana (from WITS and CERN), progressed to the local finals. Communicating science is vital to advance scientific research and also for outreach activities. To promote this skill among young scientists, we plan to become involved again in future FameLab competitions.

In terms of outreach work, we continued to establish closer contact with schools and science centres. This included the sponsorship of prizes at the Eskom Expo for Young Scientists, which gives learners an opportunity to showcase their own science projects. We also co-sponsored a postgraduate outreach trip to the Eastern Cape, which sought to grow learners' awareness of careers in science.

Post COVID-19

With the COVID-19 epidemic relaxing its hold on society, it became easier to meet in person again. NITheCS participated in person at various events, including AI Expo Africa and the World Science Forum 2022 (WSF).

At the WSF, the Abdus Salam International Centre for Theoretical Physics (ICTP) in Trieste, Italy, and NITheCS signed a Memorandum of Understanding to strengthen collaboration and support of basic and computational science in South Africa. It was signed by ICTP Director Prof Atish Dabholkar and Interim Director of NITheCS Prof Francesco Petruccione in the presence of Dr Blade Nzimande, Minister of Higher Education, Science and Innovation. Please see our news release on this event on page 33.

6.2 Summary of activities

Type of activity	Number of activities / events	YouTube views to date
Colloquia	43	2 682
Nobel in Africa Symposia Series	10	2 721
Quantum Machine Learning Meetups	6	7060
CHPC NITheCS 2022 Summer School	1	819
Math School: revision lessons for grade 12s	13	1003
Mini-schools	8	2 641
Spring School	1	
Scientific Seminar Series	1	198
Webinars	6	655
Carpentry workshops	5	100

6.3 Event details

6.3.1 Colloquia

NITheCS hosted 41 colloquia in 2022, which took place in a regular Monday slot. The presenters were mostly academic lecturers and postdoctoral researchers, but people from the private sector and recommended doctoral students were also invited to share their insights and present their research.

Speakers with international affiliation were also invited to present to our community on relevant topics.

We also presented 15-minute social events after our colloquia and mini-schools. These virtual social gatherings, launched in 2021, were well attended again. They enable community members to get to know one another and establish new networks, while NITheCS staff also interact with participants.

International Year of Basic Sciences for Sustainable Development

As 2022 was declared the International Year of Basic Sciences for Sustainable Development (IYBSSD), NITheCS committed to hosting eight events by 30 June 2023 that highlight the importance of the basic sciences in local society.

By 31 December, we had hosted seven colloquia aligned to topics of the IYBSSD. Three of these were panel discussions. The aim was to inspire dialogue on key issues that lead to sustainable development.

The IYBSSD colloquia were:

4 Jul	*Panel discussion*: The importance and impact of the 'International Year of Basic Sciences for Sustainable Development' for South Africa	Panellists: ● Prof Zurab Janelidze (SU) ● Dr Mark Nasila (FNB) ● Prof Francesco Petruccione (NITheCS) ● Dr Happy Sithole (CHPC) ● Dr Anwar Vahed (NICIS/UWC)
25 Jul	The dawn of exascale computing in the climate sciences	Prof Francois Engelbrecht (WITS)
22 Aug	*Panel discussion*: Strengthening the presence and visibility of women	Panellists: ● Prof Sarah Blyth (UCT) ● Dr Mary-Jane Bopape (SAEON) ● Prof Himla Soodyall (ASSAf) ● Prof Özlem Tastan Bishop (RU)
12 Sep	*Panel discussion*: Strengthening Education and Scientific Training in the Basic Sciences	Panellists: ● Prof David Holgate (UWC) ● Prof Will Horowitz (UCT) ● Dr Miek Messerschmidt (UP) ● Prof Loyiso Nongxa (WITS) ● Prof Francesco Petruccione (SU)
24 Oct	Artificial Intelligence for sustainable development – A systems perspective	Prof Deshen Moodley (UCT)
7 Nov	Basic Sciences for Sustainable Development: A Global Perspective and a Year of Celebrations	Prof Sandro Scandolo (ICTP, Italy)
21 Nov	Goldilocks molecules in the Anthropocene	Prof Guy Midgley (SU)

The table below sets out all the colloquia hosted by NITheCS during 2022 (including the IYBSSD colloquia):

Date	Speaker	Affiliation	Title	YouTube views to date
24 Jan	Dr Samuel A. Egieyeh	UWC	Bioinformatic, Chemoinformatic and Data Analytic Strategies for Drug Discovery and Development	78
31 Jan	Prof Özlem Taştan Bishop	RU	Two intermittently linked aspects of modern computational drug discovery: allostery and missense mutations	84
7 Feb	Prof Zurab Janelidze	SU	Noetherian information systems	66
14 Feb	Prof Frans Pretorius	Princeton University, USA	Gravitational wave astrophysics: a status report	186
21 Feb	Prof Anna Scaife	University of Manchester, UK	AI in the SKA Era: Challenges for recovering well-calibrated uncertainties from Bayesian Deep-learning	137
28 Feb	Dr Eder Kikianty	UP	Mathematics of South Africa	142
7 Mar	Dr Cerene Rathilal	UJ	Pointfree Topology: some results on the Wallman compactification in frames	145
14 Mar	Prof Jonathan Shock	UCT	A guided tour through the landscape of reinforcement learning	144
28 Mar	Prof Jacek Banasiak	UP	Fads and fallacies of mathematical modelling and applications of mathematics	102

