NITheCS

National Institute for
Theoretical and Computational Sciences

Annual Report

1 January–31 December 2021

Intelligence

is the ability to

adapt to change

~ Stephen Hawking

CONTENTS

ABBREVIATIONS

AIMS	African Institute for Mathematical Sciences
APC LAB	Astroparticle and Cosmology Laboratory
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
DUT	Durban University of Technology
ICTP	International Centre for Theoretical Physics
IFAB Int	International Foundation Big Data and Artificial Intelligence for Human Development
iThemba LABS	iThemba Laboratory for Accelerator Based Sciences
KAIST	Korea Advanced Institute of Science and Technology
KRISP	KwaZulu-Natal Research Innovation and Sequencing Platform
MIT	Massachusetts Institute of Technology
NASA	National Aeronautics and Space Administration
NASSP	National Astrophysics and Space Science Programme
NMU	Nelson Mandela University
NRF	National Research Foundation

NUS	National University of Singapore
NWU	North-West University
QuAIL	Quantum Artificial Intelligence Laboratory
QuBiT Lab	Quantum Biology Tech Lab
RU	Rhodes University
SADiLAR	South African Centre for Digital Language Resources
SASA	South African Statistical Association
SU	Stellenbosch University
UCLA	University of California, Los Angeles
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
UrQMD	Ultra-relativistic Quantum Molecular Dynamics
UWC	University of the Western Cape
WITS	University of the Witwatersrand

INTERIM DIRECTOR'S REPORT

Whereas the journey of transitioning from National Institute for Theoretical Physics (NITheP) to National Institute for Theoretical and Computational Sciences (NITheCS) is still underway, there is already much to celebrate in this first annual report under the new institutional name. In this report, we include background information about the journey of transition. The strategic intent of the roadmap there has been to step up research, training and engagement programmes by improving economies of scale, and thereby increase global competitiveness. This endeavour is embedded in the foundations of science and technology in theoretical and computational sciences: the data sciences and basic sciences drive one another in the current period of intense growth.

While the transition process continues, with some legal structures still being finalised, we have been encouraged by the reaction at the various academic institutions where we explained the transition process and roadmap during our roadshow. Many local universities have indicated they are interested in becoming NITheCS nodes in future. This process is already underway and will increase our footprint.

Like many other activities, the COVID-19 pandemic meant the roadshow had to move online. Yet, this endeavour proved valuable as a means to attract direct interaction and answer questions. Viewer numbers for the roadshow have been encouraging: a total of 402 people have participated. In the process, the new NITheCS logo has also been well received.

We are grateful to the longstanding Chairman of the NITheP/NITheCS Steering Committee, Prof Eugene Cloete, Deputy Vice-Chancellor for Research, Innovation and Postgraduate Studies at Stellenbosch University, for his exemplary services until 2021. His leadership was extremely valuable during our formative years.

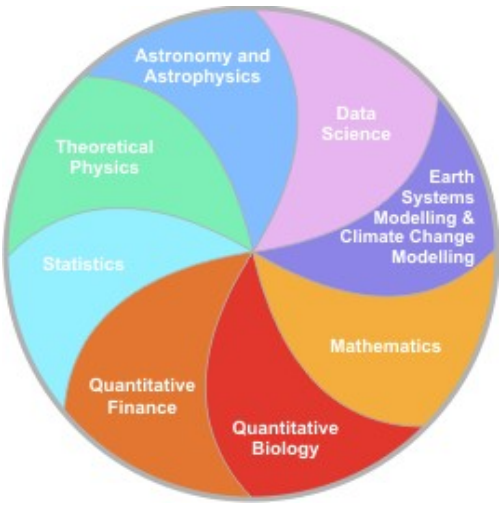
Dr Happy Sithole was elected to replace Prof Cloete as Chairman. We are indeed privileged to have someone of the stature of Dr Sithole to direct the Steering Committee. The entire NITheCS team and members will enthusiastically support Dr Sithole to drive the organisation forward and achieve its goals and support scientific endeavour in the country. Since 2019, Dr Sithole has also been the Centre Manager of the National Integrated Cyber Infrastructure System (NICIS).

Dr Sithole has stated that his aims in leading the organisation are to identify the required development in each of the eight identified thematic areas of NITheCS, and provide support for those areas. He also values collaboration across the various domains, as today's problems are multi-disciplinary and the Institute can only benefit from well-designed collaborative projects. We heartily support him in this endeavour, and also in his stated aim to ensure that we develop the necessary human capital to drive the developments in these areas, as well as a long-term sustainable funding model to ensure continuity and impact.

Strengthening collaboration

In our drive to strengthen collaboration amongst the eight themes we will, among others, include in our programme public lectures for each theme in 2022. Our new dedicated online meeting rooms will support learning and collaboration nationwide.

Thematic areas of NITheCS



The current NITheCS activities are clearly bearing fruit. Expanding the role of the organisation to embrace as many as possible of the scientific areas that can benefit from theoretical and computational science, is already opening doors and enabling work towards solving the societal grand challenges at the heart of the Department of Science and Innovation Decadal plan.

We already have more than 160 individual Associates and 11 junior Associates, and are working towards including many more: the call for new Associates remains open for individuals as well as institutions. For individuals, this relates to those who hold a position at a South African university and have a PhD in a theoretical, computational or interdisciplinary field of science relating to astronomy and astrophysics, data science, earth systems and climate change modelling, mathematics, quantitative biology, quantitative finance, statistics or theoretical physics. Institutions that focus on these fields of science may apply to become institutional associates.

This annual report details the successes and provides some statistics relating to research projects, as well as our well-received colloquia, mini-schools and other projects. The first academic papers that include NITheCS in their references have been published, and we encourage authors to continue inserting these references.

2021 Summer School

The 2021 Summer School, organised jointly by the Centre for High Performance Computing (CHPC) of the Council of Scientific and Industrial Research (CSIR) and NITheP/NITheCS, was the first to be presented as an online school due to COVID-19. The 2022 Summer School will again be an online event. This four-week programme for postgraduate students is aimed at bridging gaps between theoretical studies, data science and high-performance computing. A total of 161 students from various research institutes across Africa and around the globe participated in the 2021 Summer School.

One of our new initiatives was aimed at helping to attract and keep more women in the STEM fields. In celebration of Women's Month in August, NITheCS invited its female Associates to participate in its first Writing Retreat. It could become a permanent feature on the Institute's calendar every year, and its aim is to create the opportunity for participants to focus on work that can be done faster without the interruptions of daily life and everyday activities.

Because of the nature of our work, it has been possible to make the necessary adjustments in light of COVID-19 to conduct many of our activities online. Our small office staff has worked hard and creatively, and we have increased our activities and impact despite the additional practical challenges that have faced the globe since the pandemic started. We already use all available and relevant online facilities to conduct our work and present interesting and challenging material in our colloquia, mini-schools and other events. Many of our presentations and talks are captured via YouTube and made available via our website. Our regular newsletter and e-mail alerts about specific presentations and talks keep NITheCS Associates, interns, bursary holders, institutional partners and other interested parties up to date with our activities.

Support

We cannot continue the work of the Institute without the support of exceptional organisations and individuals. Among these are the Department of Science and Innovation (DSI), National Research Foundation (NRF), South African Institute of Physics (SAIP), local universities, our Associates and the many organisations and individuals locally and internationally who give of their time, expertise and advice to help us grow and function effectively. Many people contribute to our presentations and we are truly grateful to every person and institution. This makes it possible to look with confidence towards a year in which we continue to improve economies of scale and increase global competitiveness for our scientific community.

