Annual Report

1 January–31 December 2020

CONTENTS

ABBREVIATIONS

AIMS	African Institute for Mathematical Sciences
APC LAB	AstroParticle and Cosmology Laboratory
CHPC	Centre for High Performance Computing
CNRS	National Center for Scientific Research
CoE -MaSS	Centre of Excellence in Mathematical and Statistical Sciences
CSIR	Council for Scientific and Industrial Research
DSI	South African 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
SU	Stellenbosch University
UCLA	University of California, Los Angeles
UCT	University of Cape Town
UJ	University of Johannesburg
UKZN	University of KwaZulu-Natal
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

DIRECTOR'S REPORT

2020 was a year like no other.

Prof Frikkie Scholtz's term as Director of NITheP ended in March 2020, and we would like to acknowledge his enormous contribution to the development of Theoretical Physics in the country. Thank you very much, Frikkie!

The interim management of NITheCS started its activities in April 2020, a week after the first lockdown to prevent the spreading of Covid-19 was announced. Our first task was to move all activities online.

We introduced a weekly online Colloquium series. The first online talk on 4 May 2020 was delivered by Prof Neil Turok (University of Edinburgh) and Prof Wilfred Ndifon (AIMS), who spoke about "A strategy for finding people infected with Covid-19: optimising the efficiency of pooled testing". The talk motivated a research collaboration, supported by DSI, between NITheCS, the Krisp unit of UKZN, and Profs Turok and Ndifon.

Every month we have organised online Mini-Schools. These are training events aimed at developing the theoretical and computational skills of our students. The Mini-School concept turned out to be very successful and enjoys a vast number of followers.

Colloquia and Mini-Schools were complemented by a series of webinars on more specialised topics, addressing a more specialised audience.

Only two physical events took place in 2020. The Fourth Mandelstam Theoretical Physics School and Workshop was held in Durban from 8–17 January, while the Chris Engelbrecht Summer School 2020 took place in early February.

Hosted by NITheCS in collaboration with the Centre for High Performance Computing (CHPC), the School was devoted to the Foundations of Theoretical and Computational Sciences. Around 60 students and a team of 5 speakers spent ten days in Saldanha Bay, learning about Econophysics, Quantum Computing, Computational Chemistry on quantum computers and Machine Learning.

We have relaunched the website, and we want it to become a portal to service the community of students and academics. The aim is to offer online teaching and training materials, resources of interest, tutorials and advanced courses on the website.

We started producing a monthly newsletter, showcasing our past and future events, profiling our Associates and sharing opportunities for students and faculty.

Our flagship Internship Programme was extended from weeks to months and moved online during December 2020. We provided the internship students with data access and also supported their attendance at the 2021 SAIP conference, where they presented the results of their research.

A virtual Associate meeting was held in October 2020. It was a welcome occasion for Associates to come together and share feedback on the positive developments for the future of NITheP and outlining how NITheCS was starting to take shape.

The Bursary Holders Workshop was held virtually as well. Some students presented excellent talks, and all students prepared short videos sharing the highlights of their research.

Every crisis bears opportunity. The communication tools of the fourth Industrial Revolution facilitate collaboration with local and global partners and allow us to share information, education and training with students studying from home. We should use them to accelerate much needed societal changes and innovation.

Looking forward to the transition from NITheP to NITheCS, we are ready to serve a wider community and make a more significant impact in a world where the interdisciplinary nature of science has become its strength.

Francesco Petruccione

STAFF PROFILE

The staff profile of NITheP as on 31 December 2020 is shown below:

POSITION	INSTITUTION	CONTRACTS
Interim Director	UKZN	1 (Contract end 31 March 2021)
Deputy Directors	WITS/SU	2 (3-year contracts, renewed during 2020)
Chief Researcher	SU	1 (Contract ended 31 December 2020)
Researchers	SU/WITS/UKZN	0
Administrative	SU WITS UKZN	1 (Contract ends 31 March 2021, 5/8 position) 1 (Contract end 31 December 2022, 4/8 position) 1 (Contract ends 31 March 2021)

POSTDOCTORAL FELLOWS

The postdoctoral fellows per node as on 31 December 2020 are shown below. All positions comprise two-year contracts.

