

A scientific microscope is shown in a dark, blue-toned environment. In the center of the microscope's field of view, a glowing, stylized atomic model is visible, with a central nucleus and orbiting electrons. The background is a dark, pixelated grid pattern. A large, semi-transparent number '2024' is overlaid on the left side of the image.

# 2024

Year in Review

**NITheCS**

National Institute for  
Theoretical and Computational Sciences

“Education is the foundation of the science, technology, and innovation-based economy Africa needs in the decades ahead.”

– UN Secretary-General António Guterres

**2024: A Year in Review**

National Institute for Theoretical and Computational Sciences (NITheCS)

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# DIRECTOR'S Report

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This year was pivotal for NITheCS. Following the approval of our hosting application by Stellenbosch University (SU) and its partners, NITheCS was officially launched in April 2024. My appointment as Director followed in May, and we signed our global Consortium Agreement on 13 November.

The Consortium now includes 26 South African universities and the African Institute for Mathematical Sciences (AIMS). With its central hub located at Stellenbosch University, NITheCS operates through five coordinating regional nodes; North West, Gauteng, KwaZulu-Natal, Eastern Cape and Free State, and Western Cape.

Within the new structure, NITheCS continues to foster interdisciplinary collaboration to advance fundamental understanding and technological innovation. Our 300+ PhD-holding Individual Associates can conduct research in any of the Institute's eight key fields: astronomy and astrophysics, bioinformatics and quantitative biology, data science, earth systems and climate change

modelling, mathematics, quantitative finance, statistics, and theoretical physics.

In November we introduced our proposed research focus areas to Associates, whose valuable feedback has helped refine our plans for inclusion in the NITheCS 2025 business plan.

This report highlights our activities and achievements throughout the year, including major collaborations. Notably, 2024 marked the 60th anniversary of the International Centre for Theoretical Physics (ICTP), with which NITheCS has a collaboration agreement for joint research and education. I was invited to attend the international celebration in November.

Additionally, I was also invited to speak at the launch of the South African Centre for Digital Language Resources (SADiLaR), which creates and manages digital language resources for South Africa's official languages, and whose mission aligns with ours.

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## Looking Ahead

NITheCS continues to focus on strategic growth, operational excellence, and expanded collaboration. We aim to finalise university Consortium Agreements and relocate to our new offices in SU's Merensky Building. Strengthening our digital infrastructure and increasing our visibility remain key priorities.

In 2025, we will celebrate the International Year of Quantum Science and Technology (IYQ) with dedicated events. I will have the honour of attending its opening at the UNESCO Headquarters in Paris, marking a global push for quantum science advancements.

## Acknowledgments

A heartfelt thank you to our Associates, interim node leaders and branch heads, contributors, and mentors for their

dedication. Their involvement in our events, student mentorship, and outreach is invaluable. We also deeply appreciate the support of the Department of Science, Technology and Innovation (DSTI), National Research Foundation (NRF), and our Executive Committee.

A special thanks to our administrative team for their efforts in ensuring NITheCS continues to support groundbreaking science.

As we move into 2025, our mission remains clear: to support and advance humanity's fundamental understanding of the universe. By empowering local scientists and researchers today, we lay the foundation for tomorrow's innovations.

  
**Francesco Petruccione**  
Director

# INTRODUCTION to NITheCS

## About Us

The National Institute for Theoretical and Computational Sciences (**NITheCS**) is part of the South African science, technology and innovation landscape. The Institute is supported by the Department of Science, Technology and Innovation (DSTI), and National Research Foundation (NRF).

NITheCS operates in an independent environment, with Stellenbosch University providing administrative support. This is critical in the South African (and African) context to ensure non-alliance with a particular institution, and to maintain an independent identity.

Collaboration is central to NITheCS's success. Operating as a consortium, the Institute has contractual agreements with all public universities in South Africa, as well as the African Institute for Mathematical Sciences (AIMS South Africa).

The Institute's central **hub**, located at Stellenbosch University, handles administration, hosting, research and capacity development. During 2024, NITheCS began work to construct dedicated office space on the Stellenbosch University campus, which will be completed in 2025.

NITheCS has 26 **branches** at all public universities and affiliated research institutions in South Africa. These branches are grouped into five regional **nodes** to enhance coordination and regional relevance. The nodes, each headed by a designated university, ensures that NITheCS is locally active while remaining nationally integrated.

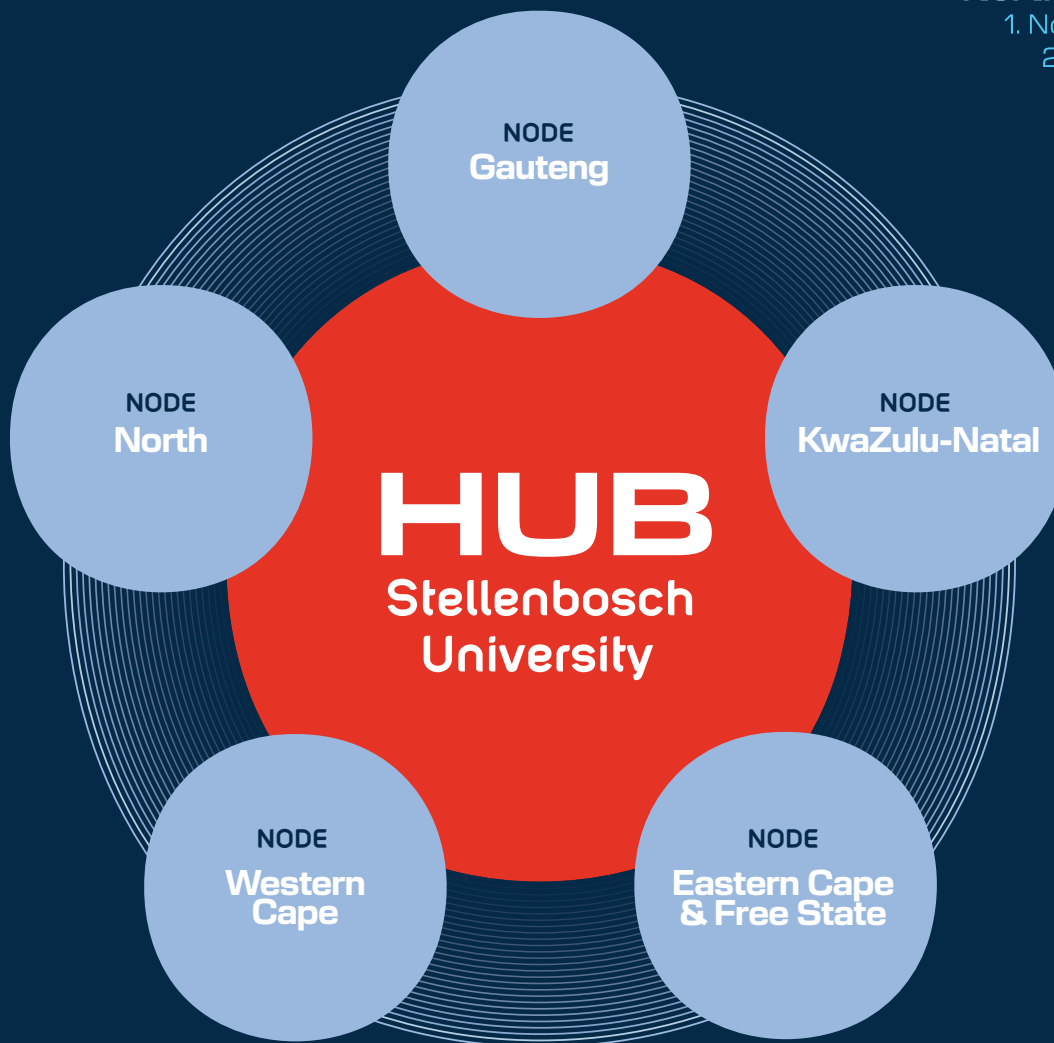
The Heads of Nodes work closely with the Director, Prof Francesco Petruccione, to ensure that each node contributes meaningfully to NITheCS's strategic vision. Under each Head of Node, Branch Heads

## Branch Heads: Tasks

- Facilitate NITheCS programmes and events in their regions.
- Engage local research communities.
- Promote collaboration aligned with NITheCS's national goals.
- Contribute to multidisciplinary research, training, and public engagement.

manage the activities of their respective institutions (*see above*).

Beyond its local partnerships, NITheCS collaborates globally with strategic partners – such as the International Centre for Theoretical Physics (ICTP) and the Africa-Europe Cluster of Research Excellence (CoRE-AI). This provides a global perspective on theoretical and computational sciences.



**North**

1. North-West University
2. University of Limpopo
3. University of Venda
4. University of Mpumalanga
5. Sol Plaatje University

**Gauteng**

1. University of the Witwatersrand
2. University of Johannesburg
3. Tshwane University of Technology
4. University of Pretoria
5. University of South Africa
6. Sefako Makgatho Health Science University
7. Vaal University of Technology

**KwaZulu-Natal**

1. University of KwaZulu-Natal
2. Durban University of Technology
3. Mangosuthu University of Technology
4. University of Zululand

**Eastern Cape & Free State**

1. Nelson Mandela University
2. University of the Free State
3. Rhodes University
4. Central University of Technology
5. University of Fort Hare
6. Walter Sisulu University

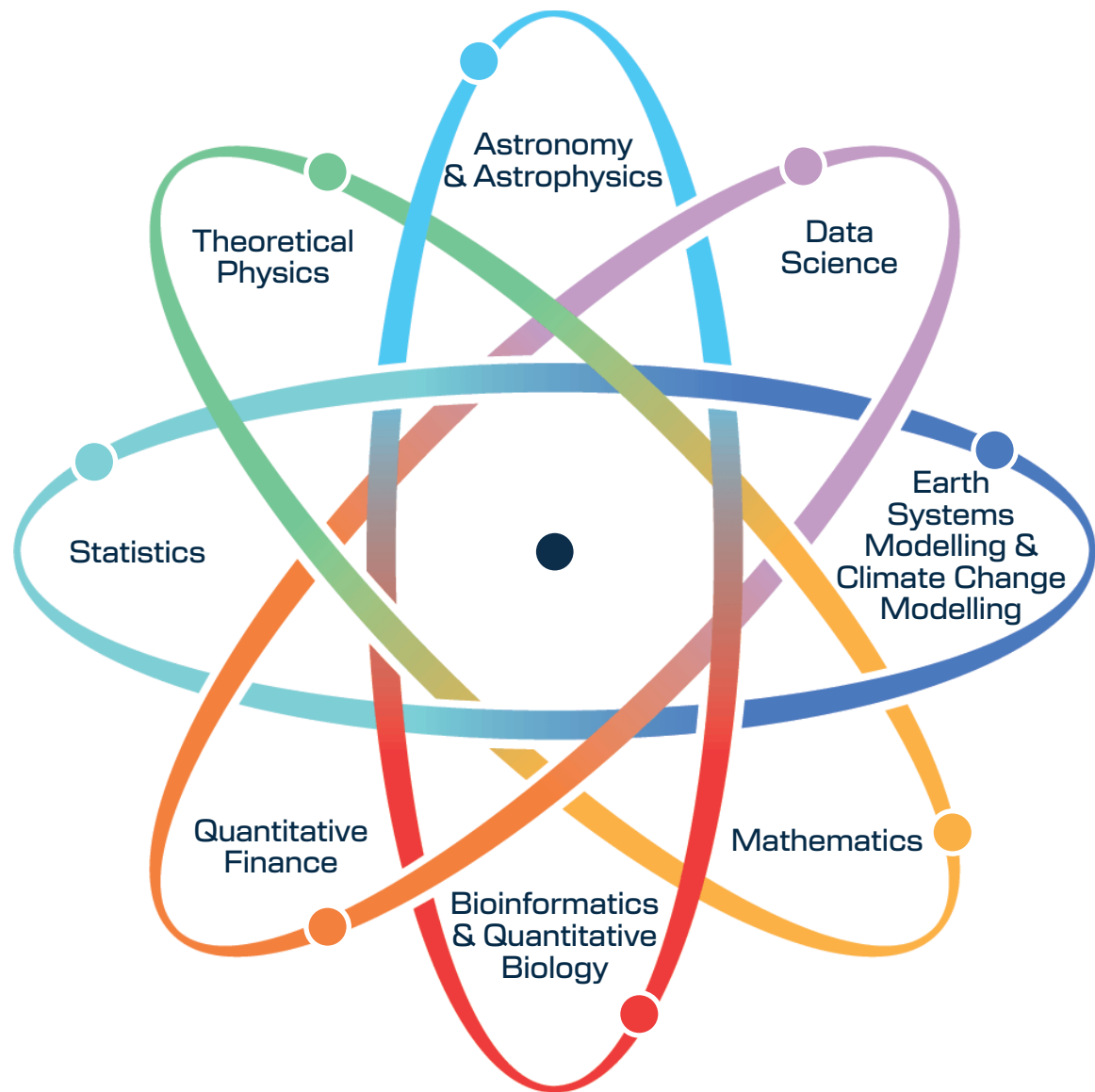
**Western Cape**

1. University of Cape Town
2. African Institute for Mathematics Sciences (AIMS)
3. Cape Peninsula University of Technology
4. University of the Western Cape