Yours sincerely,

Prof Francesco Petruccione

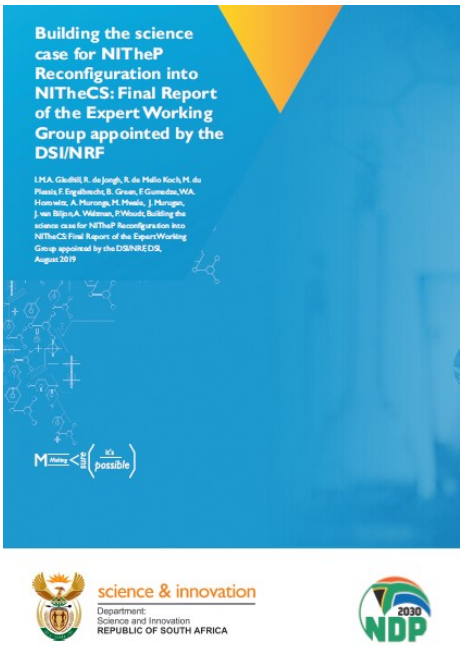
FROM NITheP TO NITheCS: A ROADMAP TO A NEW INSTITUTE

The National Institute for Theoretical and Computational Sciences (NITheCS) was formed in 2021 after starting the transition from the National Institute for Theoretical Physics (NITheP). The transition process is continuing and will conclude in 2022.

The Institute is supported by, among others, the SAIP, DSI and NRF. A 'roadmap' document to transition from NITheP to NITheCS was prepared in November 2020 by I.M.A. Gledhill and F. Petruccione, with inputs from R. de Jongh, R. de Mello Koch, M. du Plessis, F. Engelbrecht, B. Green, F. Gumedze, W.A. Horowitz, A. Muronga, M. Mwale, J. Murugan, J. van Biljon, A. Weltman, and P. Woudt.

It was prepared after intensive discussions and stated that the South African science, technology and innovation landscape supported thematic areas in which applied science is fostered, with an emphasis on moving science from research to impact. It stressed that the research capability of the nation depends on the presence of scientists with penetrating knowledge of the underlying basic principles and a thorough appreciation of the most recent achievements: traction is needed for the basic sciences to sustain and develop their underpinning foundational role.

The roadmap to transition to NITheCS



Scale of activities

The document also pointed out that the South African landscape of science and technology institutions had expanded far less than the scope and scale of its research, scientific and technological activities. NITheP, as it existed then, was one of several research and development opportunities. While limited in part due to a lack of scale, it proved its value through delivery of an exceptionally high quantity and quality of research (about 60 papers per year with a core staff of only four to five people) and critical support of world-class human capital development. Since the institute required no experimental equipment, it created notable value for relatively low investment.

Over the years, the institute stimulated a healthy interest in theoretical physics on both a national and international level through several initiatives, such as networking opportunities, mobility grants, encouraging visits from local and international physicists and physics students, bursaries, research opportunities and internships, summer schools and community service.

Strategic intent

The strategic intent of the roadmap was to step up research programmes by improving economies of scale, and thereby increase global competitiveness. Underlying this endeavour are the deep foundations of science and technology in theoretical and computational sciences: the data sciences and basic sciences drive one another in a period of intense growth.

The roadmap was in line with the policy of enhancing coherence and programme coordination to align eight themes. Coherence between these themes would enable such an institute to have greater impact on human

capital and research capacity development, and improve financial sustainability.

In alphabetical order, these themes are:

- Astronomy and Astrophysics
- Data Science
- Earth Systems Modelling & Climate Change Modelling
- Mathematics
- Quantitative Biology
- Quantitative Finance
- Statistics, and
- Theoretical Physics.

The DSI and NRF proposed in 2017 that NITheP could be repositioned to strengthen its national impact on both human capital development and research capacity development, and also improve its sustainability through this alignment.

A number of policy documents on different levels were considered in the process of planning the conversion from NITheP to NITheCS.

The science case, structure, and governance had by then already been established by an expert working group (EWG) composed of representatives of the eight proposed themes, who also consulted the communities of practice in the proposed themes. The working group report submitted in August 2019 focuses on scientific content, benefit, strategic alignment, the institutional structure in each field, collaboration, increasing research capacity, and transformation. It covers economies of scale, risks, and institutional structure. A close relationship with the Centre for High Performance Computing (CHPC) is at the centre of the design.

After the NITheP Task Team for Reconfiguration and the NITheP Steering Committee considered the EWG report, it was presented to the DSI Executive Committee. Open, transparent, science-based decisions and a shared vision of the future of science in South Africa are vital within the Steering Committee.

The roadmap sets out plans for transition from NITheP to NITheCS in a 4-phase process: the Transition, Foundational, Development and Programmatic phases. This process is still ongoing.

VIRTUAL OPERATIONS

During the COVID-19 pandemic, many theoretical and computational scientists operated and continue to function using virtual modes of communication. The Institute's operations successfully proceeded in this manner, including work on the transition process to the new NITheCS. At the same time, in-person seminars were replaced by successful webinars and mini-schools, which have increased the reach of the theoretical and computational community in South Africa globally.

Once the transition process has been completed, funding will determine the rate of growth, according to the scalability of the focus areas. During the programmatic phase the Institute will count on the continued support for its Vision and Mission of NITheCS by the Management Committee and Steering Committee, while we also look forward to setting up a permanent central location for our operations.

OUR PEOPLE

STAFF PROFILE

The staff profile of NITheCS at 31 December 2021 is shown below:

POSITION	INSTITUTION	CONTRACTS
Interim Director	UKZN	1 (Contract, renewed during 2020, ends 31 March 2022)
Deputy Directors	WITS/SU	2 (3-year contracts, renewed during 2020, end 31 March 2023)
Administrative	SU WITS UKZN	1 (Contract ends 31 March 2022, 5/8 position) 1 (Contract ends 31 December 2022, 4/8 position) 1 (Contract ends 31 March 2022, 8/8 position)

POSTDOCTORAL FELLOWS

The postdoctoral fellows per node at 31 December 2021 are shown below. All positions are two-year contracts.

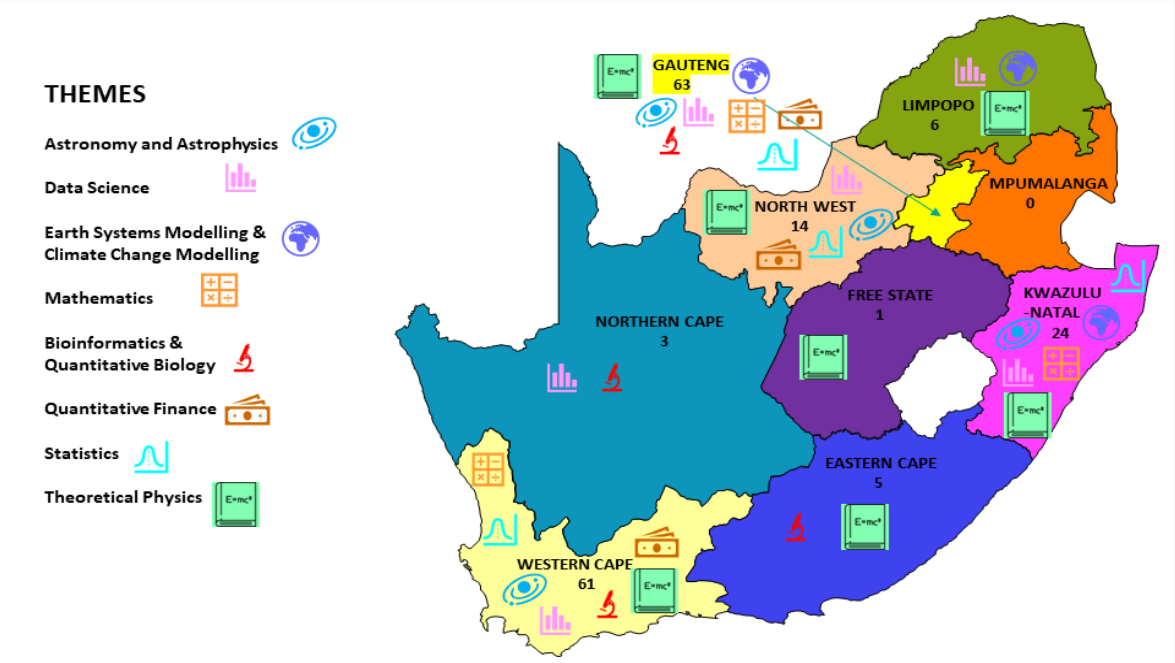
NODE	NITheCS FUNDED	EXTERNALLY FUNDED
SU	1 (Saadatmand)	0
UKZN	1 (Mongalo)	2
WITS	3 (Bhatta, Jana, Rabambi)	4
TOTAL	**5**	**6**