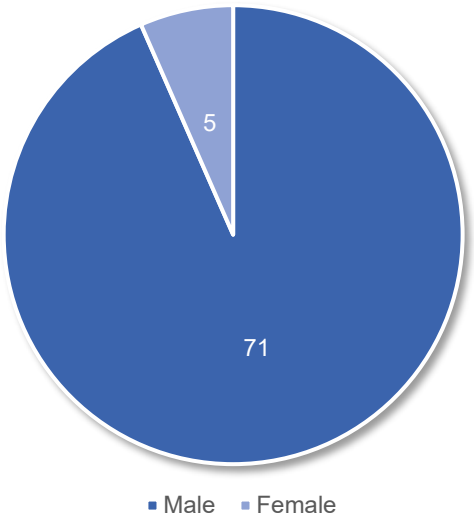
NODE	NITheP FUNDED	EXTERNALLY FUNDED
SU	1 (until April 2020)	0
UKZN	3	3
WITS	3	5
TOTAL	**7**	**7**

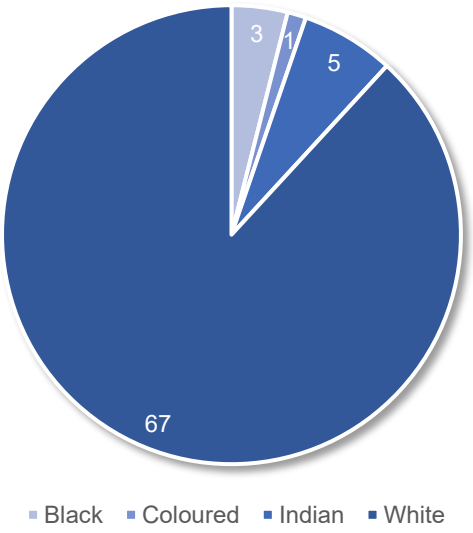
ASSOCIATES

To achieve NITheP's strategic goals, it is crucial to maintain a national network of associates throughout South Africa. On 31 December 2020, our Associates network comprised the following:

Individual Associates	76
Strategic	6
Institutional	4
Junior Associates	3
TOTAL	89

STATUS OF ASSOCIATES



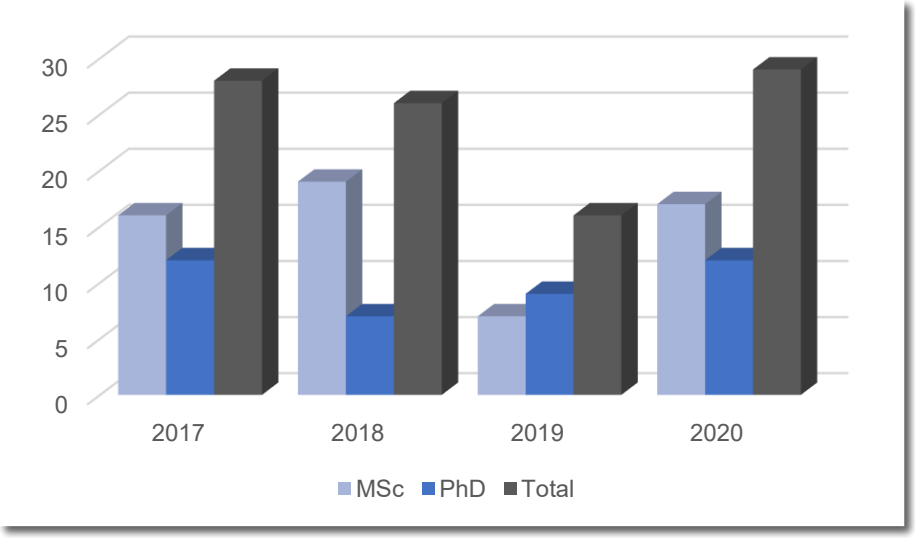


BURSARIES

BURSARIES GRANTED

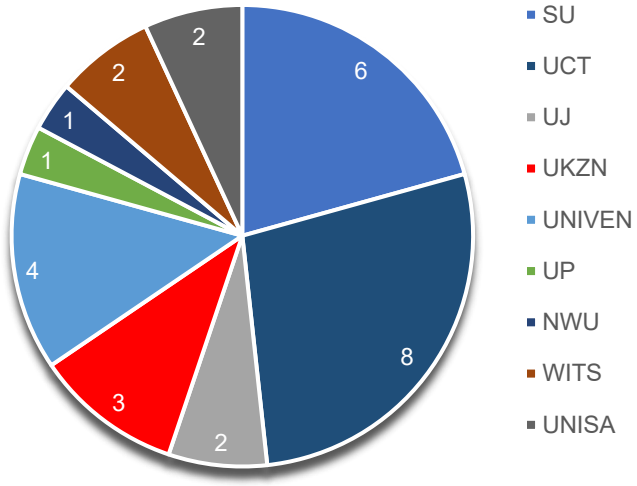
LEVEL	NUMBER OF BURSARIES	BURSARY VALUE	TOTAL
MSc	17	R80 000	R1 360 000
PhD	12	R100 000	R1 200 000
TOTAL	29		R2 560 000