## Focus Areas and Activities

NITheCS supports a range of focus areas, which reflect our commitment to advancing research and collaboration in the theoretical and computational sciences. The Institute's activities are specific to **eight thematic areas** (see figure, right) in which basic science is fostered, and its emphasis is on moving science from research to impact.

These thematic areas unite researchers, students, and institutions working on shared challenges – from fundamental physics and cosmology to data science, mathematics, and interdisciplinary applications. Through workshops, seminars, and collaborative initiatives, knowledge exchange and innovation to drive research impact in South Africa and beyond takes place.



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

Some of the activities through which NITheCS conducts its work include regular colloquiums, mini-schools, micro-schools, internships, summer schools, workshops, public lectures, other presentations, and networking opportunities.

Apart from this, NITheCS also encourages visits from local and international scientists, supports bursary holders, facilitates research opportunities, and drives community service.

## The Key Strategic Objectives of NITheCS

- Achieve equitable participation of all South African communities in its activities.
- Support the pipeline of students – from undergraduate through to postgraduate and postdoctoral research – and their early career development.
- Support major science programmes.
- Help strengthen basic scientific endeavours in the country.
- Support historically disadvantaged institutions (HDIs).
- Address socio-economic development through training and research.

# Associates

NITheCS greatly values the contributions of its national network of Associates, who play a crucial role in advancing the Institute’s strategic goals and achieving our vision. The continued growth and strength of this network supports the Institute’s aim to maintain strong international links and cooperation with relevant global partners, while ensuring it remains comparable with its counterparts across the world. Individuals as well as institutions that are engaged in a theoretical, computational, or interdisciplinary field aligned with the NITheCS themes can join us as our Associates.

## Individual Associates

Individual Associates of NITheCS are distinguished professionals who hold a PhD in a theoretical or computational field of science, or in an interdisciplinary field that falls within the eight NITheCS themes.

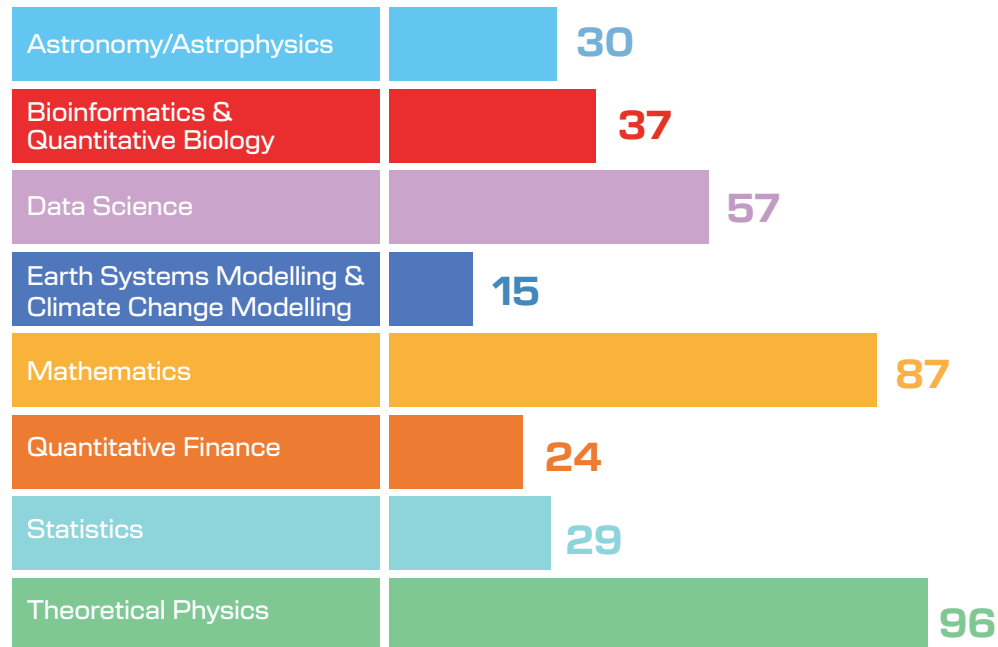
These individuals are affiliated with South African universities or corporate institutions, bringing a rich blend of academic rigor and research expertise to the NITheCS community.

Individual Associates play a crucial role in fostering a culture of excellence, innovation, and collaboration within NITheCS. Their specialised knowledge in diverse fields contributes to the interdisciplinary nature of NITheCS, enriching discussions, driving research initiatives, and mentoring the next generation of scientists and innovators.

By engaging with peers, sharing insights, and participating in collaborative research

projects, Individual Associates strengthen our capacity to address complex scientific challenges, develop solutions, and contribute to the advancement of science and technology in South Africa and beyond.

Currently NITheCS has a total number of **309 Individual Associates**. Illustrated below are the number of associates per thematic field.



## Emerging Associates

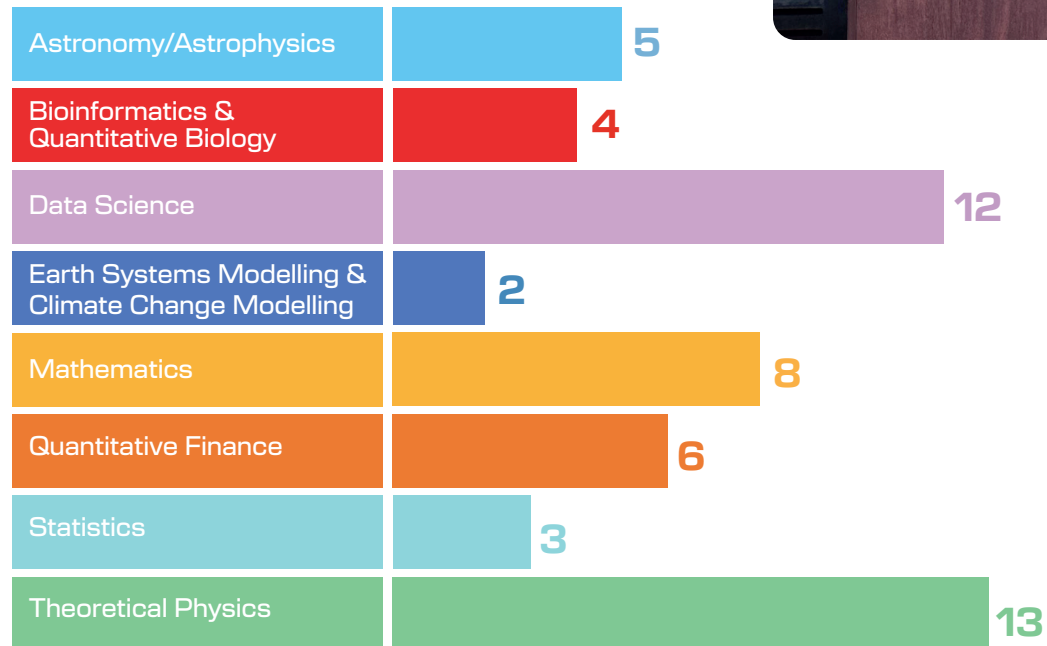
Emerging Associates at NITheCS represent the emerging talent and future leaders in the fields of science and technology. They are either staff members at South African universities enrolled in a PhD programme or South African Postdocs engaged in advanced research at these institutions.

Specialising in theoretical, computational, or interdisciplinary fields of science within the eight NITheCS themes, Emerging Associates bring fresh perspectives, enthusiasm, and a strong commitment to academic excellence and innovation. Despite being in the early stages of their careers, they demonstrate a high level of expertise and dedication to their respective fields. As Emerging Associates, they benefit from networking opportunities provided by NITheCS, which supports their professional growth and development.

Their active involvement in research projects, collaborations, and knowledge-sharing initiatives contributes to the dynamic and vibrant learning environment of NITheCS. By recognising and supporting

young talent, NITheCS encourages a continuous pipeline of skilled professionals who will contribute to the advancement of the theoretical and computational sciences in South Africa and beyond.

Currently NITheCS has a total number of **48 Emerging Associates**. Illustrated below are the number of associates per thematic field.

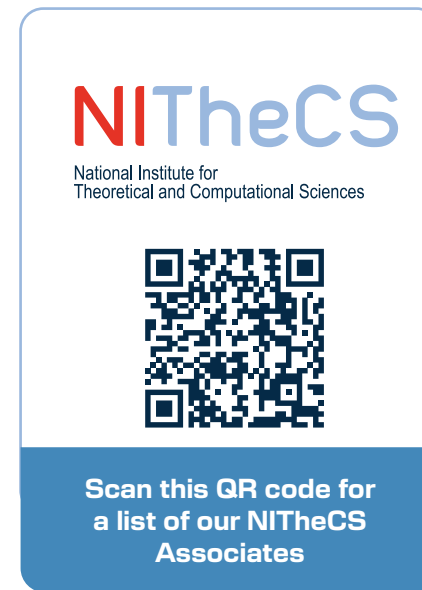
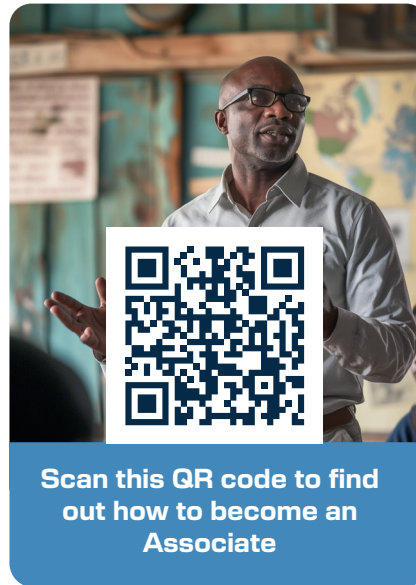


## Benefits of Becoming a NITheCS Associate

Affiliation with NITheCS offers numerous professional advantages, including:

- **Opportunities to Present:** Associates are invited to give talks at NITheCS events, including colloquia and mini-schools.
- **Research Collaboration:** Associates are encouraged to join our Research Programmes, which encourage collaboration between researchers across institutions.
- **Networking and Engagement:** Associates can participate in conferences, workshops, mobility programmes, visitor programmes, and student internships under their leadership.
- **International Connections:** The Institute's strong global links provide opportunities for collaboration with leading researchers worldwide.