ASSOCIATES

To achieve the NITheCS' strategic goals, it is crucial to maintain a national network of associates throughout South Africa. At 31 December 2021, our Associates network comprised the following members:

Individual Associates	166
Strategic Associates	6
Institutional Associates	19
Junior Associates	11
TOTAL	**202**

ASSOCIATES PER PROVINCE AND THEME



ASSOCIATES: WHO THEY ARE

Individual Associates

Astronomy/Astrophysics

- Dr Amare Abebe (North-West University)
- Prof Andrew Chen (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)
- Prof Lerothodi Leeuw (University of the Western Cape)
- Dr Stefan Lotz (South African National Space Agency)
- Prof Ilani Loubser (North-West University)
- Dr Jack Radcliffe (University of Pretoria)
- Prof Soebur Razzaque (University of Johannesburg)
- Prof Patrick Woudt (University of Cape Town)

Bioinformatics and Quantitative Biology

- Prof Tulio de Oliveira (University of Stellenbosch)
- Prof Morne du Plessis (National Institute For Communicable Diseases)
- Prof Cang Hui (University of Stellenbosch)
- Prof Tjaart Kruger (University of Pretoria)
- Dr Monica Mwale (South African National Biodiversity Institute)
- Prof Olugbenga Oluwagbemi (Sol Plaatje University)
- Dr Verena Ras (University of Cape Town)
- Prof Özlem Taştan Bishop (Rhodes University)
- Prof Vernon Visser (University of Cape Town)

Earth Systems Modelling & Climate Change Modelling

- Dr Mary-Jane Bopape (South African Weather Service)
- Prof Francois A. Engelbrecht (University of the Witwatersrand)
- Prof Colleen Vogel (University of the Witwatersrand)

Data Science

- Prof Kelvin Bwalya (University of Johannesburg)
- Dr Emmanuel Dufourq (University of Stellenbosch)
- Dr Marcel Dunaiski (University of Stellenbosch)
- Dr Samuel Egieyeh (University of the Western Cape)
- Prof Zurab Janelidze (University of Stellenbosch)
- Dr Sydney Kasongo (University of Stellenbosch)
- Prof Langa Khumalo (North-West University)
- Prof Rodney Kroon (University of Stellenbosch)
- 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)
- Prof Delia North (University of KwaZulu-Natal)
- Dr Ibidun Obagbuwa (Sol Plaatje University)
- Prof Babu Paul (University of Johannesburg)
- Dr Mpho Raborife (University of Johannesburg)
- Prof Kanshukan Rajaratnam (University of Stellenbosch)
- Prof Benjamin Rosman (University of the Witwatersrand)
- Dr Makhamisa Senekane (University of Johannesburg)
- Dr Fritz Solms (S-PLANE Automation / University of Stellenbosch)
- Prof Hossana Twinomurinzi (University of Johannesburg)
- Prof Brink van der Merwe (University of Stellenbosch)
- Prof Menno van Zaanen (North-West University)
- Prof Serestina Viriri (University of KwaZulu-Natal)

Mathematics

- 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)
- Prof Willem Conradie (University of the Witwatersrand)
- Dr Partha Pratima Ghosh (University of South Africa)
- Dr Amartya Goswami (University of Johannesburg)
- Dr Mandlenkosi Gwetu (University of KwaZulu-Natal)
- Prof Yorick Hardy (University of the Witwatersrand)
- Dr Rhameez Sheldon Herbst (University of Johannesburg)
- Dr Michael Hoefnagel (University of Stellenbosch)
- Prof Fortuné Massamba (University of KwaZulu-Natal)
- Dr Charles Msipha (Tshwane University of Technology)
- Prof Loyiso Nongxa (University of the Witwatersrand)
- Prof Delia North (University of KwaZulu-Natal)
- Prof Helmut Prodinger (University of Stellenbosch)
- Dr Cerene Rathilal (University of Johannesburg)
- Prof Benjamin Rosman (University of the Witwatersrand)
- Dr Riana Roux (University of Stellenbosch)
- Dr Ridhwaan Suliman (Council for Scientific and Industrial Research)
- Dr Vivien Visaya (University of Johannesburg)
- Dr Dawit Worku (Cape Peninsula University of Technology)
- Dr Bertin Zinsou (University of the Witwatersrand)

Quantitative Finance

- Prof Conrad Beyers (University of Pretoria)
- Prof Riaan de Jongh (North-West University)
- Prof Helgard Raubenheimer (North-West University)
- Prof Ronald Richman (Old Mutual Insure)
- Prof David Taylor (University of Cape Town)

Statistics

- 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)
- Prof Willem Schutte (North-West University)

Theoretical Physics

- Prof Igor Barashenkov (University of Cape Town)
- Dr Bruce Bartlett (University of Stellenbosch)
- 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 Hasani Chauke (University of Limpopo)
- Prof Nithaya Chetty (University of the Witwatersrand)
- Prof Fabio Cinti (University of Stellenbosch)
- Dr Chris Clarkson (University of Cape Town)
- Prof Alan Cornell (University of Johannesburg)
- Prof Marelie Davel (North-West University)
- 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)
- Dr Rocco Duvenhage (University of Pretoria)
- Prof Hans Eggers (University of Stellenbosch)
- Prof George Ellis (University of Cape Town)
- Prof Stefan Ferreira (North-West University)
- Prof Aurona Gerber (University of South Africa)
- Prof Hendrik Geyer (University of Stellenbosch)
- Prof Irvy (Igle) Gledhill (CSIR/University of the Witwatersrand)
- Dr Kevin Goldstein (University of the Witwatersrand)
- Dr Jacob Greeff (North-West University)
- Prof Shajid Haque (University of Cape Town)
- Prof Dieter Heiss (University of Stellenbosch)
- 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 (University of Stellenbosch)
- 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 (University of Stellenbosch)
- Prof Mantile Lekala (University of South Africa)
- Dr 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 (University of Stellenbosch)
- 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 Prince Mkhonto (University of Limpopo)
- Dr Shazrene Mohamed (South African Astronomical Observatory and University of Cape Town)
- Dr Bishop Mongwane (University of Cape Town)
- Prof Kavilan Moodley (University of KwaZulu-Natal)
- Prof Kristian Muller-Nedebock (University of Stellenbosch)
- Prof Azwinndini Muronga (Nelson Mandela University)
- Prof Jeff Murugan (University of Cape Town)
- 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 Martin Porrmann (University of KwaZulu-Natal)
- 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 (University of Stellenbosch)
- 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)
- Dr Ilya Sinayskiy (University of KwaZulu-Natal)
- Dr Izak Snyman (University of the Witwatersrand)
- Prof Du Toit Strauss (North-West University)
- Prof Mark Tame (University of Stellenbosch)
- Dr Gary Tupper (University of Cape Town)
- Dr Aniekan Magnus Ukpong (University of KwaZulu-Natal)
- Dr Herman Uys (University of Stellenbosch)
- Prof Mattia Vaccari (University of the Western Cape)
- Prof Judy van Biljon (University of South Africa)
- Prof Andre Weideman (University of Stellenbosch)
- Prof Herbert Weigel (University of Stellenbosch)
- Prof Heribert Weigert (University of Cape Town)
- Prof Amanda Weltman (University of Cape Town)
- Prof Konstantinos Zoubos (University of Pretoria)

Junior Associates

Astronomy/Astrophysics

- Dr Teboho Moloi (University of Cape Town)

Data Science

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

Mathematics

- Dr Mathew Aibinu (Durban University of Technology)

Statistics

- Dr Farai Mlambo (University of the Witwatersrand)

Theoretical Physics

- Dr Thuto Mosuang (University of Limpopo)
- Dr Kingsley Obodo (North-West University)
- Mr Ayanda Zungu (North-West University)

Institutional Associates

The following letters of understanding (LOUs) were finalised in 2021:

International Centre for Theoretical Physics (ICTP)

The Carpentries

Our Institutional Associates are:

- 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*
- MIT Kavli Institute for Astrophysics and Space Research*
- 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*

** Memorandums of Understanding and Letters of Understanding are still underway.*

Strategic Associates

- Prof Kanshukan Rajaratnam (Director School for Data Science and Computational Thinking at Stellenbosch University)
- Dr Joseph Kirui (Hod Physics Department UNIVEN)
- Prof Barry Green (AIMS)
- Prof Lesley Cornish (DSR/NRF CoE in Strong Materials)
- Prof Ludwig Combrinck (HartRAO)
- CEO of IThemba LABS

VIRTUAL ASSOCIATES SOCIAL EVENT INITIATIVE

A virtual Associate social initiative was launched in 2021: after every colloquium and mini-school there is a 15-minute social event. Community members could get to know one another and establish new networks at these, and NITheCS staff could also interact with participants.