BURSARY TRENDS: 2017 TO 2020



DISTRIBUTION OF BURSARY HOLDERS

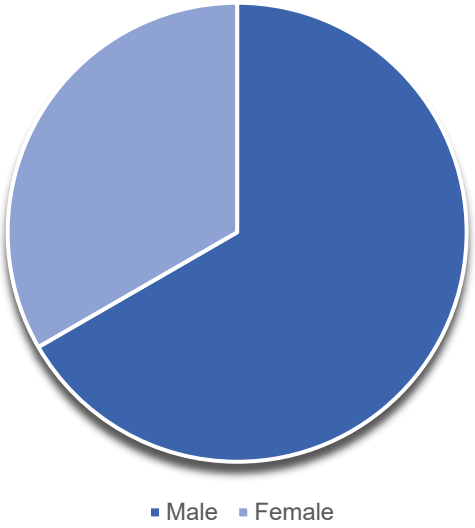
INSTITUTION	MSc	PhD	TOTAL
SU	6	0	6
UCT	6	2	8
UJ	1	1	2
UKZN	0	3	3
UNIVEN	3	1	4
UP	1	0	1
NWU	0	1	1
WITS	0	2	2
UNISA	0	2	2
TOTAL	17	12	29

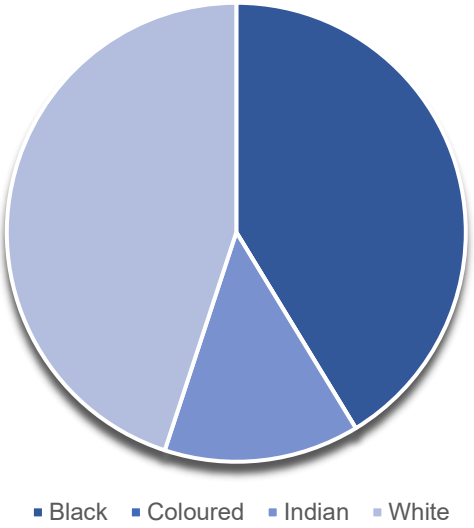


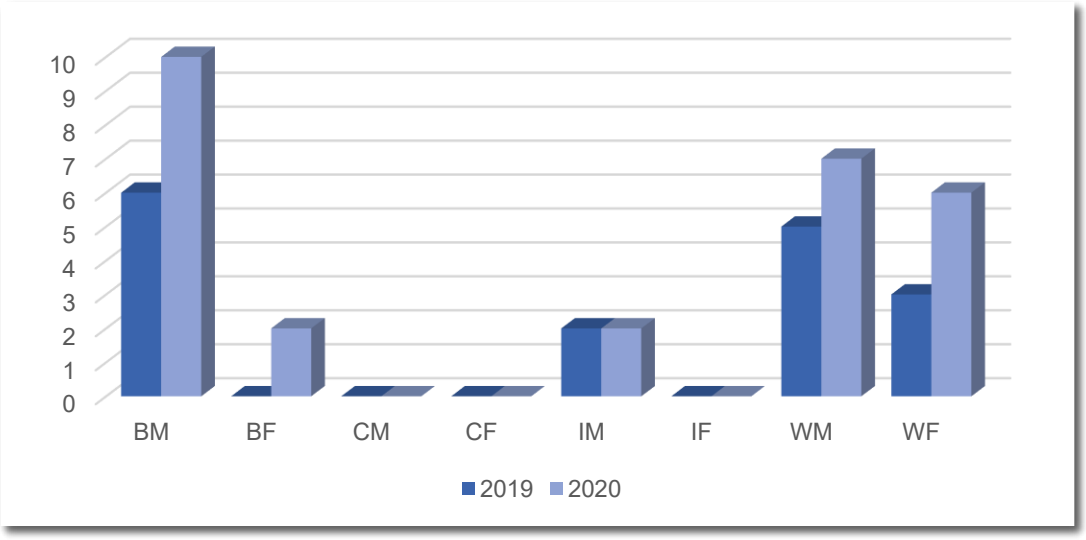
DEMOGRAPHICS OF BURSARY HOLDERS

DEGREE	BLACK		COLOURED		INDIAN		WHITE		TOTAL
	MALE	FEMALE	MALE	FEMALE	MALE	FEMALE	MALE	FEMALE	
MSc	4	2	0	0	0	0	6	5	17
PhD	6	0	0	0	2	2	1	1	12
TOTAL	10	2	0	0	2	2	7	6	29