Many Associates form long-term research partnerships through connections made at NITheCS events, strengthening both national and international scientific cooperation.





**“Our planet has got problems. We are climbing steep jagged curves of unanticipated hazards, and that’s what basic sciences are for: wading into ‘inconceivable’ territory with eye-opening practical results. The NITheCS space is designed for us to put our brains together and think, while it’s still legal.”**

– Prof Igle Gledhill  
University of the Witwatersrand

# TRAINING:

## Building the Next Generation of Researchers

At NITheCS, training is a cornerstone of our mission to develop a new generation of skilled researchers in theoretical and computational sciences. We are committed to equipping students with the knowledge, skills, and opportunities necessary to excel in academia, industry, and research institutions.

Our training initiatives are diverse, supporting students at multiple stages of their academic journey. Our flagship training initiative is the NITheCS South African Theory and Computational School (SATACS) – a formal **Teaching Programme** that delivers high-level lectures in subjects within the theoretical physics and computational sciences. Our **Internship Programme** provides hands-on experience, helping students refine their research focus and develop critical skills. Through **Bursaries**, we enable outstanding postgraduate students with financial need to pursue and complete their MSc and PhD studies.

Here is an overview of our three training initiatives and their impact in 2024.

### Teaching Programme

The NITheCS South African Theory and Computational School (SATACS) is a decentralised, hybrid national teaching programme, designed to provide world-class postgraduate education comparable to elite international programmes. Under the leadership of Prof Will Horowitz (UCT), SATACS offers specialised courses in theoretical and computational sciences, tailored for Honours and Masters students. Through SATACS, NITheCS continues to strengthen South Africa's postgraduate education in theoretical and computational sciences, preparing students for advanced research and global academic competitiveness.

Courses are delivered online and/or in

#### Impact:

1



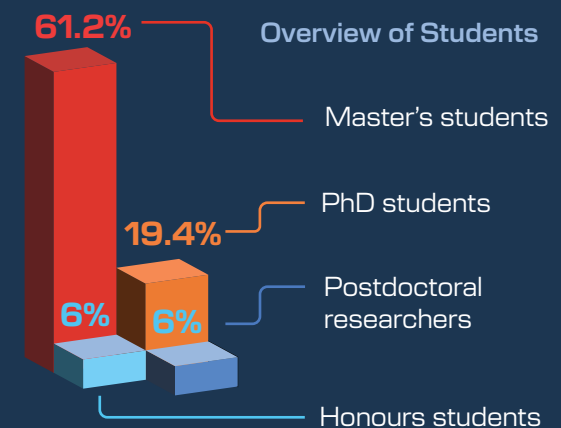
67  
students



+ 17  
institutions

Applications for the Teaching Programme

2



person, depending on the needs of instructors and participants, ensuring accessibility for students across the country. For online delivery, instructors typically use Google Classroom in combination with Zoom.

In 2024, ten courses were presented, spanning durations from a single semester to a full academic year. These included:

- Health Insurance Mathematics Linear and Longitudinal Data Modelling with R
- Answer Set Programming
- Quantum Field Theory I and II
- Category Theory
- Logics for Artificial Intelligence
- Introduction to Pointfree Topology
- Machine Learning: From Linear Regression to Deep Learning
- High-Performance Computing in Rust
- Integrable Systems

Among these, Machine Learning: From Linear Regression to Deep Learning and Quantum Field Theory I and II were the most popular.

Typically, students meet with instructors at intervals agreed upon at the start of the course. Where both the student and instructor are affiliated with the same institution, course credit may be awarded upon completion of all the course requirements.

NITheCS conducts evaluations at the end of each course to assess effectiveness and identify areas for improvement. In 2024, student feedback was overwhelmingly positive, with many highlighting the instrumental role these courses played in advancing their research careers.

**“What I love about NITheCS is how it brings together researchers across disciplines and creates real opportunities for collaboration. The sense of community is inspiring.”**

– Prof Ruan Veldman  
South African National  
Bioinformatics Institute



## Internship Programme

The NITheCS Internship Programme provides valuable training opportunities for graduate students through internships supervised by NITheCS Associates at South African universities and research institutions. The programme bridges the gap between theory and practice, allowing students to gain experience in cutting-edge research environments. A highlight of the programme is the opportunity for interns to present their research findings at the South African Institute of Physics (SAIP) annual conference, further enhancing their professional development.

### Impact:

- In 2024 the internship programme was hosted virtually across nine institutions in the mid-November to December period. This included prominent research bodies and universities.
- From a pool of 69 applicants, 23 students were selected and the cohort reflected strong national representation, with participants from 11 South African universities. The gender balance was nearly equal, with 11 female and 12 male interns.

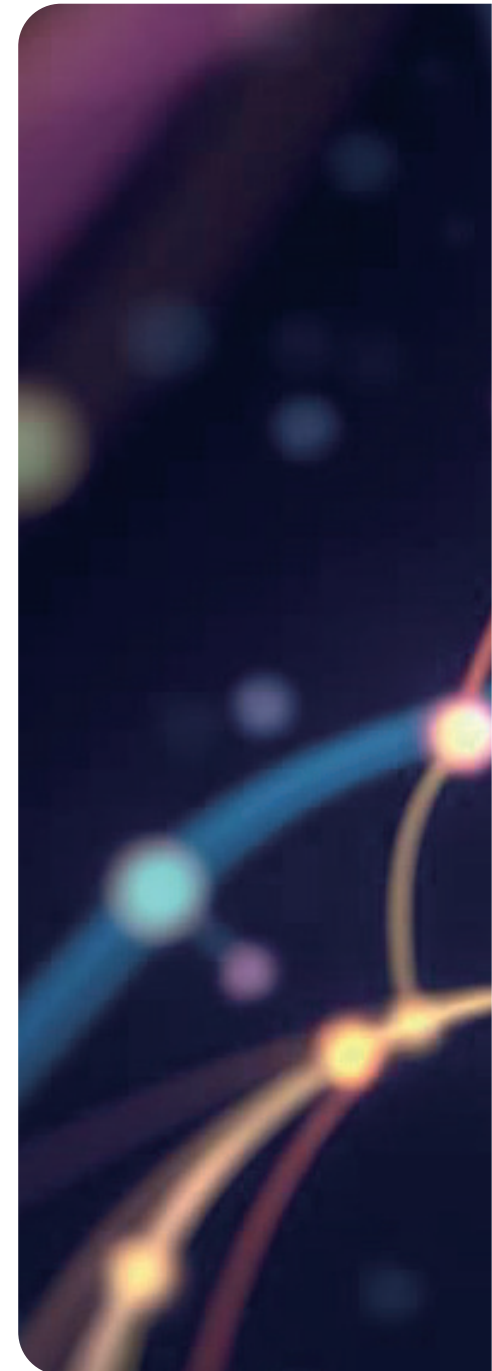


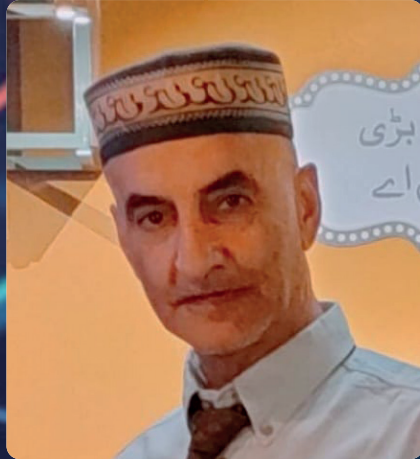
## Bursaries

Talented students pursuing MSc and PhD degrees in theoretical and computational sciences can continue their studies and focus on their research with the support of NITheCS bursaries, administered through the National Research Foundation (NRF). Allocation targets: 95% allocated to South African citizens and permanent residents, 5% allocated to students from SADC countries and beyond, 55% allocated to women.

### Impact:

- 1 NITheCS hosted a bursary-holder workshop, enabling recipients to network, present a high-level view of their research, and receive feedback on their progress.





**“NITheCS is establishing a platform for linking traditional, current, and future trends in the Mathematical Sciences and their impact on other Computational and Theoretical Sciences.”**

– Prof Abdul Kara  
University of the Witwatersrand

# ENGAGEMENT:

## Events, Sponsorships, and Communication

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NITheCS engages extensively with its community and other stakeholders through events, sponsorships, and communication. NITheCS also actively supports events presented by associate bodies. In practice, the Institute could not function efficiently without the support of its Associates and specialist bodies that engage in the theoretical and computational sciences. This support allows NITheCS to deliver a rich and far-reaching programme, with opportunities for many individuals and organisations.

### Events & Sponsorships

Most NITheCS events are conducted in a hybrid format, held both in-person and online, ensuring accessibility for participants across various geographical locations. As the Institute continues to grow, this flexibility becomes increasingly important, enabling those in our community across the country and those further abroad to engage with us. In addition, many of our events are recorded and made available on our YouTube channel, further extending our reach.

NITheCS presented and/or supported the following events in 2024:

#### 1. Colloquia

NITheCS colloquia took place in a regular Monday time slot. NITheCS Associates, visiting academics, postdoctoral researchers, and others from within the theoretical and computational sciences were invited to present at these events. The benefits of presenting a NITheCS colloquium include raising awareness among a wide spectrum of academics from many scientific disciplines. Furthermore, it encourages meaningful contact



and discussion among scholars, which frequently leads to interesting talks and future collaboration. We promote our colloquia primarily through our website, newsletters, and social media channels.

In 2024, NITheCS hosted **39 successful in-person colloquia**, which have received a total of 3 397 YouTube views.



## 2. Schools

NITheCS actively hosts, co-hosts, and sponsors various educational schools to assist in training students in the NITheCS community. In 2024, these included the inaugural Computing in High Energy Physics (HEP) and Applications CNRS-Africa Lectures (CHACAL), and our annual **Summer Schools**.

Since 2019, NITheCS has proudly partnered with the Centre for High Performance Computing (CHPC) to co-host the annual Coding Summer

School. The 2024 edition, one of the largest to date, brought together 557 participants from 30 institutions across South Africa and Kenya, with additional attendees joining via live streams from the University of Cape Town and Stellenbosch University.

The Summer School plays a vital role in equipping emerging researchers with core programming skills and introducing them

to South Africa's national computing infrastructure.

The first week of the 2024 Summer School focused on foundational tools, including Python, data science, Linux, and Bash. The second week introduced more advanced topics such as machine learning, bioinformatics, chemical simulations, and Monte Carlo methods.



Each day of Summer School featured morning lectures followed by hands-on, code-along sessions in the afternoon. The programme also included short, 15-minute invited talks by postdoctoral researchers and senior scientists, offering insights into real-world applications aligned with the school's focus areas.

To earn a certificate of completion, participants were required to attend all sessions and complete assigned quizzes and projects. This growing collaboration continues to strengthen the computational capacity of young researchers and supports the development of a data-driven research culture across the continent.

### 3. Mini-schools

NITheCS hosted **10 mini-schools** in 2024. Mini-schools generally feature a series of four one-hour lectures per month on various topics. These sessions provide our community with opportunities to broaden their knowledge and engage with diverse subject areas.