The idea is well received and these events have been well attended.

BURSARIES

BURSARIES GRANTED

LEVEL	NUMBER OF BURSARIES	BURSARY VALUE	TOTAL
MSc	10	R80 000	R800 000
PhD	8	R100 000	R800 000
PhD	1	R20 000*	R20 000
PhD	1	R50 000**	R50 000
TOTAL	20		R1 670 000

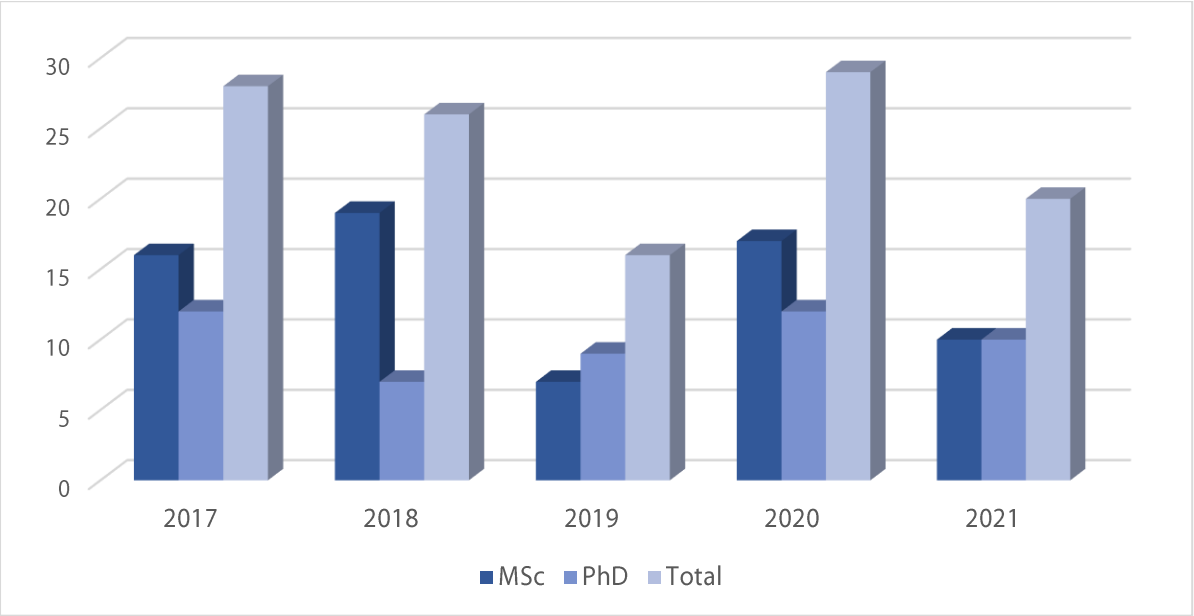
Important note about 2022 funding:

Due to contractual terms, the NITheCS UID could not allow students to apply for funding directly from NITheCS in 2022. Therefore, students applied in the general pool and notified NITheCS of their intention to apply for a NITheCS bursary. This list was forwarded to the NRF for possible 2022 funding. In addition, NITheCS plans to select students from a list of applicants in the general NRF pool, and is positive this will lead to the budgeted amount for bursaries being allocated effectively.

* PhD student Ruach Slayen (UCT) was only permitted R20k due to Shuttleworth Foundation bursary

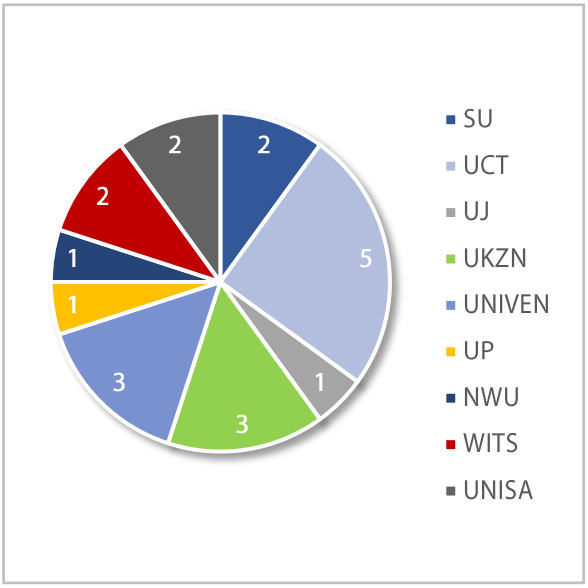
** PhD student (WITS) discontinued his studies, therefore R50k was refunded.

BURSARY TRENDS: 2017 TO 2021



DISTRIBUTION OF BURSARY HOLDERS

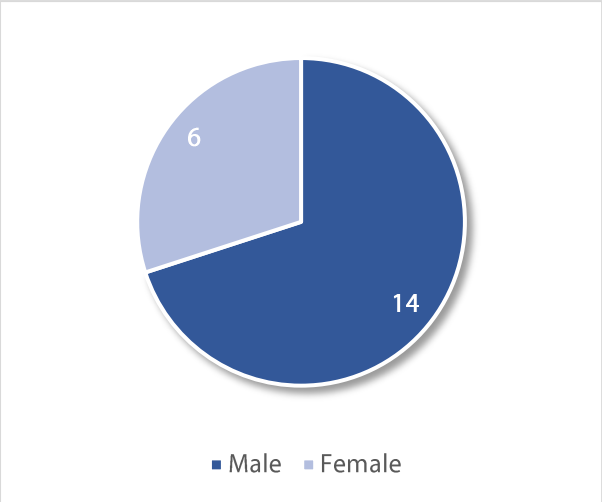
INSTITUTION	MSc	PhD	TOTAL
SU	2	0	2
UCT	4	1	5
UJ	0	1	1
UKZN	0	3	3
UNIVEN	3	0	3
UP	1	0	1
NWU	0	1	1
WITS	0	2	2
UNISA	0	2	2
TOTAL	10	10	20

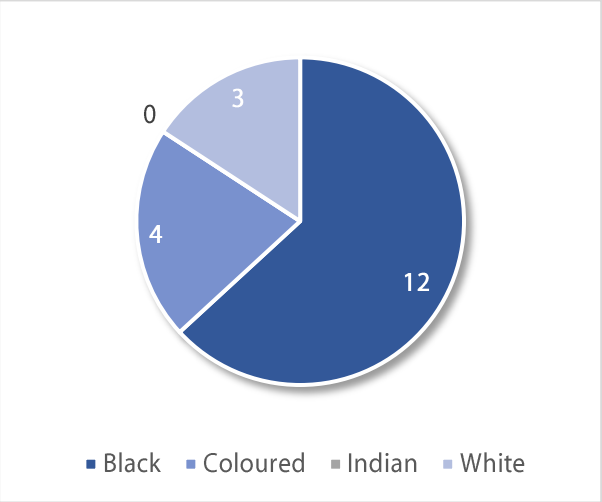


BURSARY HOLDERS' DEMOGRAPHICS

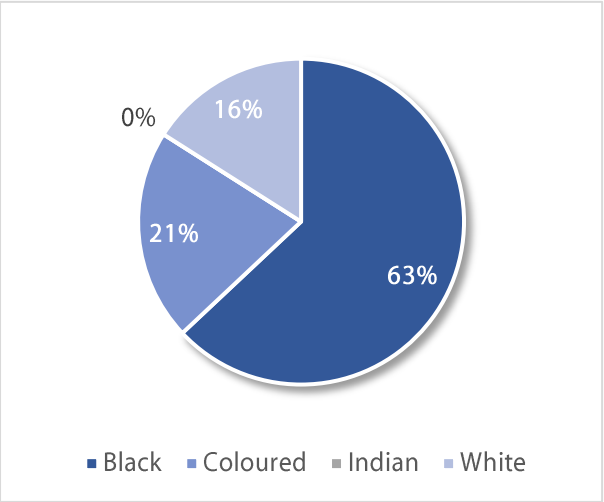
DEGREE	BLACK		COLOURED		INDIAN		WHITE		TOTAL
	MALE	FEMALE	MALE	FEMALE	MALE	FEMALE	MALE	FEMALE	
MSc	5	2	0	0	0	0	1	2	10
PhD	5	0	0	0	1	2	2	0	10
TOTAL	10	2	0	0	1	2	3	2	20