DETAILED DEMOGRAPHICS







TEACHING HOURS

NODE	NUMBER OF HOURS	
	CORE	POSTDOCS
SU	310	0
WITS	83	0
UKZN	48	48
TOTAL	**441**	**48**

ACTIVITIES

TYPE OF ACTIVITY	NUMBER OF ACTIVITIES	ATTENDEES	YOUTUBE VIEWS
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	5	1 131	5 847
Online webinars	10	294	948
Online colloquia	27	1 365	2 476
TOTAL	**42**	**2 790**	**9 271**

ONLINE MINI-SCHOOLS

DATE	NAME OF SPEAKER	TOPIC	ONLINE ATTENDEES	YOUTUBE VIEWS
July	Dr Daniel Parks (KAIST)	Quantum Computing	262	624
August	Dr Sahal Yacoob (UCT)	Introduction to Elementary Particle Physics	213	280
September	Amira Abbas (UKZN)	Basic programming for quantum machine learning	505	3 840
October	Dr Dario Rosa (KAIST)	Introduction to classical and quantum chaos	78	464
November	Dr Graeme Pleasance (UKZN)	Introduction to open quantum systems	73	639
TOTAL			**1 131**	**5 847**
GRAND TOTAL				**6 978**

ONLINE WEBINARS

DATE	SPEAKER	AFFILIATION	TOPIC	ONLINE ATTEND-EES	YOU-TUBE VIEWS
9 Apr	Clarice Aiello	UCLA	From Nanotech to Living Sensors	50	117
23 Apr	Christopher Rourk	James Walker, Dallas	Electron Transport in Catecholaminergic Neuron Groups	12	261
28 May	Prof Dariusz Chruscinski	Nicolaus Copernicus University	Universal spectra of random Lindblad operators	34	53
12 Jun	Mark Fingerhuth	ProteinQure Inc	Quantum open source software development	37	62
18 Jun	Prof Hugo Touchette	SU	Classical and quantum processes with random reset	49	100
23 Jul	Dr Garry Kemp	UJ	Lazy Open Quantum Walks	16	53
27 Aug	Dr Nina Megier	University of Milan	Local and non-local master equations	29	45
1 Oct	Revanth Reddy	InfoWorks Data	Compressed Sensing Quantum State Topography: Qubits to Qudits	20	45
19 Nov	Dr Sanjaye Rangoolam	Queen Mary University of London	Kronecker coefficients and Lattices of bipartite ribbon graphs	24	175
17 Dec	Dr Alexander Teretenkov	Steklov Mathematical Institute of Russian Academy of Sciences	Markovian approximation of non-Markovian dynamics in all orders of perturbation theory	12	37
TOTAL				294	948