### 4. Micro-schools

In June 2024, NITheCS launched micro-schools to enhance skills within its community by providing introductory insights or explanations on various topics. Each 30-minute event

consists of a 20-minute talk followed by 10 minutes of Q&A. Micro-schools promote peer-to-peer learning by connecting students and researchers from NITheCS's eight thematic areas together in a communal setting to learn from each other. This also encourages cross-discipline collaborations. A total of **13 micro-schools** were held throughout the year.

## 5. Seminars and Webinars

In 2024, NITheCS hosted both independent and joint seminars and webinars, fostering knowledge exchange and collaboration within the theoretical and computational sciences. Notably, new seminar series were launched on various campuses, including WITS (through the Mandelstam Institute for Theoretical Physics), UKZN, NWU, and SU.

These initiatives serve multiple purposes. They raise the profile of theoretical and computational sciences in local academic environments, provide a platform for local researchers and experts to present their work, and encourage interdisciplinary collaboration across the diverse fields represented by NITheCS.

By expanding these seminar series, NITheCS continues to strengthen engagement within its research community and promote cutting-edge discussions in key scientific areas.

## 6. Masterclasses

In 2024, NITheCS collaborated with CoRE AI, the African-European Cluster of Research Excellence focused on Artificial Intelligence (AI) and Computational Thinking, to host **two Masterclasses**. These sessions provided a platform for researchers, students and professionals to explore cutting-edge advancements in AI, fostering knowledge exchange between African, European and even scientific communities further abroad.

The Masterclasses covered both theoretical foundations and practical applications, equipping participants with essential AI methodologies and computational strategies. Through this collaboration, NITheCS's commitment to interdisciplinary research and international partnerships was strengthened.

## 7. Hackathons

In 2024, NITheCS co-sponsored hackathons for the first time. These events provided participants with hands-on experience in

tackling real-world challenges using cutting-edge technologies such as blockchain, artificial intelligence, and digital solutions. Students had the opportunity to apply their theoretical knowledge in a practical setting, develop critical thinking and teamwork skills, and engage with experts in their respective fields. Additionally, these hackathons connected students with industry leaders and organisations, opening doors to potential career opportunities and future research collaborations. By supporting these events, NITheCS reinforced its commitment to empowering young scientists and promoting technological advancements that address societal challenges.



The poster for the MPUMALANGA ARTIFICIAL INTELLIGENCE STUDENT HACKATHON (MAISH) features logos for the University of Mpumalanga, Tshwane University of Technology, 20 Years of Mpumalanga, and NITheCS. The main text reads: "MPUMALANGA ARTIFICIAL INTELLIGENCE STUDENT HACKATHON (MAISH) Utilising Digital Solutions to Solve Africa's Problems." It specifies the dates "24 to 26 October 2024" and the location "UMP Mbombela Campus". A QR code is provided for registration, with the text "REGISTER by 20 Sept 2024" and the URL "https://bit.ly/3B41OU2". The poster also states "Lots of Prizes to be Won!!!!" and provides contact information: "MORE INFO: email duduzile.masuku@ump.ac.za or thibact@tut.ac.za". Logos for Oxfusion and NITheCS are at the bottom.

## 8. Workshops

### Carpentry Workshops

In 2024, NITheCS hosted **six Carpentry Workshops**, equipping graduate students and researchers with essential computing skills to enhance productivity and efficiency. These hands-on sessions focused on fundamental concepts and tools, including programming skills, software design, version control, data management, and task automation. Emphasising a collaborative learning approach, participants were encouraged to support one another and apply their newfound skills to their own research challenges, enabling them to work more effectively and efficiently.

### Bursary Holder Workshop

At this annual workshop, each bursary holder delivered a brief presentation to share insights into their research, as a means to foster knowledge exchange and collaboration within the group, as well as to gauge their progress.

## 9. Other Engagement Initiatives

NITheCS sponsored or co-sponsored several initiatives during 2024 that focused on skills and knowledge development. Below are the details relating to these programmes and events.



### FameLab Contest

NITheCS again sponsored a heat of the FameLab contest, which took place in June 2024. Scientists aged 18 to 35 years in the NITheCS fields of science had the opportunity to further develop their communication skills as they were coached to explain a science concept in three minutes and could put their learning into practice.

The heat winner was Axel Dorian Piepi Toko of the University of Cape Town. The very worthy runners-up were Luyanda Mazwi (University of Johannesburg) and Iness Kyapwanyama (AIMS), who ranked in second and third place respectively. The finalists attended a masterclass in communication to prepare them for the national competition. FameLab is managed locally by the South African Agency for Science and Technology Advancement and science communication agency Jive Media Africa.

### Mathematics Programme

To inspire school learners and undergraduate students to develop a passion for mathematics, NITheCS co-sponsored an online event celebrating the International Day of Mathematics on 9 March. The event was led by Dr Cerene Rathilal (UKZN) and Dr Lungile Sitole (UJ Soweto Science Centre).

### STEM MentHER

NITheCS sponsored the STEM MentHER programme for the third consecutive year. Launched in 2022, this initiative mentors and guides aspiring female Grade 12 learners toward pursuing studies in STEM fields.

In 2024, the programme expanded from three cohorts to five, aligning with potential future studies at Stellenbosch University, the University of Cape Town, the University of KwaZulu-Natal, the University of the



Cape Town



Johannesburg



Durban

Witwatersrand, or the University of Johannesburg. NITheCS contributed funding, along with branded promotional items and marketing materials to support and promote the programme.

### Eskom Expo for Young Scientists

NITheCS is committed to inspiring young minds and fostering a passion for science through its participation in the Eskom Expo for Young Scientists. This annual



event provides school learners with the opportunity to showcase their own scientific projects. In 2024, NITheCS attended the exhibition in person, engaging with visitors at our stand and supporting the event by sponsoring several prizes.

We were also particularly pleased to celebrate the success of Witness Nkge (*pictured above*) from Gabonewe Secondary School, who received a silver medal at the 2023 Eskom Expo International Science Fair. Witness achieved six distinctions

in his Matric exams, and NITheCS was proud to have awarded him a laptop for his outstanding project in the Mathematics category. We are delighted to have played a role in his journey and to support his passion for theoretical and computational sciences.

### Teacher Development Programme

In June, NITheCS, in collaboration with the UJ Soweto Science Centre, UKZN, the South African Mathematics Foundation, and other co-sponsors, hosted an online teacher training event titled “Enhance Your Professional Development”.

Co-hosted by Dr Cerene Rathilal (UKZN) and Dr Lungile Sitole (UJ Soweto Science Centre), the programme aims to assist in the professional development of teachers on a broad scale. This year’s event successfully reached approximately 500 teachers, equipping them with valuable insights and resources to enhance their teaching practice.

### NITheCS Women’s Month Writing Retreat

To provide female researchers with dedicated time and space to focus, share ideas, and push their work forward, we invited female NITheCS Associates to apply for a grant of R10 000 to fund a self-run writing retreat in celebration of Women’s Month.



**Women's Month  
Writing  
Retreat**

NITheCS female Associates... apply for a grant to fund a Self-run Writing Retreat, so you can focus on a piece of work without the interruptions of daily life.

**Apply by:** 31 July 2024

**Details:** <https://bit.ly/4bUqo6B>



This initiative has proved popular since its launch, and more than 20 applications were received in 2024. Recipients are encouraged to add the NITheCS affiliation to publications that result following their retreat.

One of the recipients, Prof Inger Fabris-Rotelli (UP), hosted her retreat in Pretoria on 11-12 November. Led by herself, a group of her PhD students, recent graduates and staff gathered to focus, collaborate and advance their research projects.

Each participant at Prof Fabris-Rotelli's retreat leveraged the quiet, supportive environment to tackle key academic tasks. Prof Fabris-Rotelli advanced her draft papers and submitted papers to journals. She also assisted attendees with their research projects.

## SAIP Conference

NITheCS has supported the SAIP conference for the past decade as an exhibitor, and also by sponsoring student prizes in the theoretical and computational physics division. The 68th Annual Conference of the South African Institute of Physics (SAIP2024) took place at Rhodes University from 1-5 July 2024. NITheCS sponsored one of the conference tracks, provided funding to support student attendance, and contributed prizes to recognise outstanding research presentations. In addition in 2021, NITheCS provided funding to support students that took part in the internship program to present their research at the conference.

NITheCS also exhibited at the AI Expo Africa in October, and in December – both at the Science Forum and the Centre for High Performance Computing National Conference.

## Communication

NITheCS actively engages with its stakeholders to share news, invite participation in events, and disseminate information about relevant opportunities through various channels. Our communication strategy includes:

- **Monthly Newsletter:** Emailed to Associates, students, bursary holders, and other interested parties.

- **Event & Notice Emails:** These are emailed to our mailing list. We encourage all interested individuals to subscribe.

- **Website:** Our website provides information about the Institute, its members, and events.

- **Social Media:** Social media is used to share event news and relevant updates with the scientific community. Engagement on these platforms also helps expand awareness of NITheCS and its activities. We maintain active accounts on LinkedIn, X (formerly Twitter), Facebook, YouTube, and Instagram.

- **Recorded Presentations:** Colloquia, Mini-school lectures, and other presentations are recorded (subject to presenter approval) and uploaded to our YouTube channel. These serve as valuable resources for those unable to attend live sessions and thereby reach a wider audience.

- **Media Releases & Reports:** Updates are shared through media releases and annual reports.

- **Featured Scientists:** Each month, we highlight one of our Associates as a featured scientist. Their profile is published on our website and in our monthly newsletter to showcase the diverse scientific contributions of our Associates, while inspiring others to pursue careers in science.

Through these efforts, NITheCS ensures effective and inclusive communication, strengthening engagement within our community.

# 2024 Newsletter Featured Scientists:



# RESEARCH:

## Advancing Theoretical and Computational Sciences

**At NITheCS, research is at the core of our mission to advance theoretical and computational sciences in South Africa and beyond our borders. We strive to address real-world challenges and contribute to sustainable solutions that align with the United Nations' Sustainable Development Goals (SDGs).**

Our research spans cutting-edge topics, from quantum science and artificial intelligence to climate modelling and data-driven decision-making, ensuring that South Africa remains on the forefront of scientific and technological advancements on the continent.

Through our extensive network of Associates, NITheCS fosters collaborative, interdisciplinary research that not only enhances fundamental scientific understanding but also builds practical competencies for the future. By supporting innovative research projects, we equip South African scientists with the skills and resources to drive discoveries, develop new technologies, and strengthen the country's position in the international research landscape.

### Research Programmes

Launched in 2022, our research programmes are led by NITheCS Associates, who are affiliated with various South African universities, and may involve collaboration with international research partners to drive high-impact, interdisciplinary research. Each programme runs for a minimum of 12 months, ensuring sustained exploration of complex scientific challenges and fostering long-term research excellence.

Another positive outcome of the research programmes is the opportunity to build the next generation of scientific leaders. When investigators integrate graduate students and postdoctoral researchers in their programmes, these young people can develop critical research skills, engage in hands-on problem-solving, and collaborate with leading experts in their fields. This not only strengthens South Africa's scientific capacity, but also enhances the country's contribution to knowledge and innovation.

In 2024, the research programmes continued to operate in their existing form for the final year. During this time, calls for new programmes were made, leading to the formation of new groups and the development of new research topics, which will be reported on in 2025.



# 1. Genomics, Bioinformatics, and Advanced Medicine

In 2024, this programme focused on two main areas: improving genomic computing and using large language models (LLMs) to tackle mental-health challenges.

A major activity was a March training course, “Parallel Computation with GPUs: An Introduction to Programming with CUDA,” which drew more than 120 postgraduate students and academics across South Africa as part of the NITheCS Mini-School Programme.