4 Apr	Emeritus Prof Hans Roosenschoon	SU	The man who (unknowingly) mistook his music for mathematics	127
11 Apr	Dr R. Srikanth	Poornaprajna Institute of Scientific Research, India	Counterfactual security of quantum key distribution	79
14 Apr	• Prof Sir Peter Knight (Imperial College, UK) • Prof Francesco Petruccione (SU) • Wenmiao Yu (Cofounder of Quantum Dice, UK)		Fulfilling our quantum ambitions: Research and technology efforts in quantum in SA and the UK	191
25 Apr	Prof Devis Tuia	Swiss Federal Institute of Technology Lausanne (EPFL), Switzerland	Machine learning supporting ecology, supporting machine learning	35
9 May	Dr Bruce Bartlett	SU	The geometry of the classical and quantum 6j symbols	101
16 May	Prof Andrew Forbes	WITS	Quantum-like classical light	79
23 May	Prof Mark Solms	UCT	A new approach to the hard problem of consciousness	438
30 May	Isabella Rammala	RU	Compact Radio Sources in the 1.28 GHz MeerKAT Galactic Center Mosaic	45
6 Jun	Dr Kim Martin	SU	Research Software Engineering (RSE) as a component of a healthy academic ecosystem	136
13 Jun	Dr Lorène Jeantet	AIMS	Deep learning: computer science for wildlife monitoring	99
20 Jun	Prof Sahal Yacoob	UCT	A W-Boson by Any Other Mass	39
27 Jun	Dr Mawande Lushozi	UCT	Physics of the Fragmentation Region: Nuclear Compression, Baryon Stopping, and Coloured Glass	68
4 Jul	• Prof Zurab Janelidze (SU) • Dr Mark Nasila (FNB) • Prof Francesco Petruccione (NITheCS) • Dr Happy Sithole (CHPC) • Dr Anwar Vahed (NICIS/UWC)		*Panel discussion*: The importance and impact of the 'International Year of Basic Sciences for Sustainable Development' for South Africa	45
11 Jul	Dr Carsten Blank	data cybernetics ssc GmbH	A compact quantum distance-based binary classifier – how entanglement is a resource	65
18 Jul	Prof Roger Deane	WITS	The shadow of the supermassive black hole in the centre of our Milky Way	33
25 Jul	Prof Francois Engelbrecht	WITS	The dawn of exascale computing in the climate sciences	47
1 Aug	Dr Martin Weigt	NMU	Generalised B-algebras with applications to quantum mechanics	43
12 Aug	Prof Martin Bucher	Université Paris Cité/CNRS, France	Mapping the Initial Conditions of the Universe using the Cosmic Microwave Background	64
15 Aug	Prof Julian D. May	UWC	Big data, blockchain and biltong: opportunities for data science in food system analysis	45
22 Aug	• Prof Sarah Blyth (UCT) • Dr Mary-Jane Bopape (SAEON) • Prof Himla Soodyall (ASSAf) • Prof Özlem Tastan Bishop (RU)		*Panel discussion*: 'Strengthening the presence and visibility of women'	27
29 Aug	Prof Jeff Murugan	UCT	The Mathematical Physics of Quantum Batteries	121

5 Sep	Prof Yin-Zhe Ma	UKZN	Using South Africa's MeerKAT to constrain Axion dark matter	Video not available online
12 Sep	• Prof David Holgate (UWC) • Prof Will Horowitz (UCT) • Dr Eder Kikianty (UP) • Dr Miek Messerschmidt (UP) • Prof Loyiso Nongxa (WITS) • Prof Francesco Petruccione (SU)		*Panel discussion*: 'Strengthening Education and Scientific Training in the Basic Sciences'	42
19 Sep	Prof Stefan Lotz	NWU and SANSA	Knowledge Discovery in Time Series Data	42
26 Sep	Dr Adriana Marais	Foundation for Space Development Africa	Extreme environment economics	29
3 Oct	Prof Hugh Patterton	SU	Bioinformatics – a personal journey	28
10 Oct	Dr Marco Mariola	UKZN	Africhino: Open-hardware for Teaching and Learning	20
17 Oct	Dr Uljana Hesse	UWC	The Rooibos Genomics Program	30
24 Oct	Prof Deshen Moodley	UCT	Artificial Intelligence for sustainable development – A systems perspective	23
7 Nov	Prof Sandro Scandolo	Abdus Salam ICTP, Italy	Basic Sciences for Sustainable Development: A Global Perspective and a Year of Celebrations	72
14 Nov	Prof Emil Roduner	University of Stuttgart and UP	The origin of irreversibility in thermodynamic processes – or is 'memory' a new parameter for the physical state of matter?	30
21 Nov	Prof Guy Midgley	SU	Goldilocks molecules in the Anthropocene	29
28 Nov	• Dr Liam Baker (SU) • Phil Labuschagne (JIMCOBSA)		Mathematical Contests in South Africa, Africa and the World	85
TOTAL				**2 682**