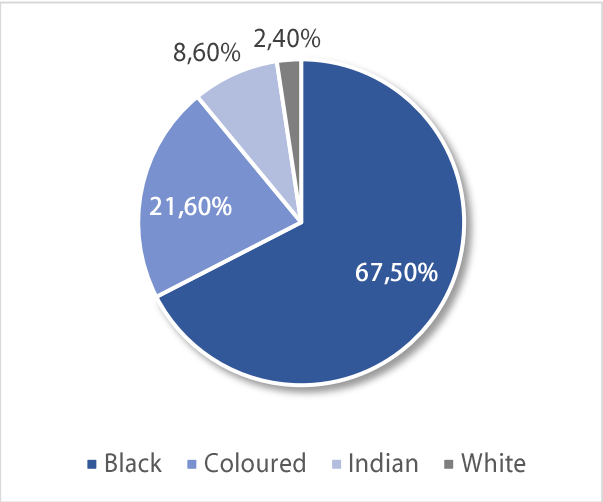
Detailed demographics

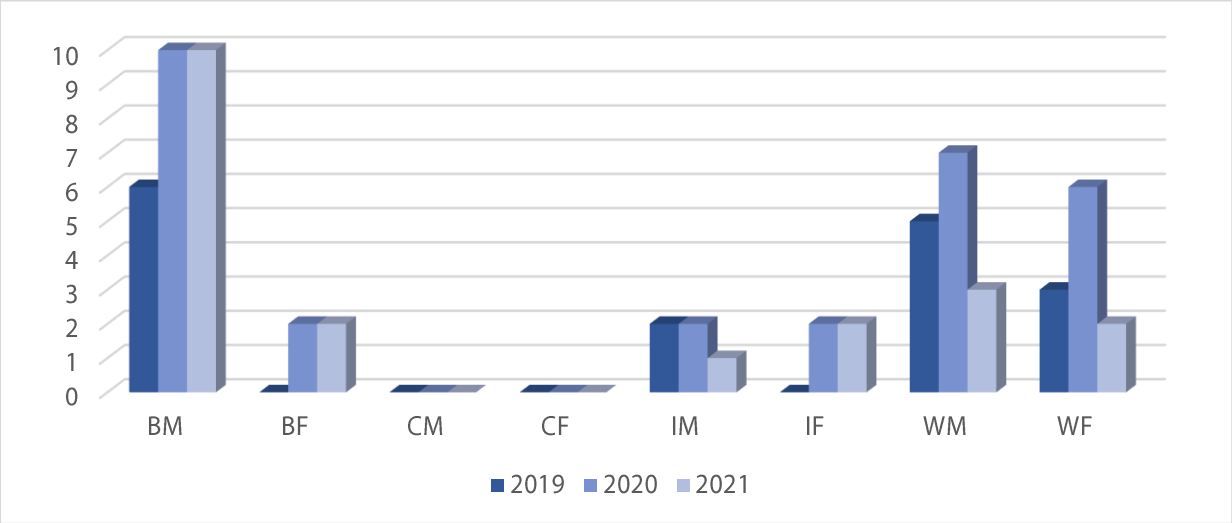




BURSARY HOLDERS' DEMOGRAPHICS VERSUS THE SOUTH AFRICAN POPULATION







Bursary demographics for Black males (BM), Black females (BF), Coloured males (CM), Coloured females (CF), Indian males (IM), Indian females (IF), White males (WM) and White females (WF).

VIRTUAL BURSARY HOLDERS WORKSHOP

A bursary holders workshop took place on 25 November 2021 via Zoom. About 80% of NITheCS bursary holders attended the workshop led by Prof Francesco Petruccione. He updated the students about the NITheCS implementation plan and answered questions.

Another workshop will be held around April 2022.

ACTIVITIES FOR 2021

TEACHING HOURS

Teaching hours for staff (Interim Director, Deputy Directors and Postdocs) are reflected in the table below:

NODE	NUMBER OF HOURS	
	CORE	POSTDOCS
SU	250	0
WITS	83	0
UKZN	48	48
TOTAL	**381**	**48**

ACTIVITIES

TYPE OF ACTIVITY	NUMBER OF ACTIVITIES	ATTENDEES	YOUTUBE VIEWS TO DATE
PHYSICAL			
Long-term visitors	0*	0*	n/a
Mobility	0*	0*	n/a
Research workshops	0*	0*	n/a
Capacity development workshops	0*	0*	n/a
CHPC/NITheP Summer School	1	65	n/a
Chris Engelbrecht Summer School	1	43	n/a
ONLINE			
Mini-schools	9	3 483	3 406
Online webinars	10	246	661
Online colloquia	43	2 270	4 047
Roadshows	15	402	n/a
Data@Breakfast	13	1 121	1 145
Quantum Machine Learning Meetup	3	642	3 292
TOTAL	**95**	**8 272**	**12 551**

* Due to COVID-19 no physical activities could take place, but our usual activities will resume if conditions allow during 2022.

ONLINE MINI-SCHOOLS

DATE	NAME OF SPEAKER	TOPIC	NUMBER OF ATTENDEES	YOUTUBE VIEWS TO DATE
March	Prof Nico Orce (UWC)	Mathematical modelling of COVID-19	646	617
April	Prof Uwe Jaekel (Hochshule Koblenz, University of Applied Sciences, Germany)	Introduction to Monte Carlo Methods	263	413
May	Prof Kanshu Rajaratnam (SU Data School)	Introduction to Python Programming	1 349	1 000
June	Prof Vishnu Jejjala & Dr Pallab Basu (WITS), and Dr Anirbit Mukherjee (University of Pennsylvania, USA)	Machine learning in high energy theory	193	338
July	Prof Kanshu Rajaratnam and Dr Juan Klopper (SU Data School)	School for Data Science and Computational Thinking: Series of online lectures in data science and computational thinking	Data not available	Data not available
Aug	Prof Bruce Mellado, Dr Xifeng Ruan & Prof Deepak Kar (WITS)	Introduction to Big Data and machine learning for particle physics	277	260
Sept	Prof Martin Bucher (UKZN)	Mapping the Initial Conditions of the Universe: Exploring the Cosmic Microwave Background	192	166
Oct	Dr Amartya Goswami (UJ) and Prof Zurab Janelidze (SU)	Elementary Introduction to Category Theory	297	342
Nov	Prof Brink van der Merwe (SU) and Prof Yorick Hardy (WITS)	Getting started with Haskell	266	270
TOTAL			3 483	3 406

ONLINE WEBINARS

DATE	SPEAKER	AFFILIATION	TITLE	NUMBER OF ATTENDEES	YOU-TUBE VIEWS TO DATE
21 Jan	Dr Anton Trushechkin	Steklov Mathematical Institute of the Russian Academy of Sciences	Unified master equation of weak-coupling limit type	Data not available	93
29 Mar	Dr Paola Andrea Concha Obando	Brazilian Center for Research in Physics (CBPF)	Macro-to-micro quantum mapping and the emergence of nonlinearity	31	44
22 Apr	Dr Kade Head-Marsden	Harvard University, USA	Dilation based quantum algorithms for the time-evolution of open quantum systems	24	185
17 Jun	Dr Bertus Jordaan	Data scientist, Payment24	Towards essential nodes in a simple quantum network based on photons	22	38
25 Jun	Dr Ismael Galván	National Museum of Natural Sciences, Madrid, Spain	The quantum basis of organic evolution	78	78
2 Jul	Dr Daniel Burgarth	Macquarie University, Sydney, Australia	Eternal adiabaticity and KAM-stability	19	53
9 Jul	Dr Denise Welsch	Rey Analytical Research, Germany	Contribute to Statsomat and make data analysis automatically interpretable	27	40
22 Jul	Dr Adrián Budini	National Scientific and Technical Research Council (CONICET), Bariloche, Argentina)	Quantum non-Markovianity: an approach from past-future correlations	26	51
30 Sep	Prof Rocco Duvenhage	UP	Optimal quantum channels		28
19 Nov	Dr Fabio Anza	University of California, USA	A kinetic theory of information transport	19	51
TOTAL				246	661