ONLINE COLLOQUIA

DATE	SPEAKER	AFFILIATION	TOPIC	ONLINE ATTEND-EES	YOU-TUBE VIEWS
4 May	Neil Turok & Wilfred Ndifon	Perimeter/AIMS	A strategy for finding people infected with COVID-19: optimising the efficiency of pooled testing	245	336
25 May	Bruce Bassett	UCT	How hard will COVID-19 hit South Africa? A story in three parts.	122	151
15 Jun	Azwinndini Muronga	NMU	Diversity, Equity, and Inclusion in Science	77	81
9 Jul	Kavan Modi	Monash University	Reduction in neural complexity and temporal asymmetry due to application of general anaesthesia	11	47
20 Jul	Robert de Mello Koch	WITS	Is Deep Learning an RG Flow?	86	90
27 Jul	Freedom Gumedze	UCT	Network meta-analysis with random inconsistency effects and outliers	26	27
3 Aug	Kanshu Rajaratnam	SU	Consumer Lending Models	50	50
17 Aug	Artur Ekert	NUS/Oxford	Privacy for the paranoid ones - the ultimate limits of secrecy	59	52
24 Aug	Amanda Weltman	UCT	Fundamental Physics in the Radio Sky	69	44
31 Aug	Michael Kastner	SU	Equilibration timescales of isolated quantum systems	44	40
7 Sep	Maalik Maaza	iThemba LABS	On the tunnelling of wave-matter neutron wavepackets, neutron trapping & Neutron life-time	56	52
14 Sep	Jianshu Cao	MIT	Stochastic Formalism and Simulation of Quantum Dissipative Dynamics	28	71
21 Sep	Jeff Murugan	UCT	Scrambling in Quantum Networks	37	85
28 Sep	Matthias Troyer	Microsoft	A Quantum Future of Computation	85	148
5 Oct	Filip Wudarski	NASA, QuAIL	Quantum computing activities at Quantum Artificial Intelligence Laboratory (QuAIL)	31	79
12 Oct	Ashleigh Hutchinson	WITS, CoE MaSS	Navigating turbulent waters	26	42
19 Oct	Betony Adams	UKZN	Quantum effects in the brain: How much do we know?	51	385
26 Oct	Cora Dvorkin	Harvard	Unveiling the Nature of Dark Matter with Cosmological Observables	36	144

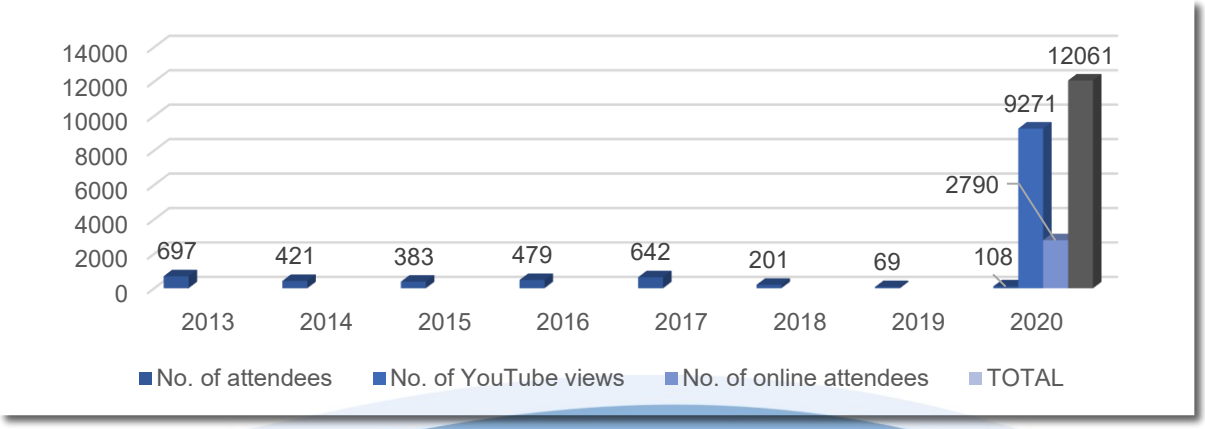
2 Nov	Sir Peter Knight	Imperial College	Creating the UK National Quantum Technology programme	51	85
9 Nov	Camille Lombard Latune	UKZN	An introduction to Quantum Thermodynamics	25	40
16 Nov	Dr Sanjaye Rangoolam	Queen Mary University of London	Quantum Mechanics in Combinatoric algebras, tensor models and Kronecker coefficients	24	236
30 Nov	Dr Stephan Woerner	IBM Research	Towards Quantum Advance in the Financial Service Sector	86	73
08 Dec	Prof Gershon Kurizki	Weizmann Institute of Science, Israel	The Observer and the World: Does Science describe the Universe?	26	52
14 Dec	Dr Mawande Lushozi	University of Washington	Evolution of the fragmentation region in ultrarelativistic heavy ion collisions	25	66
TOTAL				1 365	2 476

EXPOSURE

TOTAL VIEWS: ONLINE PROGRAMMES

PROGRAMME	NUMBER OF ATTENDEES	NUMBER OF YOUTUBE VIEWS	TOTAL
Mini-Schools	1 131	5 847	6 978
Webinars	294	948	1 242
Colloquia	1 365	2 476	3 841
TOTAL	2 790	9 271	12 061

TOTAL ATTENDEES DURING PREVIOUS WORKSHOPS



2020/2021 RESEARCH PROGRAMMES

The Research Programmes launched in 2020/2021 span the network of NITheP Associates and involve South African universities as well as several international collaboration partners.