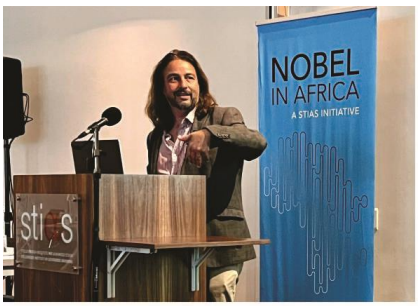
6.3.2 Conferences

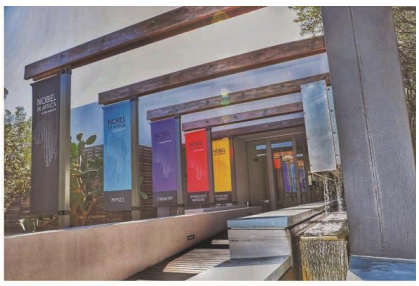
The 1st International Congress on Advanced Computational Modelling of Materials (CAMOM) was held in September. Local and international speakers addressed attendees at this hybrid event, which ran over five days. It was organised by NITheCS Associates Dr Kingsley Obodo, Dr Aniekan Ukpong and Dr Tjaart Kruger.

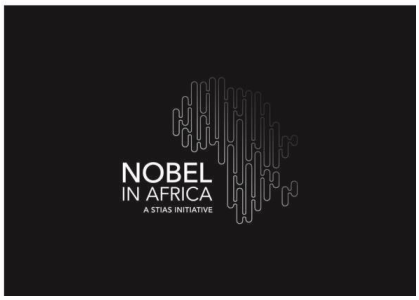
6.3.3 Nobel in Africa Symposia Series

In October and November NITheCS participated in Nobel in Africa – a Stellenbosch Institute for Advanced Study (STIAS) initiative in partnership with Stellenbosch University under the auspices of the Nobel Foundation and the Royal Swedish Academy of Sciences (KVA)with funding from the Knut & Alice Wallenberg Foundation

NITheCS was involved in organising one of the symposia that formed part of Nobel in Africa, while we also organised and sponsored a series of public lectures at several campuses across South Africa.







The full set of lectures in the outreach programme are listed below:

Date	Speaker	Affiliation	Venue	Title	YouTube views to date
18 Oct	Prof Yin-Zhe Ma	UKZN	UWC	Cosmology: A Golden Era	*
20 Oct	Prof Viatcheslav Mukhanov	Ludwig-Maximilians-Universität, Germany	UCT	The Quantum Universe	*
20 Oct	Prof Erik Aurell	Royal Institute of Technology (KTH), Sweden	SU	The Mystery of Black Hole Entropy	*
21 Oct	Prof Francesco Petruccione	SU	AIMS	Entanglement: From Theory to Quantum Computers	*
21 Oct	Dr Thifhelimbilu Daphney Bucher	CPUT	NMU	Rise and Take Your Position	*
	Prof Neil Turok	University of Edinburgh	AIMS	Universe	356
24 Oct	Prof Sir Michael Berry	Bristol University	SU	How Quantum Physics Democratised Music: A Meditation on Physics and Technology	256
31 Oct	Prof Neil Turok	University of Edinburgh	UKZN	Universe	1 800
	Prof Armita Nourmohammad	University of Washington	WITS	Learning the shape of the protein universe	65
31 Oct	Prof Mogens Hogh Jensen	University of Copenhagen	UKZN	Complexity in science	97
	Prof Angelo Vulpiani	University of Rome	UKZN	Predicting the future: An old problem from a modern perspective	
1 Nov	Prof Erik Aurell	Royal Institute of Technology (KTH)	UKZN	Fluctuation Relations	91
	Prof Luca Gammaitoni	Università di Perugia	UKZN	Why it is difficult to find something if you do not know what you are looking for	
2 Nov	Prof Armita Nourmohammad	University of Washington	WITS	Learning the shape of the immune and protein universe	56
TOTAL					**2 721**

** The event was either not recorded or the video clip was not published on YouTube at the speaker's request.*

6.3.4 Quantum Machine Learning Meetups

Quantum Machine Learning Meetup (QML Meetup) is a series of talks by QML researchers to discuss their work, with time for a Q&A session afterwards.