ONLINE COLLOQUIA

DATE	SPEAKER	AFFILIATION	TITLE	NUMBER OF ATTENDEES	YOU-TUBE VIEWS TO DATE
25 Jan	Prof Sera Markoff	University of Amsterdam, Netherlands	Putting hair on black holes	74	120
15 Feb	Prof Nico Orce	UWC	COVID-19 situation in South Africa using new epidemiological models	47	170
8 Feb	Prof Morten Hjorth-Jensen	Michigan State University, USA; University of Oslo, Norway	Machine learning and quantum mechanics for many interacting particles	113	405
22 Feb	Prof Ilya Sinayskiy	UKZN	Open quantum walks	56	158
1 Mar	Prof Ofer Aharony	Weizmann Institute of Science, Israel	Towards a theory of quantum gravity	59	198
8 Mar	Prof Gerard Milburn	University of Queensland, Australia	Learning time: clocks and analogue machine learning	51	95
15 Mar	Prof Oluwule Daniel Makinde	SU	Nanofluid dynamics and its engineering cooling applications	34	295
29 Mar	Prof Dariusz Chruscinski	Nicolaus Copernucius University, Torun, Poland	On universal constraints for relaxation rates for quantum dynamical semigroups	32	111
12 Apr	Prof Shiraz Minwalla	Tata Institute for Fundamental Research, Mumbai, India	Bose Fermi dualities in three spacetime dimensions	58	76
14 Apr	Prof Yasser Omar	IT & IST, University of Lisbon, Portugal	Tackling particle tracking with quantum computation (World Quantum Day)	121	127
19 Apr	Dr Aniekan Magnus Ukpong	UKZN	High performance computing: insights from condensed matter and materials physics	38	67
26 Apr	Prof Michael Laidlaw	Retired, ex UKZN	Topology and quantum mechanics 50 years ago	34	178
3 May	Prof Azwinndini Muronga, Ms Thuthukile Khumalo, Ms Khodani Mafune, Mr Bradley Nemutudi	NMU, WITS/iThemba LABS, UNIVEN, UL	Statistical and thermal models for heavy-ion collisions and astrophysics	54	144

10 May	Prof Nico Orce	UWC	How atomic nuclei polarize	48	125
17 May	Prof Nithaya Chetty	WITS	Aim for the sky, but keep your feet on the ground	59	57
24 May	Prof Daniel Harlow	MIT, USA	Symmetry in field theory and gravity	49	109
31 May	Prof Ilya Mandel	Monash University, Melbourne, Australia	The promise of gravitational-wave astrophysics	35	65
7 Jun	Prof Mattia Vaccari	UWC	The Ilifu cloud computing facility & X-Informatics data-intensive research	62	42
14 Jun	Prof Erik Aurell	KTH Royal Institute of Technology, Stockholm, Sweden	The case for the necessity to quantize the quantum gravitational field or the lack of it	51	73
21 Jun	Prof Kavilan Moodley	UKZN	Dark energy and cosmological cross-correlations with HIRAX 21cm intensity mapping	34	67
28 Jun	Prof Francesco Petruccione	UKZN, NITheCS	The transition from NITheP to NITheCS	60	45
5 Jul	Dr Laure Gouba	ICTP Trieste, Italy	The beauty of quantum mechanics	62	257
12 Jul	Prof Deshen Moodley	UCT, Co-Director of National Centre for Artificial Intelligence Research (CAIR) at UCT	Designing adaptive and cognitive computer systems in South Africa	42	53
19 Jul	Prof Bruce Bassett, Prof Wolfram Decker, Prof Barry Green, Prof Bernardo Rodrigues	UCT, TU Kaiserslautern, AIMS	*Panel discussion*: Computation as a tool for solving theoretical questions	31	63
26 Jul	Prof Judy van Biljon	UNISA	Machine Learning for the developing world: towards a research agenda	95	63
2 Aug	Prof Ina Schaefer, Prof Bruce Watson, Tobias Runge	Technical University of Braunschweig, Germany; SU	Designing Correct Algorithms	34	72
16 Aug	Dr Eric Maluta	UNIVEN	Theoretical Studies of brookite TiO_2 as a material for dye-sensitized solar cells	36	99
23 Aug	Prof Erik Aurell	KTH Royal Institute of Technology in Stockholm, Sweden	Lessons learned on SARS-CoV-2 genomics from GISAID	44	68
30 Aug	Dr Monica Mwale	SANBI	South African species reference DNA databases: General gap analysis of vertebrates	23	not uploaded

6 Sep	Dr Emmanuel Dufourq	SU & AIMS	Machine learning for ecology	59	90
13 Sep	Dr Sydney Kasongo	SU	Genetic algorithm in domain of intrusion detection systems	35	33
20 Sep	Prof Langa Khumalo	South African Centre for Digital Language Resources (SADiLaR)	Locating SADiLaR as a strategic centre for developing computational resources for African languages in the Context of 4IR	78	35
27 Sep	Prof Nico Orce	UWC	On the universality of the r-process (or why we see the same abundance of elements around us)	28	54
4 Oct	Prof Regina Maphanga	CSIR	From density functional theory to machine learning	49	
11 Oct	Dr Amartya Goswami	UJ	An invitation to visit the world of categories	47	
18 Oct	Dr Japie Greef	NWU	Aligning student and educator capstone project preferences algorithmically	21	
25 Oct	Dr Mark Nasila	FirstRand Risk (FNB)	The critical role of design thinking in artificial intelligence and machine learning applications	87	87
8 Nov	Prof Fritz Solms	S-PLANE Automation/SU	Some thoughts on software architecture	42	43
15 Nov	Prof Aleks Kissinger	Oxford University, UK	Picturing quantum software	78	78
22 Nov	Dr Jonathan Blackledge	Technological University Dublin, Ireland; UWC, UKZN	Knowledge economies and the future of higher education	120	126
29 Nov	Dr Mary-Jane Bopape	SA Weather Service	Forecasting at the South African Weather Service	14	17
06 Dec	Prof Steven Karataglides	UJ	Two problems of nuclear structure in the sd shell	43	47
13 Dec	Dr Cari van Schalkwyk	SU	The potential for cervical cancer elimination in South Africa	33	35
TOTAL				**2 270**	**4 047**

ONLINE ROADSHOWS

Prof Francesco Petruccione was the speaker at the following roadshows about the transition from NITheP to NITheCS:

DATE	PRESENTED FOR	NUMBER OF ATTENDEES
20 May	University of Venda	22
20 May	Stellenbosch University	17
20 May	South African Statistical Association	15
27 May	University of Limpopo	24
3 June	Nelson Mandela University	32
10 June	University of the Witwatersrand	42
11 June	CoE-MaSS	15
24 June	Free State University	26
1 July	Sol Plaatje University	40
1 July	Northwest University	14
15 July	University of Johannesburg	27
15 July	University of the Western Cape	29
23 Sept	Mangosuthu University of Technology	21
30 Sept	University of Pretoria	29
7 Oct	General roadshow	49
TOTAL		402