RESEARCH PROGRAMMES AND PIs:

Computational Studies of Optoelectronic Properties and Material Engineering of Photoactive Layer in Perovskite Solar Cells

PIs: Dr NE Maluta (UNIVEN) in collaboration with Prof RR Maphanga (CSIR) and Dr E. Maphasha (UP)

Theoretical and Computational Astrophysics Foundations for HIRAX Big Data

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 Modelling for Genomic Contact Tracing

Proposers: Prof Martin Bucher (PI) (UKZN/CNRS/APC), Prof Bruce Bassett, (AIMS), Prof Steven Gratton (Princeton), Sinoxolo Nene (UKZN), Prof Tulio de Oliviera (KRISP/UKZN) and Prof Ilya Sinayskiy (UKZN)

Machine Learning meets Theoretical Physics

PIs: Prof Vishnu Jejjala (WITS), Prof Jonathan Shock (UCT), Dr Pallab Basu (WITS), Prof Robert de Mello Koch (WITS)

Big Data Science applied to Nuclear Physics

PI: Prof Nico Orce (UWC)

South African Theory School (SATS)

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)

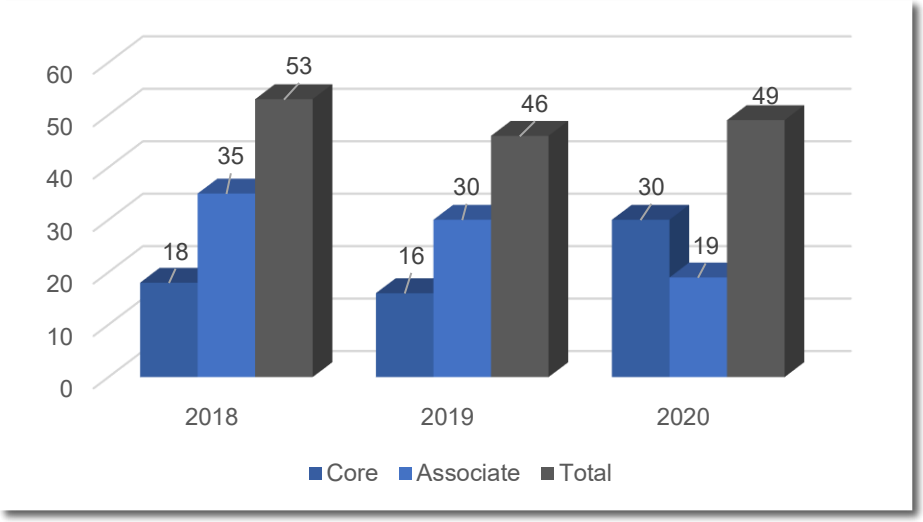
Faculty and university partners: Prof Azwinndini Muronga (NMU), Profs Amare Abebe and Christo Venter (NWU), Prof Stefan Ferreira (NWU/NASSP), Profs Makaiko Chithambo and Denis Pollney (RU), Prof Kevin Goldstein (WITS), Prof Alan Cornell (UJ), Dr Eric Maluta and Prof Joseph Kirui (Univen), Profs Nico Orce and Roy Maartens (UWC), Dr Betty Kibirige (Unizulu).

PUBLICATIONS

SOURCE

	NUMBER OF PUBLICATIONS
Core staff	30
Associates	19
TOTAL	49

NUMBER OF PUBLICATIONS: 2018 - 2020



WORKSHOPS

VIRTUAL ASSOCIATE WORKSHOP

The associate workshop was held for the first time in a virtual setting on 19 November 2020. Going forward, associate meetings are likely to be a blended format of physical and virtual.

For 2021, there are plans to hold one meeting in the first half of the year and another in the second half.

In future, we also plan to add a virtual cocktail event after the meeting, so associates can interact with one another – possibly on a platform such as "Run The World".

The current NITheP Associate Representative is Prof Will Horowitz.