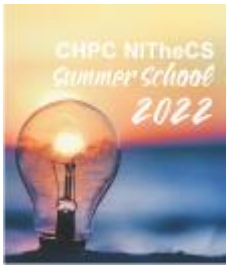
Date	Speaker	Affiliation	Title	YouTube views to date
4 Feb	Antal Száva	Quantum software developer at Xanadu	Using PennyLane for Quantum Differentiable Programming	**340**
31 Mar	Matthias Caro	Technical University of Munich	Generalization guarantees for variational quantum machine learning	568
TOTAL				**908**

6.3.5 Schools

NITheCS hosted and participated in several schools in 2022:

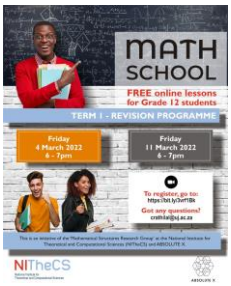
7th Biennial African School of Fundamental Physics and Applications
This was held as a hybrid event with in-person attendance at Nelson Mandela University from 28 November to 9 December. The overall theme was '100 Years of Physics in Africa – Past, Present and Future'. In addition to the scientific programme, attendees could participate in workshops, outreach programmes, tutorials and forums.

CHPC NITheCS 2022 Summer School: *'The 12th CHPC Introductory Programming School and The 4th NITheCS Summer School on the Foundations of Theoretical and Computational Science'*
This school introduces postgraduate students to programming, as well as the theoretical and computational sciences. Due to the COVID-19 lockdown, it took place online from 31 January to 25 February.



Math School: revision lessons for grade 12s
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'.

This new initiative, driven by Dr Cerene Rathilal (UJ), provided online mathematics revision lessons to grade 12 students, covering term 1, 2 and 3. Lessons were held online and recordings are accessible via the NITheCS YouTube channel. The NITheCS community was informed of the revision and encouraged to share the information.



Summary of the math revision lessons in 2022:

Date	Topic	Title	YouTube views to date
4 Mar	Term 1 revision	Basic Arithmetic; Number Patterns and Series	197
11 Mar		Euclidean Geometry (Part 1) and Proportionality	143
21 Apr	Term 2 revision	Euclidean Geometry	128
5 May		Analytic Geometry	93
19 May		Calculus (Part 1)	94
2 Jun		Calculus (Part 2)	73
5 Aug	Term 3 revision	General revision	150
19 Aug			90
2 Sep			80
12 Sep			91
TOTAL			**1 139**

Mini-schools
NITheCS hosted eight mini-schools during 2022. Each mini-school comprises a series of lectures that extend over three to four weeks and the topics change monthly. Our community is invited to attend these lectures to expand their knowledge.

Date	Speaker and affiliation	Topic	No. Of attendees	YouTube views to date
March	Dr Fabio Anzà (University of Washington & Templeton Research Fellow, University of California, Davis, US)	Geometric Quantum Mechanics of finite-dimensional systems	55	L1: 184 L2: 125 L3: 48 L4: 47
April	Dr Krishna Govender (CHPC)	An introduction to computer aided drug design	175	L1: 217 L2: 279 L3: 263
May	• Dr Kingsley Obodo (NWU) • Dr Cecil Ouma (Next-Einstein Forum Fellow)	Quantum ESPRESSO	79	L1: 186 L2: 102 L3: 78
July	Ian Joel David (UKZN)	A Practical Introduction to Quantum Computing with Qiskit	48	L1: 167 L2: 95 L3: 77 L4: 65
Aug	• Dr Amartya Goswami (UJ) • Prof Zurab Janelidze (SU)	Elementary Introduction to Set Theory	85	L1: 128 L2: 46 L3: 61 L4: 50
Sept	Dr Henri Laurie (UCT)	The Julia language: easy, generic, fast (but no free lunch)	76	L1: 91 L2: 46 L3: 36 L4: 49
Oct	Dr Laure Gouba (ICTP, Italy)	Green's Functions for Ordinary Differential Equations	35	L1: 50 L2: 32 L3: 20 L4: 24
Nov	• Prof Martin Bucher (CNRS, France) • Dr Japie Greeff (NWU)	Phylogenetic Inference and Machine Learning	78	L1: 21 L2: 10 L3: 22 L4: 22
TOTAL			**631**	**2 641**

Spring School on Theoretical and Computational Foundations of Quantum Technologies
The School aimed to provide an introduction to Quantum Computing, Machine Learning for Quantum Physics, Quantum Communication and Quantum Machine Learning It was attended by postgraduate students in physics, mathematics, applied mathematics and computer science who are interested in both theoretical and computational aspects of quantum technologies. Scholarships were available to cover successful applicants' local travel, accommodation and meals.

The 4-day school was held at Alpine Heath Resort, Northern Drakensberg, in November.