DATA@BREAKFAST

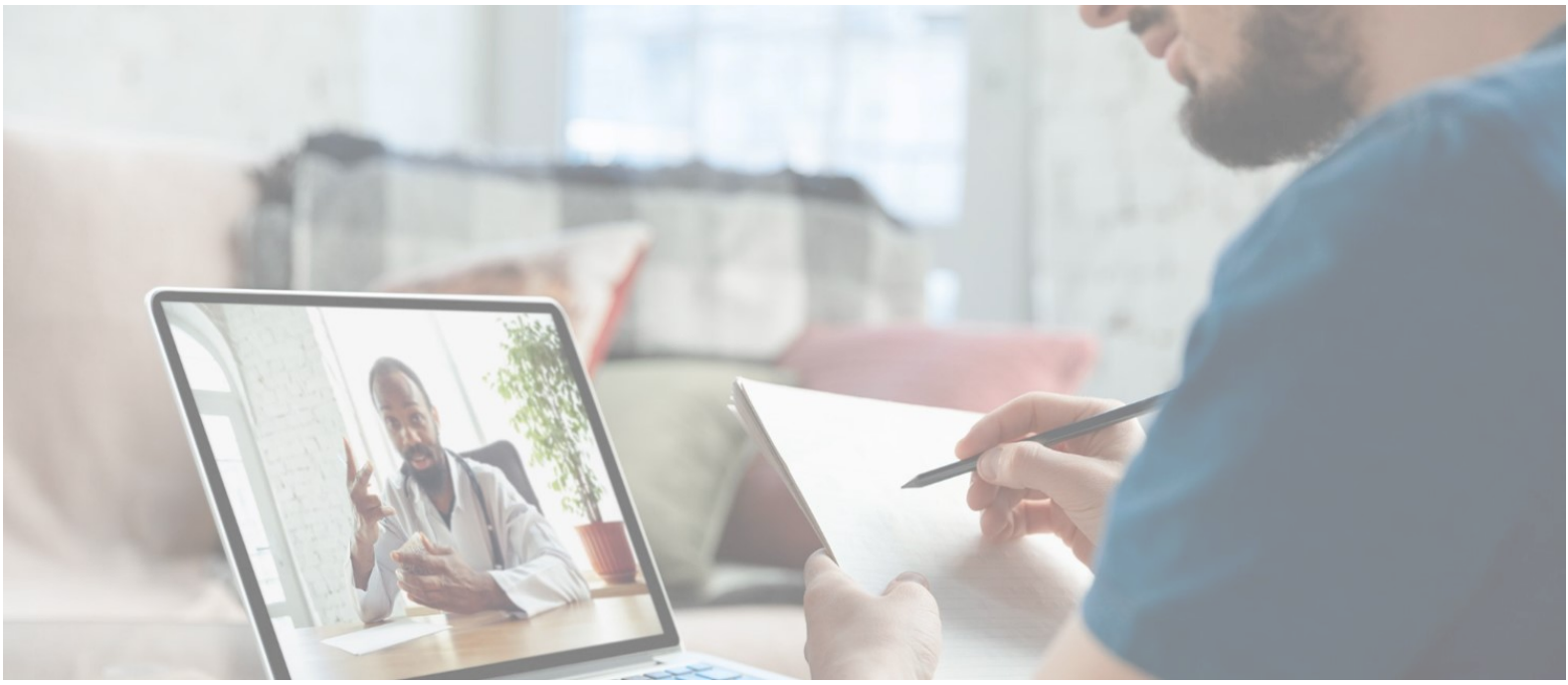
Data@breakfast is a platform to discuss current topics relating to big data, artificial intelligence, quantum computing, machine learning and related issues.

DATE	SPEAKER	AFFILIATION	TITLE	NUMBER OF ATTENDEES	YOUTUBE VIEWS TO DATE
5 Feb	Mr Farai Mazhandu	One Quantum Africa	Introduction to the quantum tech ecosystem and why Africa needs to build a robust quantum community now	104	66
19 Feb	Prof Yin-Zhe Ma & Dr Wei-Ming Dai	UKZN	The puzzle of Hubble constant: a holographic universe solution	52	56
26 Feb	Dr Paul Plantinga	HSRC	Getting more from government (meta) data	48	23
5 Mar	Dr Makhamisa Senekane	UJ	A hands-on introduction to Quantum Information Processing	25	173
12 Mar	Prof Simon Connell	UJ	Nuclear energy in the mix: Can it power Africa sustainably?	110	38
19 Mar	Dr Jarrad Wright	CSIR	Least-cost energy systems… or not?	126	38
26 Mar	Prof Bruce Bassett	UCT &AIMS	Predictions for COVID-19 IN South Africa 2021 and beyond	142	134
16 Apr	Dr Denise Welsch	Rey Analytical Research	Statsomat.com-Apps for automatic data analysis and learning	31	27
23 Apr	Prof Francesco Petruccione	UKZN & NITheCS	The National Institute for Theoretical and Computational Sciences	28	186
2 Jul	Prof Tulio de Oliveira and Dr Richard Lessells	UKZN	An update on COVID-19 in South Africa	269	171
23 Jul	Dr Guy Lamb	SU	The determinants of community violence and its policing in South Africa	157	80
30 Jul	Dr Ridhwaan Suliman	CSIR	COVID-19 and trends: the devil in the details		129
1 Oct	Dr Angelique Trusler	The Carpentries	The Carpentries: An open access community	29	24
TOTAL				1 121	1 145

QUANTUM MACHINE LEARNING MEETUP

Quantum Machine Learning Meetup (QML Meetup) is a series of talks by QML researchers discussing their work, with Q&A discussions afterwards.

DATE	SPEAKER	AFFILIATION	TITLE	NUMBER OF ATTENDEES	YOUTUBE VIEWS TO DATE
29 Apr	Dr Maria Schuld	UKZN	Taking stock of machine learning-a critical perspective	321	1 812
24 Jun	Dr David Sutter	IBM Research, Zurich	The power of quantum neural networks	195	791
26 Aug	Hsin-Yaun (Robert) Huang		Power of data in quantum machine learning	126	689
TOTAL				642	3 292



WORKSHOPS

WORKSHOPS SPONSORED

South African Conference for Artificial Intelligence Research (SACAIR2021)
AI for Science, Technology and Society
Sponsorship: R60 000

Deep Learning IndabaX
Sponsorship: R30 000

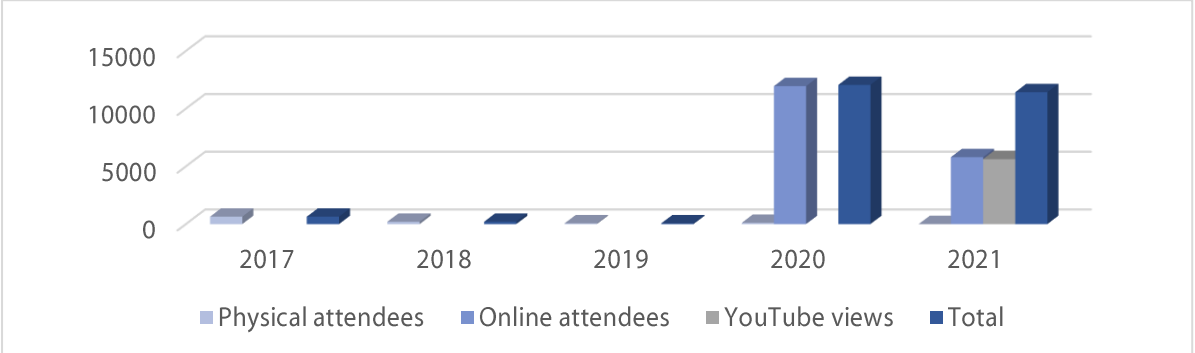
Two-day workshop to celebrate the 60th Anniversary of the Paper on Dynamical Maps by E.C.G. Sudarshan, P.M. Mathews and J. Rau.

3rd NITheP Summer School on the Foundations of Theoretical and Computational Science
February 2021

OTHER WORKSHOPS DURING 2021, AND ONGOING PROGRAMMES

- Virtual Associate workshop – November 2021
- Virtual bursary workshop – November 2021
- Virtual internship programme culminating in 2022 SAIP event
- Research focus areas call (ongoing)
- Associates call (remains open)
- Call for nodes and contracting sites (ongoing)
- 4th Foundations of Theoretical and Computational Science Summer School – February 2022 via Zoom

TOTAL ATTENDEES DURING PREVIOUS WORKSHOPS



PROGRAMMES

2020/2021 RESEARCH PROGRAMMES

The research programmes launched in 2020/2021 involved the entire network of Associates attached to South African universities, as well as several international collaboration partners.