As part of the programme, PhD candidate Hanitriniala Malalatiana Rakotondrasoa (Stellenbosch University) is developing faster ways to detect recombination in large viral genome datasets using parallel programming. Viruses normally copy themselves with only small mutations, producing genome “family trees.” In the early days of genomics, when datasets were small, scientists could analyse all possible trees to find the best one. But with modern sequencing generating enormous datasets – more than 17 million SARS-CoV-2

genomes alone – these old methods no longer work. Instead, researchers must use smarter, scalable algorithms that run efficiently on modern hardware.

Although people often talk about Moore’s Law and rapidly improving computers, single-processor performance has largely plateaued. Today, progress comes from using many processors at once. Graphics Processing Units (GPUs), which can contain tens of thousands of processing cores, now play a major role in high-performance computing. However, they require specialised programming. NVIDIA addressed this by developing CUDA, a language extension that makes GPU programming easier. The Mini-Course taught participants the basics of CUDA, parallel computing, and performance optimisation.

Recombination – when a virus mixes genetic material from two different “parents” – is rare but important, because it can create new, sometimes more dangerous variants. Rakotondrasoa is working on ways to detect these events in huge datasets.

The programme also explores how AI can

support mental-health research. Ian Masaga (MSc, North-West University) is training LLM-based classifiers to recognise psychological markers. He uses synthetic conversations that mimic real clinical cases, comparing the AI’s assessments with those of a consulting psychologist.

Another MSc student, Shiksha Dhedha (North-West University), is using generative AI to build a narrative-based serious game that helps users explore anxiety disorders. Working with Profs Reolyn Heymann and Marita Heyns, the team is creating an immersive interactive-fiction experience guided partly by fantasy author and YouTube creator Marie Mullany.

The programme is also developing custom GPT systems with Dr Tamlynn Jefferis (North-West University). One project, “Glimmer,” is trained on psychological theories including Polyvagal Theory, Cognitive Behavioural Therapy, and Somatic Experiencing. Early tests have been very promising. The work is now expanding into play-therapy and game-based learning for young children, combining Glimmer’s psychological principles with the “Amazing Tales” role-playing system to teach social and educational skills through imaginative play.

## 2. Advancing Biodiversity Informatics and Ecological Modelling (ABIEM)

### A data-driven Compass for Conservation in a Changing World

In 2024, ABIEM shifted from proof-of-concept to proof-of-impact. Our teams combined ecology, mathematics, and open data systems to answer a key question: How do we turn huge amounts of biodiversity data into information that parks, people, and policymakers can actually use?

*MacFadyen et al.* (2023) introduced a “spiral pipeline” for doing exactly this – later called a “lifeboat” by *Hui et al.* (2024). It shows how raw observations move through cleaned datasets, models, and dashboards to support real conservation decisions.

### Science that travels from Code to Conservation

Aligned with ABIEM's goals – better biodiversity data workflows, stronger ecological models, cross-disciplinary teamwork, and training new talent – we balance time at our computers with time

in the field. Regular field trips, retreats and small workshops in natural settings help us verify our data, observe ecological processes first-hand, and refine research questions. These sessions strengthen collaboration and ensure our models stay realistic and grounded in nature.

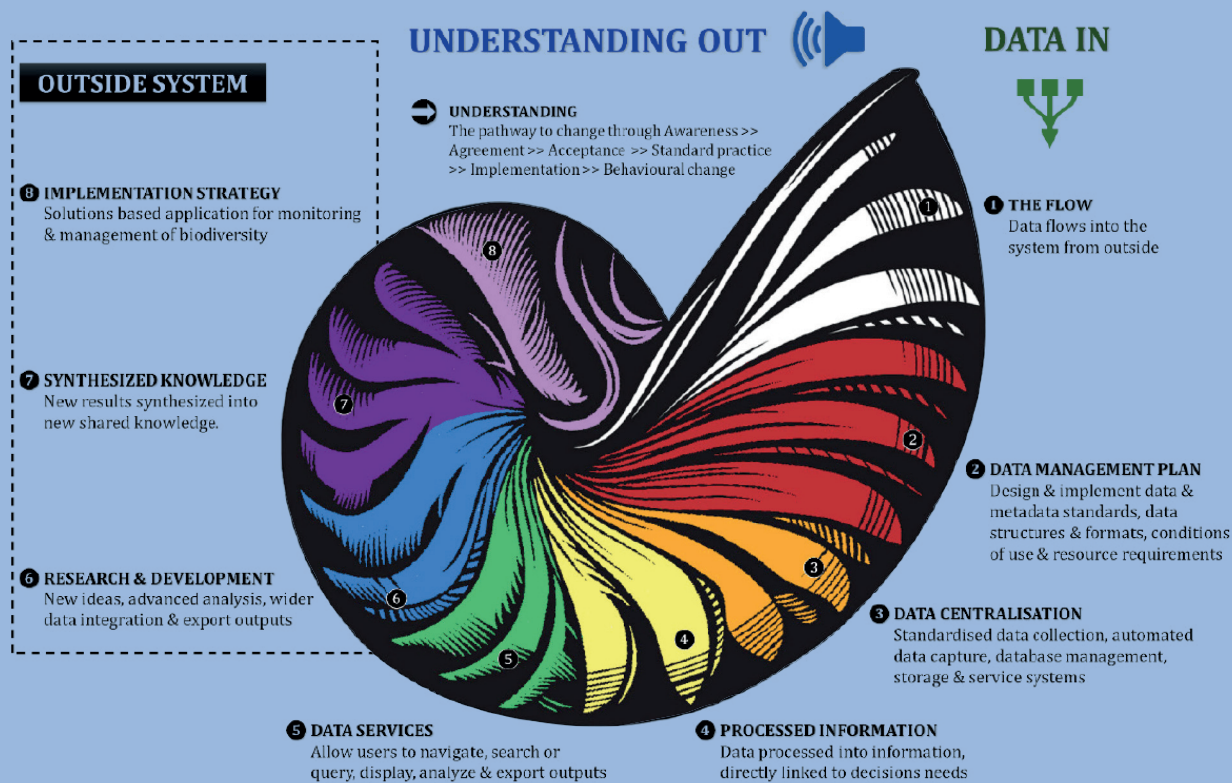
In 2024, ABIEM researchers produced 16 peer-reviewed publications that delivered practical, decision-ready insights.

Highlights included:

- An AI pipeline that detects lemur calls in Madagascar's rainforests (*Batist et al.*).
- The first woody-cover map of Kruger National Park from the 1940s – vital for fire-management planning (*Riccardi et al.*).
- New understanding of savanna grass-herbivore diversity patterns (*Čuda et al.*) and drivers of insect turnover across Africa (*Basel et al.*).
- Theory-driven work on eco-evolutionary feedbacks using rock-paper-scissors models (*Kubyana et al.*).

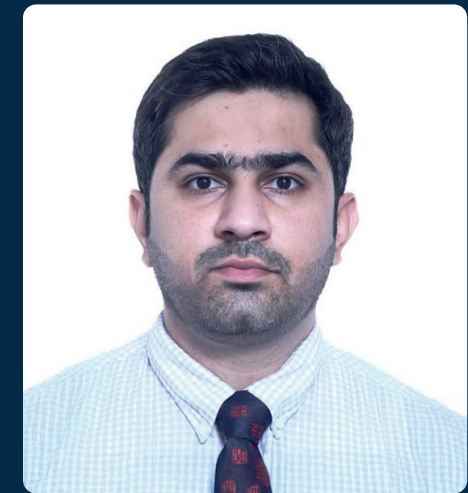
*MacFadyen et al* (2023) charts the path from raw biodiversity observations to conservation action. Data move from a metadata-governed workspace, through a central repository with automated quality checks, into tailored information products that answer management questions. Online services then make these products discoverable and usable, allowing researchers to integrate datasets, build predictive models and generate knowledge for managers. The nautilus-shell design – echoing the golden ratio – symbolises the iterative, interconnected nature of biodiversity data, supporting ABIEM's goals of strengthening data workflows, ecological modelling, cross-disciplinary collaboration and training along the full data-to-decision pipeline.

- Global syntheses, including the biodiversity-informatics “lifeboat” framework (*Hui et al.*) and evidence supporting invasive-species targets for the CBD (*Roy et al.*).
- Modelling studies on pollination networks (*Yahaya et al.*), cassava disease



“I enjoy working with NITheCS because it provides an inclusive, dynamic environment for researchers to share ideas. NITheCS creates a space where innovation feels natural.”

– Dr Ali Raza Bhatti  
Stellenbosch University



spread (*Sikazwe et al.*), and how animals navigate patchy landscapes (*Gibbs et al.*).

- A Nature Ecology & Evolution study linking wood density to global carbon stocks (*Mo et al.*).

Together these publications show how ABIEM turns data pipelines into real-world conservation action – producing open, rigorous science used by ecologists, modellers, and policymakers worldwide.



## Building People, not just Pipelines

### Conferences

ABIEM believes that building people is just as important as building models.

At the 2024 Savanna Science Network Meeting (SSNM) in Skukuza, five early-career researchers translated advanced mathematical theory into actionable insights for conservation managers. Their work spanned modelling mammal movement, informing river corridor design, analysing the genetics of invasive wasps, disentangling fire-rainfall-herbivore interactions, and improving approaches to rhino population monitoring.

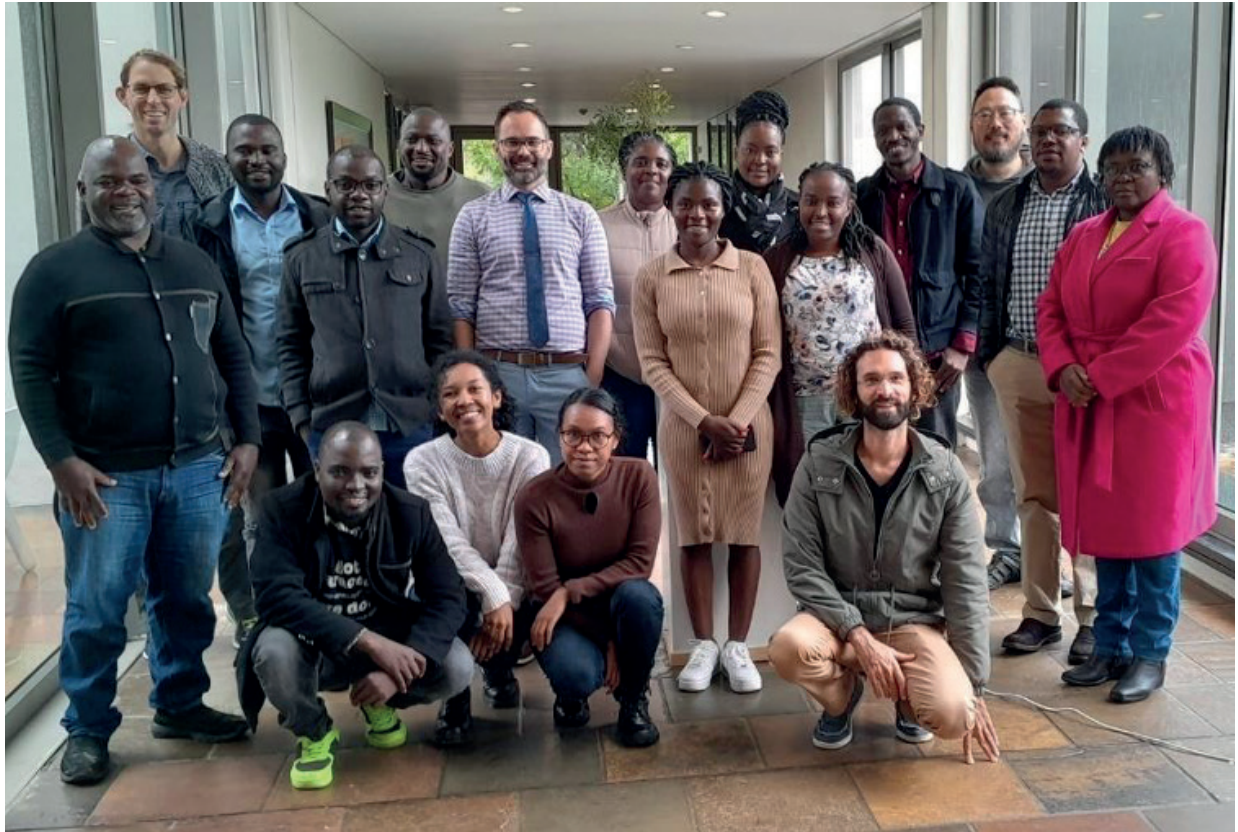
By placing students and postdoctoral researchers at the centre of mixed academic-SANParks engagements like (SSNM), these forums function as “living classrooms,” enabling emerging scientists to translate cutting-edge models into tangible conservation action.