6.3.6 Scientific Seminar Series

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

Date	Speaker	Affiliation	Title	YouTube views to date
24 Aug	Prof Francesco Petruccione	SU	Bad vibrations: Quantum tunnelling and SARS-CoV-2 infections	131
23 Sep	Prof Ilya Sinayskiy	UKZN	Quantum Simulation of Open Quantum Systems	67
TOTAL				198

6.3.7 Symposia

Biodiversity Informatics – 'Drowning in Data, Thirsty for Information and Starved for Understanding'
NITheCS sponsored this symposium, which took place at Stellenbosch University from 28-30 November. The event sought to bring together key biodiversity stakeholders with distinctive expertise to encourage the establishment of transdisciplinary, collaborative networks. The event organisers hoped to demonstrate the importance of building partnerships and developing a culture of cooperation and interoperability to establish operational workflows for biodiversity data synthesis. Challenges were discussed, opportunities were highlighted and innovative solutions for biodiversity informatics in South Africa were encouraged.

6.3.8 Webinars

We held six webinars during 2022, focused on topics relating to theoretical physics. Here are the details:

Date	Speaker	Affiliation	Title	YouTube views to date
21 Jan	Mo Kordzanganeh	University of Manchester	Quantum Machine Learning for Radio Astronomy	139
25 Mar	Lea Lautenbacher	Federal University of Pernambuco, Brazil, and University of Ulm, Germany	Approximating Invertible Maps by Recovery Channels: Optimality and an Application to Non-Markovian Dynamics	74
9 Apr	Prof Francesco Petruccione (SU) Dr Garry Kemp (UJ) Dr Yaseera Ismail (UKZN) Ms Betony Adams (UKZN)		What is Quantum?	155
14 Apr	Prof Barry Sanders	University of Calgary, Canada	Observing a changing Hilbert-space inner product	92
27 May	Mark Fingerhuth	Co-founder and Head of R&D ProteinQure Inc	Learning Curves of Quantum Kernel Machines	58
24 Jun & 1 Jul	Pratik Nandy	Centre for High Energy Physics, Indian Institute of Science, India	Recent progress on Krylov complexity	Part 1: 102 Part 2: 35
TOTAL				**655**

6.3.9 Workshops

Several workshops were held in 2022, some of which we hosted while others were sponsored.

Carpentry workshops

NITheCS hosted five Carpentry workshops in 2022. The aim was to provide graduate students and other researchers in our community with opportunities to learn valuable computing skills that would 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	Description	Number of attendees
4-8 Apr	Software Carpentry	Basic research computing skills	33
3-6 May	Software Carpentry	Basic research computing skills	31
1-3 Jun	Carpentries Instructor Training	The first step towards certifying and participating as a Carpentries Instructor	29
1-5 Aug	Data Carpentry	(Genomics) Workshop	34
14-18 Nov	Software Carpentry	Shell, Git, Plotting and Programming in Python	39
TOTAL			166

South African Conference for Artificial Intelligence Research (SACAIR2022)

NITheCS hosted a day-long workshop at SACAIR2022, 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 in December.

RSE@SUN Workshop

This event was presented in person by Dr Jannetta Steyn (Newcastle University, UK) on The Internet of Things (the 'five senses of the Internet') at Stellenbosch University in September.

Associates' Workshop

The annual workshop for NITheCS Associates was held in person in November at the three NITheCS nodes, namely Stellenbosch University, the University of KwaZulu-Natal and the University of the Witwatersrand, in November. To connect with Associates who were unable to attend in person, the workshop was also held virtually in December.

Bursary Information Session Workshop

NITheCS hosted a workshop at a National Research Foundation event in June 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 and its associated call.

Bursary holders' Workshop

The annual workshop for NITheCS bursary holders was held in November. The 30 bursary holders were invited to attend and given an opportunity to provide insight into their research. Three guest speakers recounted their achievements and thereby motivated the bursary holders.

Engagement

NITheCS sponsored and co-sponsored several initiatives during 2022 that focused on skills and knowledge development. We also engaged through events that encouraged learners to consider careers in the fields of science covered by NITheCS.

Here are the initiatives in which we were engaged in 2022:

International Year of Basic Sciences for Sustainable Development
As 2022 was declared the International Year of Basic Sciences for Sustainable Development (IYBSSD), NITheCS committed to hosting eight events by 30 June 2023 that highlight the importance of the basic sciences in local society. By 31 December, we had hosted seven colloquia aligned to topics of the IYBSSD. Three of these were panel discussions. The aim was to inspire dialogue on key issues that ultimately lead to sustainable development. For more information please view section 6.3.1.

International Day of Mathematics

High school learners were made more aware of mathematics through an online celebration of the International Day of Mathematics in March. A photo challenge also sought to grow awareness of Mathematics in everyday life.

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 winner of the heat, Onesimo Mtintsilana (WITS/CERN), progressed to the national finals in October.