Prof Will Horowitz

VIRTUAL BURSARY HOLDERS WORKSHOP 2020

The bursary holders' workshop was held on 10 December 2020. All students submitted a short presentation and a few were selected to deliver their talks live. These students are:

- Ian Pittaway (SU) – "A Review of the Measurement Problem in Quantum Mechanics" https://bit.ly/37dUPFA
- Anna Chrysostomou (UJ) – "On the computation of black hole quasinormal modes: a study of half-integer perturbations in asymptotic limits" https://bit.ly/37c5ssN
- Celeste Johnson (WITS) – "A bilocal description of the conformal algebra at the critical point in 3 dimension" https://bit.ly/37bIWjI
- Sipho Lukhozi (UJ) – "A survey of N-body and Hydrodynamic Simulations in Higher Spin f(R) gravity" https://bit.ly/3jiN5If

INTERNSHIPS

VIRTUAL INTERNSHIP PROGRAMME

Two students were hosted by Professors Petruccione and Sinayskiy (UKZN). A further 30 students were hosted by Prof Muronga, (NMU) along with seven tutors.

The students were grouped based on their strengths, knowledge and fields such as physics, mathematics and computer sciences.

The following topics were covered:

- 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 UrQMD
- Landau Hydrodynamics for high-energy nuclear collisions
- Bjorken Hydrodynamics for high-energy nuclear collision
- Mathematical modelling of COVID-19 using South African data
- Quantum computing.

BURSARY HOLDERS' HIGHLIGHTS

AMIRA ABBAS

Amira is a predoc researcher and a member of the IBM Quantum Computing Research team in Zurich and the IBM Quantum Education team in South Africa.

Her current research focuses on the intersection of quantum mechanics and machine learning theory to solve problems that are not possible to compute classically. Recently, she co-authored a paper that demonstrates the potential of quantum machine learning models.

Amira holds an undergraduate degree in actuarial science, an honours degree in quantitative finance and a master's degree in physics. She is Africa's first recipient of Google's PhD Fellowship for quantum computing.

She is an active member of numerous community-driven initiatives that are centered around strengthening science and technology in Africa. Furthermore, she is frequently invited to conferences and events to discuss her work on quantum machine learning.

BETONY ADAMS

Betony published a review paper with Prof Petruccione, covering current developments in quantum neurobiology. This included proposed quantum mechanisms related to anaesthetic action, neurotransmitter reception, the effects of electromagnetic radiation on the brain as well as entangled neural activation.

The paper brought about some interest and opportunities to collaborate, including with UCLA QuBiT Lab to test the hypothesis that entangled Posner molecules influence neural activation.

A cover article was also published in *Physics World* magazine, and Betony discussed the ideas on the *Physics World* podcast. She was also invited to deliver presentations for Neural Engineering Research Venture (NERV), the NITheP Colloquium lecture series and the Space4Women Show.

BURSARY HOLDERS' REFLECTIONS ON 2020

CLARENCE VUSI MABASO, MSC STUDENT, UNIVEN

"Different events in my life have directed me toward this path. Wanting to be a better person, I took it upon myself to become an academic.

To engage in a scientific research project without funding had me under pressure. However, NITheP become my 'Thanos' by wiping away my financial problems.

Personally, 2020 was an achievement! Working under the COVID-19 regulations had everyone on tiptoes, trying to adapt to a new normality.

Working at home with not enough resources and struggling to keep contact with my promoter were some of the challenges. However, the greatest highlight was that I had all day, every day to prevail a working strategy toward progress. Communication and support from NITheP kept me motivated and I remained consistent."

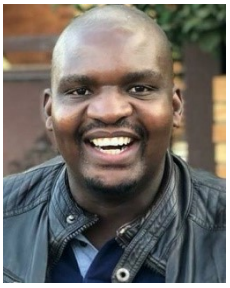
THABANG DOREEN LEBESE, PHD STUDENT, WITS

"The year 2020 was the hardest year for me, as a lot happened. Due to Covid-19, the national lockdown and not receiving my bursary money from NITheP, I was unable to pay my landlord for rent. As a result, I was evicted from my accommodation near the university. I returned to my home in Limpopo, leaving all my belongings in storage as an assurance that I would return and pay the outstanding rent.

I then could not attend weekly meetings with my supervisors due to poor internet signal and not having money for data.

I usually worked at night, from midnight to 5h00, and managed to write a paper, which is 95% complete."

KAGISO MPSHE, PHD STUDENT, UNISA



"My research employs Computational Fluid Dynamics to study aerodynamic shape design, focusing on wind turbine blades.

The previous year was the most challenging in my academic calendar. Covid-19 restrictions, limited resources and conditions in my township, such as continued power cuts due to some illegal connections, affected me negatively. The support and counsel I received from my supervisor helped me to remain focused.