## Workshops

In June 2024, Andrew Reid Bell's short course taught more than 20 participants how to build game-based models that explore how people and the environment interact. Using NetLogo, they learned to simulate resource use, conflict, cooperation and decision-making under uncertainty.

The workshop created an active online community where participants continue sharing code and ideas – supporting ABIEM's goal of data-driven, people-centred ecosystem management.



## Mini-Schools

In October 2024, Sandra MacFadyen and Maarten Trekels led an online NITheCS mini-school on using “data cubes” to combine satellite imagery with species records.

Over 35 young scientists learned to build cloud-optimised cubes, apply metadata standards and run reproducible analyses – skills often

inaccessible in resource-limited regions.

The virtual format removed travel barriers, and follow-up support has helped participants keep learning and collaborating. The result: stronger human capacity to turn raw environmental data into real conservation decisions.

## Impact Beyond Academia

- **Policy influence:** ABIEM's modelling contributed to a Nature E&E paper that shaped the wording and metrics of CBD Target 6 on invasive species, adopted at COP-16 – showing these targets are both urgent and achievable.
- **Protected-area management:** Historical woody-cover maps (1939–44) and new vegetation-mapping workflows are now feeding into SANParks' fire-management dashboards. Herbivore–grass models inform grazing quotas in Limpopo reserves.
- **Global standards:** As Africa's partner in the EU Horizon B-Cubed project, ABIEM co-develops “occurrence cubes” and biodiversity indicators now being piloted by GBIF. The collaboration also delivered an international mini-school training researchers from 20 countries, ensuring African perspectives shape future biodiversity-monitoring systems.

By embedding our open-data, open-code ethos in a broader complexity framework, ABIEM's 2024 innovations will continue to steer conservation decisions – keeping science, software and society tightly coupled in the years ahead.



“It would be wonderful if NITheCS could actively collaborate with the University of Namibia. Strengthening engagement and activities here would make a big difference for students and researchers.”

– Mr Ireneus Kashinduka  
University of Namibia



### 3. Machine Learning in Support of Theoretical and Computational Science

Artificial intelligence is now part of almost every aspect of daily life, keeping **machine learning (ML)** and **deep learning (DL)** at the centre of research and public discussion. Universities interact with these technologies in many ways – from developing the models society relies on, to adapting to the growing use of large language models by students and academics.

As an ML Research Programme (RP), we are fortunate to have both the mandate and support to explore the frontiers of fundamental and applied deep learning. Our goals are twofold:

- (1) Develop new, specialised ML techniques.
- (2) Apply ML to scientific modelling challenges.

Below are some highlights from 2024, and what lies ahead.

#### KnowIt: Opening New Doors in Deep Learning

One of our major achievements was the development of **KnowIt (arxiv:2507.06009)**, a toolkit from the MUST Deep Learning group at NWU. KnowIt helps researchers uncover patterns in data that change over time – whether predicting river flow or spotting early signs of health concerns.

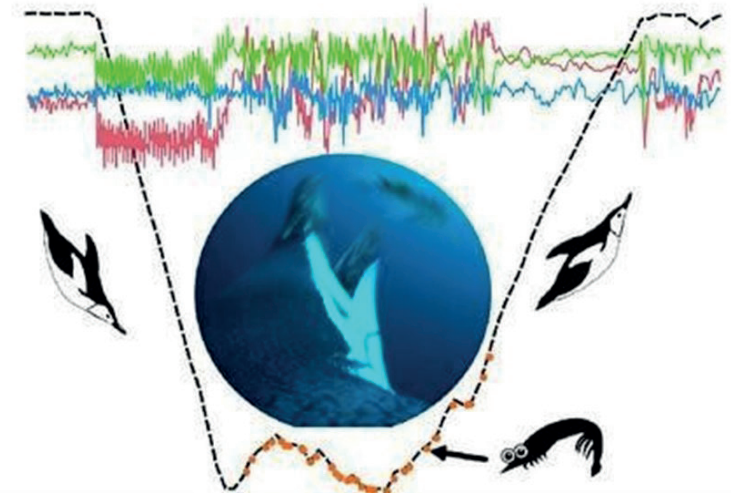
In 2024, our team refined KnowIt into a reliable, well-documented framework and released it publicly on **GitHub**. Postgraduate students are already using it to explore new questions in deep learning, and we are preparing a research paper on KnowIt for 2025. Our long-term vision is for KnowIt to support discoveries across fields like healthcare, climate science, and engineering.



#### Deep Learning for Penguin Conservation

NITheCS associate Dr Stefan Schoombie (UCT) is developing innovative camera- and sensor packages for Chinstrap and Adélie penguins. By combining video, GPS, accelerometer and depth data, researchers can identify and count prey captured by penguins – key indicators for monitoring krill populations and overall ecosystem health. This work contributes to CCAMLR's Ecosystem Monitoring Program.

Dr Schoombie and collaborators created DL models to detect prey-capture events using accelerometer and depth data, along with an open-source interface that synchronises video and sensor streams. Users can load trained models and automatically map



predictions onto the time-series data, making this tool essential for future studies. An MSc student from our programme contributed code to this software, gaining valuable hands-on experience.

In 2024, Dr Schoombie presented this work at the 8th International Bio-Logging Science Symposium in Tokyo and at the SCAR Open Science Conference. It also featured in Nature Africa, and two related papers were published in Royal Society Open Science and Methods in Ecology and Evolution.

### **Space Physics Provides a Rich Laboratory for Time Series Problems**

The modelling and forecasting tasks in space physics often take the form of multivariate regression problems, with nonlinear interactions and non-stationary time dependencies between inputs and outputs. Our collaboration with the South African National Space Agency (SANSA) geomagnetic observatory in Hermanus gives us access to expertise and compelling problems to solve.

In November, Prof Stefan Lotz from SANSA presented at the European Space Weather Week in Coimbra, Portugal, discussing the use of transfer learning to predict geomagnetic disturbances from space-borne solar wind measurements.

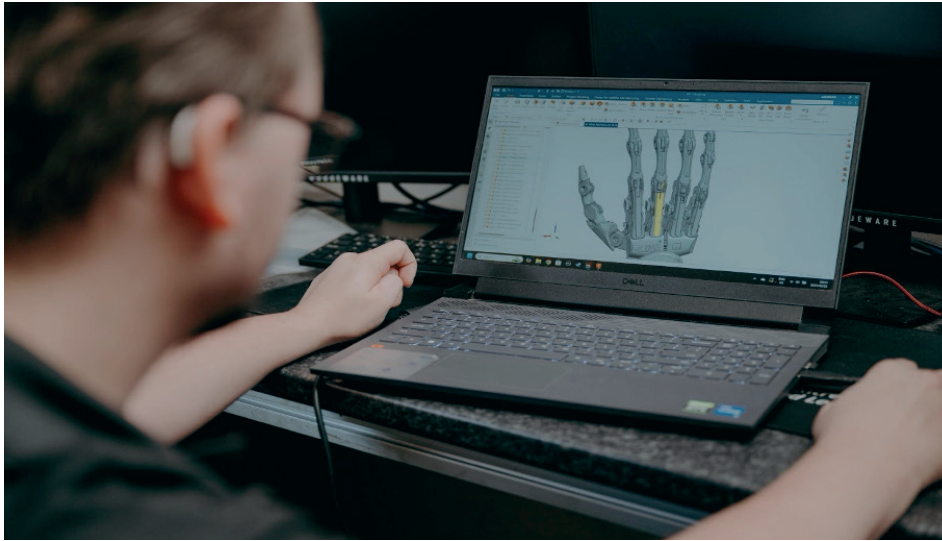
His talk, part of the session “Applications of Artificial Intelligence to Space Weather and Space Climate,” highlighted the broad applications of deep learning and the multidisciplinary collaborations it enables.

### **MUST Hosted Their Annual Deep Learning Bootcamp**

Held at North-West University (NWU) and sponsored by NITheCS, this intensive five-day training brought together researchers, students, and industry professionals to explore AI and deep learning – from fundamentals to advanced models. Over 350 participants joined on-site and online, reflecting strong enthusiasm for advancing deep learning research and its real-world applications.

The bootcamp began with deep learning basics, including neural network architectures and mathematical foundations. The remaining days focused on practical concepts such as optimisation, regularisation, and different network types, including recurrent and convolutional networks. The final day taught practical methods and best practices, equipping participants to apply deep learning beyond tutorials and pursue new insights in their research.





### **Beyond Limits Collaboration**

At the end of the year, we launched a collaboration with the **Beyond Limits group at NWU's Faculty of Engineering**. Beyond Limits develops assistive technologies such as prosthetic legs, arms, and customised sockets.

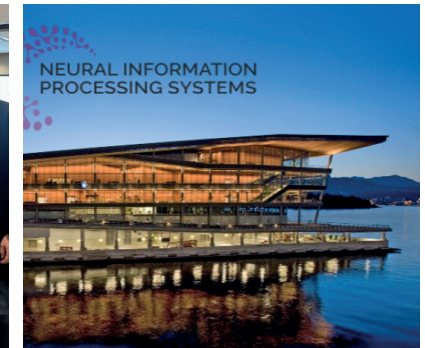
Through MUST, our machine learning research programme will help interpret electromyography (EMG) signals – electrical signals from residual muscles – to translate intent into action. This enables users to intuitively move hands and wrists and perform increasingly complex tasks with precision. This collaboration exemplifies how AI can enhance human potential, combining engineering with empathy.

### **Not Forgetting the Fundamentals**

Despite advances in AI, deep learning is still a relatively new field, and we don't yet fully understand all the factors that enable these systems to perform at high levels.

Towards the end of 2024, a small contingent of our research programme – including Prof Marelie Davel – attended the Workshop on Scientific Methods for Understanding Deep Learning in Vancouver during the NeurIPS conference. There, they exchanged knowledge with leading experts on theoretical developments in the field.

Earlier in the year, at the AAAI Conference on Artificial Intelligence (held at the same venue), our team published a paper predicting neural network performance from internal measurements, further contributing to understanding deep learning fundamentals.