STEM MentHER

The STEM MentHER programme was launched in 2022 to guide and streamline aspiring female Grade 12 students into the STEM fields. The intention is among others for successful candidates to become role models for other girls. A total of 16 girls in Gauteng were selected in June to participate in the programme, led by Dr Cerene Rathilal (UJ). NITheCS provided branded materials for the programme, including badges, certificates and T-shirts, as well as marketing materials to advertise the programme.

SAIP Conference

The Department of Physics at Nelson Mandela University hosted the SAIP2022 Conference as an online event from 1 to 8 July. NITheCS sponsored one of the tracks at the conference and provided funding to students to attend the conference.

We also donated 10 prizes of R3 000 sponsorships, which were awarded to learners in various categories**:**

Chemistry and Biochemistry

- Mpho Bongwe (Soshanguve Technical School)
- Xolane Kunene (Sir Pierre Van Ryneveld High)

Computer Science and Software Development

- Yash Ghela (Star College Pretoria)
- Lulama Majoko (Star College Pretoria)
- Yu Tan Shan (St Johns College)

Earth Science

- Jade Fajana (Hoerskool Langenhoven)

Engineering

- Adam von Wielligh (Hoerskool Centurion)

Mathematics

- Refilwe Nchabeleng (Bona Lesedi Secondary School)

Renewable Energy

- Tsholo Mokebe (H.B Nyathi Secondary School)
- Siphiwe Sithomo (H.B Nyathi Secondary School)

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. We attended the exhibition in person and welcomed visitors to the NITheCS stand. We also sponsored some of the prizes, which were awarded to Jade Fajana, Xolane Kunene and Yu Tan Shan.

Teacher Development Programme

Also in July, an online teacher training event focused on the topic '*Assessing student learning by applying or incorporating different classroom techniques*.' Hosted by Dr Cerene Rathilal (UJ), it reached some 500 teacher attendees. The programme sought to promote the professional development of teachers on a broad scale.

Career Fest 2022

In August, this online event was hosted to inform high school students about various careers and vocations, including those in the fields of science.

Outreach trip to the Eastern Cape

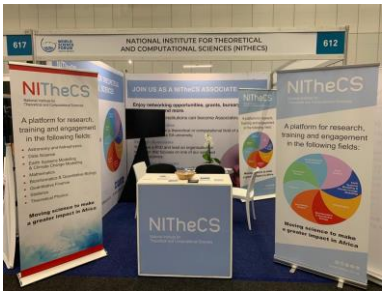
Seven postgraduate students from the Department of Physics at Stellenbosch University undertook an outreach road trip to the Eastern Cape in early September. The aim of the trip, supported by NITheCS and Optica, was to grow high school learners' awareness of careers in science. Over 280 students from five high schools in the Eastern and Western Cape attended demonstrations of a range of physics experiments this year. These interactive sessions also provided the opportunity for students to ask questions.

Fundamano

A first-of-its-kind theatrical production, *Fundamano*, was produced by students at Stellenbosch University. Its theme was 'Explore the secrets of understanding mathematics'. The project 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, which gained much positive feedback, took place at the Drostdy Theatre in Stellenbosch on 4 November.

World Science Forum (WSF2022)

In December, the WSF2022 took place for the first time in Africa, attracting many prominent local and international scientists, as well as decision makers, representatives of civil society and the media. Prof Francesco Petruccione (SU), our interim Director, was among the speakers at the event. NITheCS also participated in the exhibition.



The WSF2022 was also the venue for NITheCS and the Abdus Salam International Centre for Theoretical Physics (ICTP), Trieste, Italy, to sign a Memorandum of Understanding (MoU) to strengthen their collaboration and support of basic and computational science in South Africa.

Programmes

8.1 NITheCS Internship Programme

This flagship NITheCS programme offers students an outstanding 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 to December
- *Second phase*: mid-January to mid-April

The 2021/2022 internships, which were attended virtually, ended in April 2022 and the interns submitted their reports for the 2022 SAIP conference. Three of the papers were selected to be published in the conference proceedings.

2022/2023 programme
In July a call was issued to NITheCS Associates to suggest topics for the 2022/2023 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.

Thereafter, 26 topics were submitted across six of the eight themes. From the proposals, the following topics were selected:

1. Compact Stars as Laboratories for Matter at Extremes and Fundamental Physics
2. Physics and Evolution of the Early Universe
3. Physics of Core-collapse Supernovae
4. Relativistic Fluid Dynamics in Heavy-Ion Collisions and Particle & Nuclear Astrophysics
5. Relativistic Kinetic Theory in Heavy-Ion Collisions and Particle & Nuclear Astrophysics
6. Statistical and Thermal Physics in Heavy-Ion Collision and Particle & Nuclear Astrophysics
7. The IYBSSD and the IUPAP centenary-100 years of physics in Africa (the past, present and future)
8. Theoretical & Computational Biophysics
9. Theory and Phenomenology of Relativistic Heavy-Ion Collisions

As COVID-19 restrictions had been relaxed, the 2022/2023 NITheCS Internship Programme could resume in person. A call was issued for students to register for an internship in July. A record number of 36 students were selected to participate as interns in the current cohort. Some of the interns had participated in our 2021/2022 internship programme, but they re-applied to experience the internship in person.