Although I could not achieve all my desired targets, I am motivated by the fact that there was some progress in my work. As Covid-19 restrictions were relaxed towards the end of the year and the bursary funds became available, life became much better. I am thankful to NITheP for the bursary and assistance."

FURTHER ACTIVITIES: 2020/21

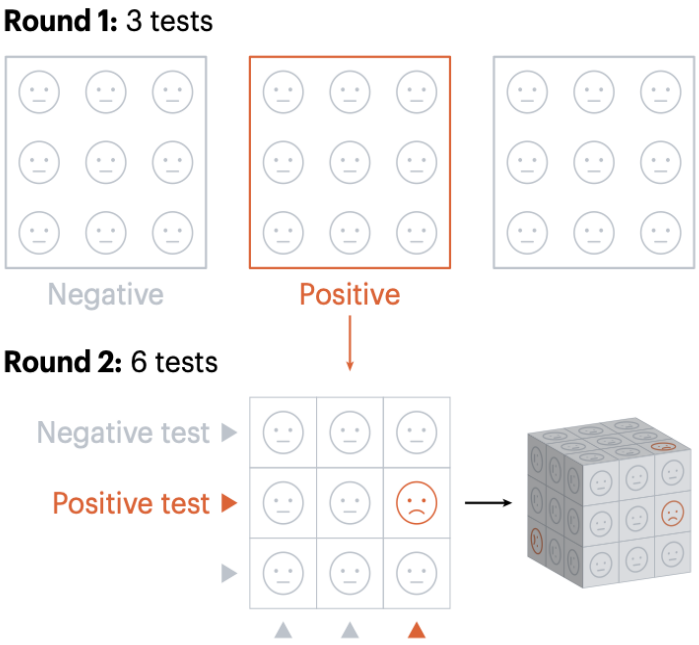
NITheP Workshop:
"Quantum Thermodynamics"
23 – 27 November 2020
Durban

South African Science Forum 2020:
"National Big Data Hubs and the Strategic Role of International Collaboration"
Italian Embassy, DSI, NITheP, IFAB Int. Foundation for Big Data and Artificial Intelligence for Human Development
December 2020

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

RESEARCH GRANTS

Massive screening for Covid-19 using pooled testing
(DSI, R2Mio)



STATEMENT OF INCOME AND EXPENDITURE

FOR THE PERIOD ENDING:	30/07/2021	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	5 884 810.00	5 047 912.33
CURRENT EXPENDITURE		
Advertisements: general	15 000.00	0.00
Bursary postgraduate	1 641 300.00	2 600 739.73
Cell phone airtime	46 000.00	30 000.00
Computer materials	0.00	699.00
Copy and printing	0.00	850.00
Foreign exchange loss	668.52	0.00
General office costs	481 006.00	0.00
Gifts	0.00	529.90
Internet network email levy	16 922.00	1 385.00
Marketing costs	2 660.00	28 205.00
Prizes and medals	3 500.00	4 000.00
Research publications	21 699.27	0.00
Research contract conduit payment	3 171 000.00	50 000.00
Services	312 385.59	361 020.46
Telephone: calls	237.21	7 147.24
Telephone: rent	6 626.25	13 776.52
Total remuneration	165 805.16	1 708 145.50
Travel: accommodation	0.00	193 141.80
Travel: daily allowance, air, car rental	0.00	48 272.18
ASSET TRANSACTIONS		
Asset scrapping/transfers	0.00	-122 542.22
Depreciation	5 968.72	12 069.33
Income: internal assets	-5 968.72	110 472.89
OPERATING (SURPLUS) / SHORTFALL FOR PERIOD	-11 487 716.83	-5 455 667.67
FUNDS TRANSFERS	224 172.00	0.00
Transfers from	224 172.00	0.00
NET (SURPLUS) / SHORTFALL FOR THE PERIOD	-11 263 544.83	-5 455 667.67
PLUS: ACCUM (FUNDS) / SHORTFALL ON 01/01/2021	-10 148 554.23	-4 692 886.56
ACCUM (FUNDS) / SHORTFALL ON 30/07/2021	-21 412 099.06	-10 148 554.23
MINUS: BALANCE SHEET ITEMS	1 000.00	1 000.00
Petty cash control account	1 000.00	1 000.00
FUNDS AVAILABLE ON 30/07/2021	-21 411 099.06	-10 147 554.23

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