## 4. Advanced Computational Modelling of Materials

During the 2024 reporting period, this NITheCS-supported research programme delivered strong scientific, training, and societal outcomes across condensed matter physics, materials science, biophysics, catalysis, and renewable energy. The programme integrates theoretical, computational, and data-driven methods to address fundamental challenges in energy conversion, optoelectronics, and biological light harvesting, while supporting South Africa's priorities in climate action, skills development, and global scientific engagement. Its interdisciplinary focus spans physics, chemistry, materials science, and computational modelling, with particular emphasis on non-carbon-based materials and bio-inspired systems, translating fundamental theory and machine learning into predictive frameworks for materials design.

Significant progress was achieved across key research thrusts in 2024. Ukpong advanced understanding of lattice geometry, phase transitions, and carrier dynamics relevant to

optoelectronic optimisation. Krüger generated new insights into bio-inspired polymer solar cells and photosynthetic light-harvesting systems using advanced spectroscopy and quantum chemical modelling. Esterhuysen applied computational chemistry to clarify intermolecular interactions in catalysis-related materials, while Obodo contributed to hydrogen economy research, 2D materials for photocatalysis, and theoretical method development. These efforts resulted in peer-reviewed publications and strengthened international collaborations.

The programme demonstrated high productivity and international visibility through refereed journal articles, review papers, doctoral theses, and conference presentations. Training and mentorship were central, with multiple degrees awarded and intensive skills development in scientific computing and machine learning. Outreach activities further enhanced employability in data science and engineering.

Beyond academia, the programme supported science education and communication by attracting MSc students into research pathways and producing a publicly accessible report on biophysics in Africa. Strongly aligned with NRF priorities and the Sustainable Development Goals – particularly Quality Education, Gender Equality, and Climate Action – the programme achieved a high return on investment despite limited resources. While not focused on



Bertus van Heerden (left), a former NITheCS bursary holder (for 1 year during his PhD), was selected to participate in the 2024 Lindau Nobel Laureate Meeting. Here he stands next to Eric Betzig, one of the 2014 Nobel Laureates in Chemistry.



The 2024 NITheCS funds allowed us to co-fund Dr Mamaru Alem, a postdoctoral research assistant, for 3 months, to work on several computational projects. Pictured above (right), he received the presentation award at the 12th International Conference of the African Materials Research Society (AMRS2024), 16-19 December 2024, University of Rwanda.

Our open-source software suite was highlighted on the front cover of Biophysical Reports.



B2 rating awarded to Prof Tjaart Krüger (left).

immediate commercialisation, it lays a strong foundation for future advances in energy, catalysis, and environmental remediation.

In 2024, the Advanced Computational Modelling of Materials research programme strengthened South Africa's research capacity through impactful science, high-level training, and meaningful societal engagement, positioning it well for continued impact in future funding cycles.

## 5. Mathematical Structures and Modelling

**In 2024, the Mathematical Structures and Modelling research programme slowed its South African collaborative activities after an intensive 2022–2023 period. Instead, programme members focused on advancing their individual research trajectories, without expending NITheCS funds.**

### International Engagements

Prof Zurab Janelidze (Stellenbosch University) visited several European universities (Portugal, Belgium, Estonia, Italy), delivered five invited talks and laid the groundwork for future collaboration with Prof Maietti's Logic group at the University of Padova.

Prof Watson and Dr Kuo (University of the Witwatersrand) published in the Proceedings of the American Mathematical Society with Dr Kalauch (Technische Universität Dresden), and gave lectures at the CIMPA school "Ordered Structures and their Applications in Finance and Machine Learning" in Tunisia.

Dr Goswami (University of Johannesburg) received a C2 NRF rating for his work in algebra and lattice theory.

Prof Moshokoa (Tshwane University of Technology) visited Patras University, Greece, to collaborate on topology and analysis.

Dr Rathilal (University of KwaZulu-Natal) co-organised a Topology for Tomorrow session at the AIMS Siyakhula Festival, featuring a talk on Topological Data Analysis by Prof Ulrike Tillmann. Dr Rathilal also presented joint work in Korea, and participated in a workshop at the Isaac Newton Institute.

### New Talent

One of the programme's biggest achievements in 2024 was attracting two postdoctoral researchers, Dr Caviglia and Dr Mesiti, specialising in category theory, algebra, and logic. They collaborated across universities and disciplines, organised the Future Mathematicians Programme at the South African Mathematical Society Congress, and hosted Prof Dorette Pronk for a keynote and visits to work with them and Dr Rathilal.

### Strategic Vision

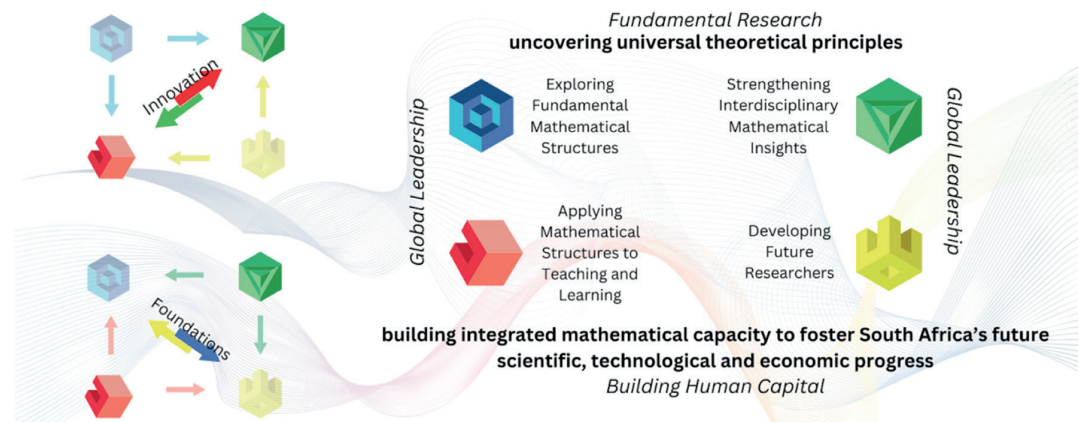
The most significant achievement of 2024 was the development of a framework for the proposed Focus Area in Mathematical Structures for Foundations and Innovation (2025–2026). This framework reflects a vision where South African mathematics

contributes to national prosperity, global scientific leadership, and education.

Investment in theoretical mathematics cultivates abstract reasoning and structural thinking – the very skills driving innovation in cryptography, machine learning, and space science. Yet, much of South Africa’s mathematical talent exists in silos, limiting its impact. By fostering collaboration across disciplines, institutions, and generations, the Focus Area aims to:

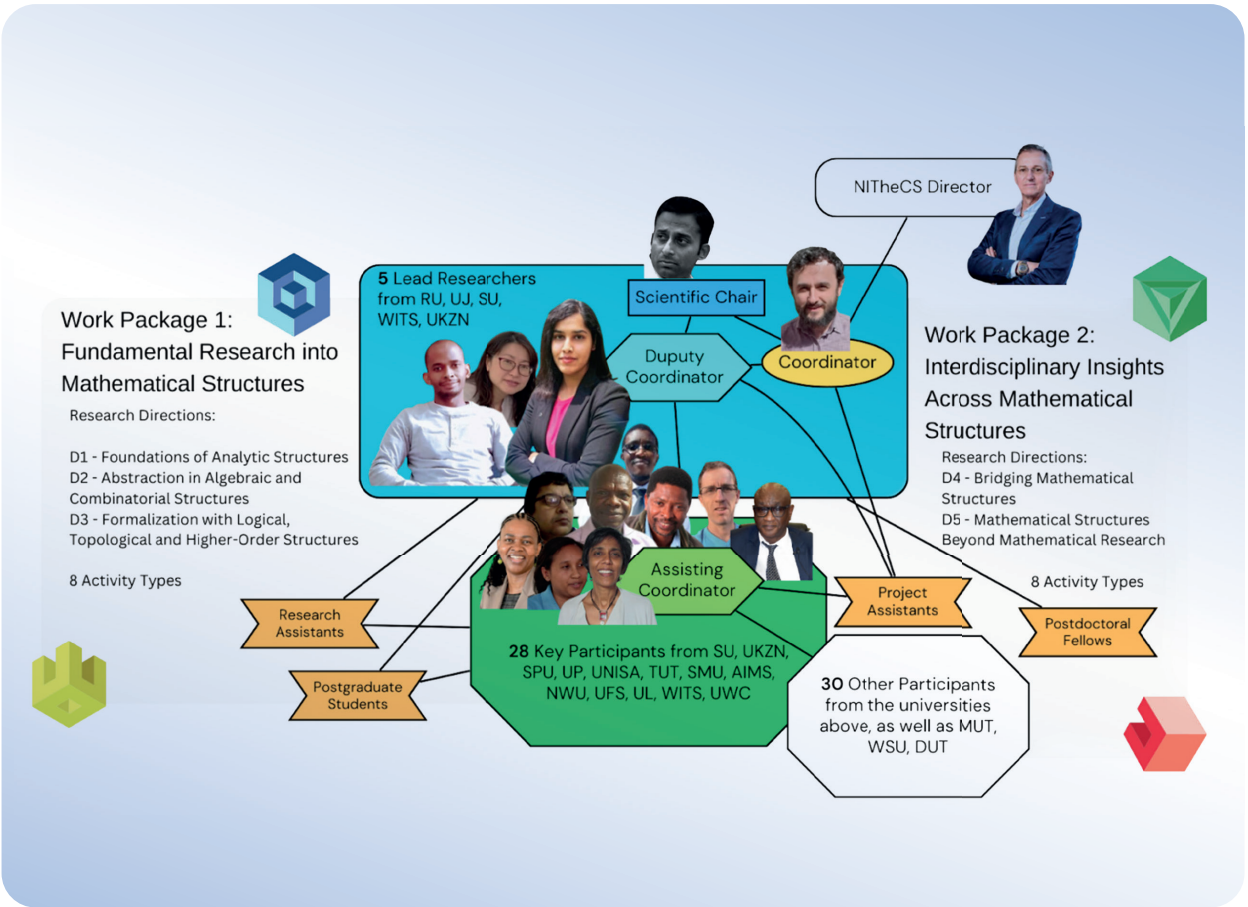
- Break down silos in theoretical research.
- Connect foundational mathematicians with educators and school learners.
- Address challenges in mathematics teaching and learning.
- Translate abstract research into societal impact and national innovation.

The 2024 framework structures the work into two work packages and five research directions, with five lead researchers coordinating up to 60 collaborators across South African universities. This approach strengthens the community of mathematicians while linking research excellence to education and societal advancement.



**“2024 was a year of change and progress.”**

– Prof Andronikos Paliathanasis  
Durban University of Technology



**“What I love about NITheCS is its commitment to nurturing emerging scholars and strengthening South Africa’s research ecosystem. Being part of this community has been truly energising.”**

– Prof Dephney Mathebula  
 University of Fort Hare



**“NITheCS has allowed me to follow important classes through the links posted. It has been a great platform of learning.”**

– Miss Eunice Ngomba  
 Rhodes University



## 6. Quantitative Finance



As 2024 draws to a close, the Quantitative Finance Research Program (QFRP) at NITheCS reflects on a year of growth, collaboration, and impactful contributions to

quantitative finance. Under the leadership of Prof Mesias Alfeus (*above*), the program continues to advance research at the intersection of mathematics, finance, and technology, with a strong focus on real-world applications that benefit both the financial industry and broader society.

### Advancing Knowledge and Collaboration

In 2024, QFRP made significant strides in theoretical and applied finance. Key projects explored novel methodologies in financial risk management, particularly in understanding market dynamics in emerging markets. Highlights include ongoing studies of the Cox-Ingersoll-Ross (CIR) model with jumps to model the forward spread between JIBAR and ZARONIA, providing insights into South

Africa's risk-free rate. Researchers also contributed to the South African Fine Wine Index (SAFW10), using stochastic modeling to identify high-quality investment opportunities in the wine sector.