Based on their strengths, knowledge and fields of study, the interns were grouped into the various topics, which are being supervised by five NITheCS Associates. In total, 12 tutors also work collaboratively with the groups.

Student affiliation	Gender		Total
	Female	Male	
Nelson Mandela University	1	1	2
North-West University	2	-	2
Stellenbosch University	2	1	3
University of Cape Town	-	2	2
University of Johannesburg	3	2	5
University of KwaZulu-Natal	1	-	1
University of the Western Cape	1	3	4
University of Venda	4	3	7
University of Zululand	2	6	8
Walter Sisulu University	2	-	2
TOTAL	**18**	**18**	**36**

8.2 Research programmes

NITheCS initially launched research programmes in 2020/2021. They seek to involve the entire network of Associates attached to South African universities, as well as several international collaboration partners. Their duration is at least 12 months.

The 2022 research programmes are listed below.

Research programmes and principal investigators (PIs)

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	• 38 Papers published • Funds leveraged: R2 million • 22 Students supervised
• Prof Marelie Davel (NWU) • Dr Stefan Lotz (SANSA)	Machine learning in support of theoretical and computational science	• 7 Researchers • 2 Research workshops • 11 Papers published
• Prof Martin Bucher (UKZN) • Dr Japie Greeff (NWU)	Genomics, bioinformatics, and advanced medicine	• 1 Research Workshop • 4 Collaborators • 2 Papers published
• Dr Shajid Haque (UCT) • Prof Thomas Konrad (UKZN) • Prof Jeff Murugan (UCT) • Prof Ilya Sinayskiy (UKZN)	Quantum technologies for sustainable development	• 5 Researchers • 10 Students supervised
• Prof Tjaart Kruger (UP) • Dr Aniekan Ukpong (UKZN) • Dr Kingsley Obodo (NWU)	Advanced computational modelling of materials	• 7 Researchers • 1 Research workshop
• Dr Vernon Visser (SANBI) • Prof Cang Hui (SU) • Dr Sandra MacFadyen (SU) • Dr Emmanuel Dufourq (SU)	Advancing biodiversity informatics and ecological modelling	
• Prof Zurab Janelidze (SU) • Dr Yorick Hardy (WITS) • Dr Partha Ghosh (UNISA)	Space-like mathematical structures and related topics in algebra, logic and computation	• 20 Researchers • 8 Research workshops • 24 Collaborators • 14 Papers published or in process of going to press • 17 Papers submitted for publication • 32 Papers in progress

8.3 South African Theory and Computational School (SATACS)

The NITheCS South African Theory and Computational School (SATACS) is a decentralised, semi-virtual, national teaching programme in theoretical physics and computational sciences. Launched as the South African Theory School in 2021, the programme was renamed 'SATACS' in 2022 to reflect the wider range of courses.

Under the directorship of Prof Will Horowitz, SATACS' goal is to provide teaching of the highest quality, pitched at Honours / Masters level. This is at a level similar to that found in elite postgraduate programmes around the world.

In 2022 SATACS expanded its range with three additional courses. A total of 51 students, representing 12 universities, participated in these courses.

Presenter(s)	Topic	Duration
Prof Jonathan Shock	Machine Learning for Theoretical Physicists	2 semesters
Dr Shajid Haque (UCT)	Differential Geometry	1 semester
Prof Konstantinos Zoubos (UP)	Introduction to General Relativity	1 semester
Prof Amare Abebe (UCT)	Introduction to Cosmology	1 semester
Prof Amanda Weltman (UCT)	Extreme Gravity or An Introduction to Black Holes and Gravitational Waves	1 semester
Dr Makhamisa Senekane	Introduction to Privacy-Preserving Schemes for Applications in Artificial Intelligence	1 semester
• Dr Partha Pratim Ghosh (UNISA) • Prof Yorick Hardy (WITS) • Prof Zurab Janelidze (SU) • Dr Cerene Rathilal (UJ)	Mathematical Structures	1 semester
Prof Jeff Murugan (UCT)	Advanced Methods for Mathematical Physics	1 semester
Prof Charalampos (Haris) Skokos (UCT)	Non-linear Hamiltonian Dynamics and Chaos	1 semester
Prof Will Horowitz (UCT)	Quantum Field Theory I	1 semester
Prof Will Horowitz (UCT)	Quantum Field Theory II	1 semester
TOTAL		