RESEARCH PROGRAMMES AND PRINCIPAL INVESTIGATORS (PIs)

INVESTIGATORS/PROPOSERS	TOPIC
PI: Dr N.E. Maluta (UNIVEN) in collaboration with Prof R.R. Maphanga (CSIR) and Dr E. Maphasha (UP)	Computational Studies of Optoelectronic Properties and Material Engineering of Photoactive Layer in Perovskite Solar Cells
PI: Prof Amanda Weltman (UCT) **Co-PI:** Prof Kavilan Moodley (UKZN) **Co-investigators:** Prof Roy Maartens (UWC), Prof Mario Santos (UWC), Dr Michelle Lochner, (UWC), Prof Matt Hilton (UKZN), Prof Bruce Bassett (AIMS), Prof Aritha Pillay (DUT), Prof Oleg Smirnov (RU)	Theoretical and Computational Astrophysics Foundations for HIRAX Big Data
PI: Prof Martin Bucher (UKZN/CNRS/APC) **Co-PI:** **Co-investigators:** Prof Bruce Bassett, (AIMS), Prof Steven Gratton (Princeton), Sinoxolo Nene (UKZN), Prof Tulio de Oliviera (KRISP/UKZN) and Prof Ilya Sinayskiy (UKZN)	Theoretical Modelling for Genomic Contact Tracing
PIs: Prof Vishnu Jejjala (WITS), Prof Jonathan Shock (UCT), Dr Pallab Basu (WITS), Prof Robert de Mello Koch (WITS)	Machine Learning meets Theoretical Physics
PI: Prof Nico Orce (UWC)	Big Data Science applied to Nuclear Physics
PI: Prof WA Horowitz (UCT) **Co-PIs:** Prof Robert de Mello Koch (WITS), Prof Jeff Murugan (UCT), Prof Jonathan Schock (UCT), Prof Amanda Weltman (UCT) **Faculty and university partners:** Prof Azwinndini Muronga (NMU), Profs Amare Abebe and Christo Venter (NWU), Prof Stefan Ferreira (NWU/NASSP), Profs Makaiko Chithambo and Denis Pollney (RU), Prof Kevin Goldstein (WITS), Prof Alan Cornell (UJ), Dr Eric Maluta and Prof Joseph Kirui (Univen), Profs Nico Orce and Roy Maartens (UWC), Dr Betty Kibirige (Unizulu).	South African Theory School (SATS)

INTERNSHIP PROGRAMME

For the first time, the NITHeCP internship programme went online due to travel restrictions imposed by COVID-19. The programme hosted about 30 interns from universities across South Africa. The programme is aimed at building capacity in nuclear physics, particle physics and astrophysics.

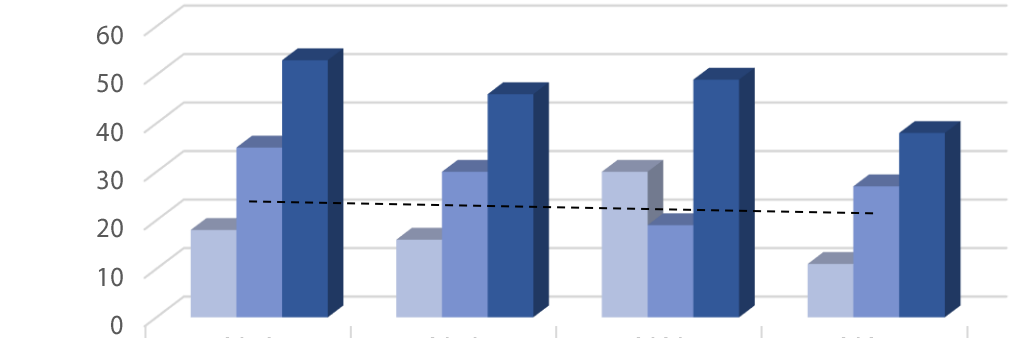
Seven tutors worked collaboratively with the groups of students. Based on their strengths and knowledge, as well as fields such as physics, mathematics and computer sciences, students were grouped into various topics, namely:

- Statistical and thermal models for heavy ion collisions and astrophysics
- Equation of state of neutron stars and gravitational waves from neutron star collisions
- Modelling particle production from heavy ion collisions
- Relativistic kinetic theory and the particle phase space analysis using Ultra-relativistic Quantum Molecular Dynamics (UrQMD)
- Landau hydrodynamics for high-energy nuclear collisions
- Bjorken hydrodynamics for high-energy nuclear collision
- Mathematical modelling of COVID-19 using South African data.

STUDENT AFFILIATION	GENDER	NUMBER
University of Western Cape	Female	2
University of Free State	Female	1
University of Venda	Female	5
University of Venda	Male	2
University of Witwatersrand	Male	4
University of Wits/Venda	Female	2
Northwest University	Male	1
Sol Plaatjie University	Male	1
University of Limpopo	Male	2
University of Limpopo	Female	1
University of Pretoria	Female	1
University of Zululand	Female	1
University of Zululand	Male	1
Nelson Mandela University	Female	2
Nelson Mandela University	Male	2
University of South Africa	Male	1
University of South Africa	Female	1
TOTAL		30

PUBLICATIONS

NUMBER OF PUBLICATIONS: 2018--2021



	2018	2019	2020	2021
Core	18	16	30	11
Associate	35	30	19	27
Total	53	46	49	38

Core Associate Total Linear core - - - - -

PUBLICATIONS 2021

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STATEMENT OF INCOME AND EXPENDITURE - NITheP

FOR THE PERIOD ENDING:	31/12/2021	31/12/2020
TOTAL INCOME	-17 372 526.83	-10 503 580.00
Income: NRF apportioned	-17 372 526.83	-10 503 580.00
TOTAL EXPENDITURE	10 743 060.93	5 047 912.33
CURRENT EXPENDITURE		
Advertisements: general	24 750.00	0.00
Bursary post graduate	3 661 300.00	2 600 739.73
Cell phone airtime	46 000.00	30 000.00
Computer materials	0.00	699.00
Consultation fees	48 160.38	0.00
Copy and printing	4 730.64	850.00
Foreign exchange loss	668.52	0.00
General office costs	481 006.00	0.00
Gifts	0.00	529.90
Graphic design	7 590.00	0.00
Internet network email levy	36 922.00	1 385.00
Marketing cost	231 309.76	28 205.00
Prizes and medals	3 500.00	4 000.00
Research publications	11 792.88	0.00
Research contract conduit payment	4 713 502.00	50 000.00
Services	1 060 289.28	361 020.46
Telephone: calls	266.83	7 147.24
Telephone: rent	15 335.04	13 776.52
Total remuneration	318 687.60	1 708 145.50
Travel: accommodation visum pa	0.00	193 141.80
Travel: daily allowance, air, car rental	0.00	48 272.18
Workshops	60 000.00	0.00
ASSET TRANSACTIONS		
Asset scrapping/transfers	0.00	-122 542.22
Depreciation	12 067.87	12 069.33
Income: internal assets	-12 067.87	110 472.89
Asset purchases	17 250.00	0.00
OPERATING (SURPLUS) / SHORTFALL FOR PERIOD	-6 629 465.90	-5 455 667.67
FUNDS TRANSFERS	224 172.00	0.00
Transfers from	224 172.00	0.00
NET (SURPLUS) / SHORTFALL FOR THE PERIOD	-6 405 293.90	-5 455 667.67
Plus: ACCUM (FUNDS) / SHORTFALL ON 01/01/2021	-10 148 554.23	-4 692 886.56
ACCUM (FUNDS) / SHORTFALL ON 31/12/2021	-16 553 848.13	-10 148 554.23
Min: BALANCE SHEET ITEMS	43 410.00	1 000.00
Debtors control account	50 000.00	0.00
Petty cash control account	1 000.00	1 000.00
Sundry creditors	-7 590.00	0.00
FUNDS AVAILABLE ON 31/12/2021	-16 510 438.13	-10 147 554.23

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