The programme advanced sustainable investment strategies by exploring how quantitative methods can improve portfolio decisions, especially under climate-related risks. Collaborations with industry leaders and policymakers ensured that QFRP's research remains relevant to both financial and environmental sustainability goals.

### Fostering Academic and Industry Partnerships

QFRP strengthened partnerships with academic institutions and industry stakeholders, notably through the SU-GARP Academic Partnership at Stellenbosch University. Participation in high-profile conferences – including the 15th Annual Financial Market Liquidity Conference in Budapest and the Quantitative Methods in Finance conference in Sydney – expanded the program's impact and provided a platform for sharing new research.

Research on the role of financial instruments in supporting sustainable development gained attention from policymakers.

Analyses that include emerging markets are helping shape discussions on how financial innovation can drive inclusive and sustainable economic growth.

### Engaging the Next Generation of Researchers

Mentorship and training remain a cornerstone of QFRP. In 2024, the program hosted seminars, workshops, and guest lectures, giving students and early-career researchers exposure to cutting-edge quantitative finance research. The September NITheCS-QFRP Workshop, which attracted leading academics and practitioners worldwide, was a standout event fostering collaboration and learning.

### Outreach and Societal Impact

QFRP's societal contributions extend beyond academia and industry. Research on wine investment, exemplified by the SAFW10, bridges finance and agriculture while boosting South Africa's global wine presence. Work on climate-related financial risk models supports global efforts to tackle climate change, demonstrating the program's commitment to research that generates tangible societal value.



## 7. New Insights into Astrophysics and Cosmology

During 2024, the **New Insights into Astrophysics and Cosmology** project made substantial progress towards its scientific and capacity-development objectives. Research activities focused on advancing theoretical models in astrophysics and cosmology and confronting them with cutting-edge observational data from multi-messenger and cosmological surveys.

Key scientific outputs were achieved across the project's core themes. In multi-messenger astrophysics, the team produced high-impact work on high-energy neutrinos, gamma-ray bursts, compact binary mergers, and ultra-luminous X-ray sources, combining observational data with advanced machine-learning and neural-network techniques. Several studies addressed neutrino propagation, quantum complexity, and transient source identification using IceCube, LIGO-Virgo, and gamma-ray datasets. In cosmology and gravity, significant progress was made on modified gravity theories, interacting dark energy models, dynamical systems approaches, and large-scale structure probes, including correlations involving the

thermal Sunyaev–Zel’dovich and integrated Sachs–Wolfe effects.

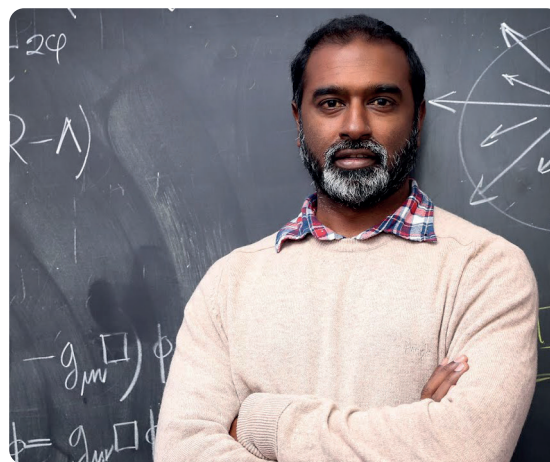
These efforts resulted in a strong publication record during the reporting period, including multiple papers published in leading international journals such as JCAP, Monthly Notices of the Royal Astronomical Society, The Astrophysical Journal Supplement Series, and European Physical Journal C. The breadth and quality of outputs demonstrate clear alignment with the project’s original objectives and international competitiveness.

The project continued to play a significant role in human-capacity development. Postdoctoral researchers, PhD candidates, and MSc students across several South African institutions were actively involved in research, co-authoring publications and gaining advanced training in data analysis, theoretical modelling, and computational techniques. Collaboration across institutions was maintained, strengthening national research networks and contributing to skills development in priority areas of astrophysics and cosmology.

Overall, the 2024 activities reflected strong progress, effective use of resources, and measurable scientific impact, having

involved over 20 researchers, including postdocs and postgraduate students, and with over 20 papers published during the stated project year.

## 8. Quantum Technologies for Sustainable Development



The 2024 NITheCS focus area on **Quantum Technologies** fostered collaboration between prominent research groups led by PIs mentioned above. These teams pursued cutting-edge investigations across quantum computing, quantum complexity, quantum

communication, and quantum machine learning, with possible applications to future Universal Fault-Tolerant quantum devices and currently existing Noisy Intermediate-Scale Quantum (NISQ) devices. The programme produced significant outputs in complexity theory, algorithm development, theoretical assistance to experimental optics, and training of postgraduate students.

### Key milestones included:

- Demonstrating Krylov complexity as a diagnostic tool for quantum criticality.
- Introduction of a scalable multi-class quantum kernel classifier.
- Accurate characterisation of the Markovian quantum noise in NISQ devices.

Turn over to the next spread to see the **Quantum Technologies 2024 Highlights** within Research, Collaborations and Partnerships, and Human Capacity Development.

## Research Highlights

### Haque & Murugan Group:

- Studied quantum complexity in many-body systems to understand chaos and phase transitions.
- Used the Kitaev chain to show that Krylov complexity detects topological phase transitions.
- Analysed Krylov complexity and spectral form factors in noisy random matrix models, identifying novel sensitivity to decoherence.
- Extended Krylov complexity methods to Jacobi coherent states in quantum optics.

### Konrad Group:

- Investigated local entanglement in Mathieu-Gauss vector modes, demonstrating Bell inequality violations in spatial-polarisation modes.
- Developed nonlinear optical techniques for correcting distorted spatially-structured light.
- Published a high-impact study in Nature Communications showcasing quantum teleportation of spatial modes using nonlinear detectors.
- Explored teleportation schemes for full light states and proposed optimal quantum cloning with structured light.

### Sinayskiy Group:

- Designed a novel multi-class quantum kernel classifier using a SWAP test architecture that remains qubit-efficient and noise-robust.
- Simulated convex mixtures of Markovian and non-Markovian quantum channels on NISQ hardware.
- Developed a hardware-agnostic framework for modelling quantum device noise.
- Investigated optimiser performance for QAOA under realistic noise, identifying SPSA and ADAM optimisers as top performers.
- Introduced hybrid genetic methods for designing quantum feature maps and ensemble-based quantum classifiers.

## Collaborations and Partnerships

### Strong academic partnerships:

- 1. Haque & Murugan:** Collaborated with Caputa (Warsaw) and Bhattacharyya (IIT-Gandhinagar).
- 2. Konrad:** Partnered with Forbes (Wits) and Perez-Garcia (Mexico).
- 3. Sinayskiy:** Continued long-standing collaboration with Petruccione (SU).

These collaborations were critical in delivering high-impact research and supporting transcontinental knowledge exchange.

### Outputs:

A total of 14 peer-reviewed journal articles were published in 2024.

- 1. Haque & Murugan:** 3 papers, including JHEP articles on quantum complexity.
- 2. Konrad:** 5 papers, including in Nature Communications and Advanced Photonics.
- 3. Sinayskiy:** 6 papers in Scientific Reports, EPJ Quantum Technology, and Quantum Machine Intelligence.

## Human Capacity Development

- Students Graduated: 4 (3 MSc, 1 PhD).
- Total Personnel Trained: 13 (10 students, 3 postdocs).

# PUBLICATIONS

At NITheCS, research is not only about discovery – it is about contributing to the global body of knowledge through publication. By sharing their findings in peer-reviewed journals, conference proceedings, and book chapters, our Associates play a crucial role in shaping the theoretical and computational sciences both locally and globally. Publications help to validate research outcomes, facilitate scientific discourse, and inspire new lines of inquiry within and beyond their respective disciplines.

Beyond advancing knowledge, publication enhances the credibility and visibility of our Associates. A well-documented track record of published research increases public trust, strengthens their reputations, and can open doors to funding opportunities, international collaborations, and interdisciplinary projects. It also enables our Associates to contribute meaningfully to the scientific landscape, reinforcing our commitment to research and innovation.

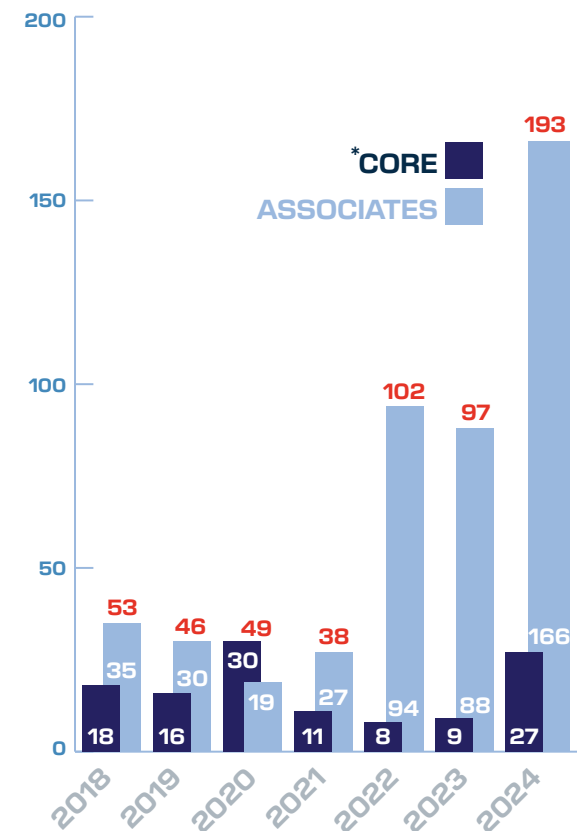
In 2024, we are pleased to report a significant increase in publications by NITheCS Associates. This growth is partially

due to both the rising number of NITheCS Associates and the supportive research environment that NITheCS fosters – one that actively encourages researchers to conduct high-quality studies and publish their findings.

Since 2018, NITheCS publications have grown from 53 to 193 by 2024, reflecting a significant increase in community engagement and a strong adoption of NITheCS as an affiliation in publications. In 2025, NITheCS will continue to encourage its associates to include the affiliation in their publications to further demonstrate the community’s activity and impact.



Number of publications per year:



\* Publications by NITheCS Executive Management Committee members or Postdoctoral Researchers.

# GOVERNANCE

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

Although Stellenbosch University provides administrative support, NITheCS operates in an independent environment.

The leadership structure of NITheCS is designed to ensure strategic coherence, research excellence, and effective regional implementation. It comprises three interconnected bodies: Steering committee, Scientific Advisory Board, and Executive Management Committee

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## The NITheCS Team

Our team is the foundation of our mission to advance theoretical and computational sciences across South Africa and beyond.

Our dedicated staff bring a wealth of expertise, experience, and enthusiasm to their roles, working collaboratively to support research, education, and public engagement.

From operations and administration to academic coordination and outreach,

each team member plays a vital part in ensuring the success and impact of NITheCS initiatives.

The Hub team at Stellenbosch University (*pictured right*), handles administration, hosting, research and capacity development and work closely with the Nodes and Branches to ensure that everyone contributes meaningfully to NITheCS's strategic vision.



**Prof Francesco Petruccione**  
Director



**René Kotzé**  
Institute Manager



**Nelisiwe Mncube**  
Senior Administrative Assistant



**Farah-Naaz Samuels**  
Senior Administrative Assistant



**Mbali Kunene**  
Administrative Officer

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**NITheCS**

National Institute for  
Theoretical and Computational Sciences