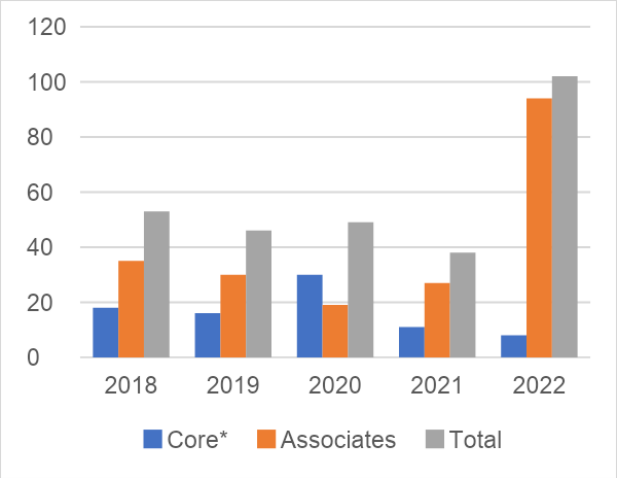
Publications

9.1 Number of publications per year: 2018-2022

The total number of publications increased by 168% from 2021. The increase can mainly be attributed to the larger number of Associates who have joined NITheCS over the past 24 months, who include the NITheCS affiliation on their publications.

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

** Publications by NITheCS Directorate and Postdocs*



9.2 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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Statement of income and expenditure

For the period ending:	31/12/2022	31/12/2021
TOTAL INCOME	**-16 168 030.77**	**-17 372 526.83**
Income: bursary	-460 000.00	0.00
Income: NRF apportioned	-15 661 000.05	-17 372 526.83
Interest receive: internal all	-554.20	0.00
Profit: exchange rate foreign	-5 624.75	0.00
Sundry interest received	-1 108.77	0.00
Sundry income: non taxable	-39 743.00	0.00
TOTAL EXPENDITURE	**19 264 594.47**	**10 743 060.93**
CURRENT EXPENDITURE		
Advertisements: general	12 730.50	24 750.00
Affiliation & registration exp	10 700.00	0.00
Bursary postgraduate	4 672 522.00	3 661 300.00
Cell phone airtime	22 913.16	46 000.00
Consultation fees	13 344.00	48 160.38
Copy and printing	1 533.18	4 730.64
Courses	9 500.00	0.00
Entertainment general	68 274.20	0.00
Flowers (not gifts)	500.00	0.00
Foreign exchange loss	0.00	668.52
General office costs	0.00	481 006.00
General research costs	1 786 426.00	0.00
Gifts	1000.00	0.00
Graphic design	6 302.00	7 590.00
Internet network email levy	900.00	36 922.00
Maintenance of apparatus	2 980.00	0.00
Marketing cost	433 505.39	231 309.76
Photographic expenditure	3 650.00	0.00
Postage and courier services	298.28	0.00
Prizes and medals	54 000.00	3 500.00
Promotional material	15 144.35	0.00
Research conferences	99 000.00	0.00
Research publications	43 534.83	11 792.88
Research contract conduit payment	6 183 931.63	4 713 502.00
Services	3 061 309.23	1 060 289.28
Smaller furniture and equipment	4 041.84	0.00
Stationery	11 644.34	0.00
Subscription and membership fees	415 268.36	0.00
Telephone: calls	2 797.84	266.83
Telephone: rent	13 685.58	15 335.04
Total remuneration	1 966 629.07	318 687.60
Travel: accommodation visum pa	54 908.47	0.00
Travel: foreign travel subsistence	23 749.85	0.00
Travel: daily allowance, air, car rental	93 109.92	0.00
Workshops	171 410.45	60 000.00
ASSET TRANSACTIONS		
Depreciation	10 676.90	12 067.87
Income: internal assets	-10 676.90	-12 067.87
Asset purchases	3 350.00	17 250.00
OPERATING (SURPLUS) / SHORTFALL FOR PERIOD	**3 096 563.70**	**-6 629 465.90**
FUNDS TRANSFERS	**-647 867.81**	**224 172.00**
Transfers from	0.00	224 172.00
Transfers to	-647 867.81	0.00
NET (SURPLUS) / SHORTFALL FOR THE PERIOD	**2 448 695.89**	**-6 405 293.90**
***Plus*: ACCUM (FUNDS) / SHORTFALL ON 01/01/2022**	**-16 553 848.13**	**-10 148 554.23**
ACCUM (FUNDS) / SHORTFALL ON 31/12/2022	**-14 105 152.24**	**-16 553 848.13**
***Min:* BALANCE SHEET ITEMS**	**-137 536.51**	**43 410.00**
Creditor provision balancing	-257 135.00	0.00
Debtors control account	120 851.77	50 000.00
Petty cash control account	1 000.00	1 000.00
Sundry creditors	-2 253.28	-7 590.00
FUNDS AVAILABLE ON 31/12/2022	**-14 242 688.75**	**-16 510 438.13**

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