

Developing a Sustainable High Performance Computing Ecosystem: A Case Study of Southern Africa

Dr Happy Sithole

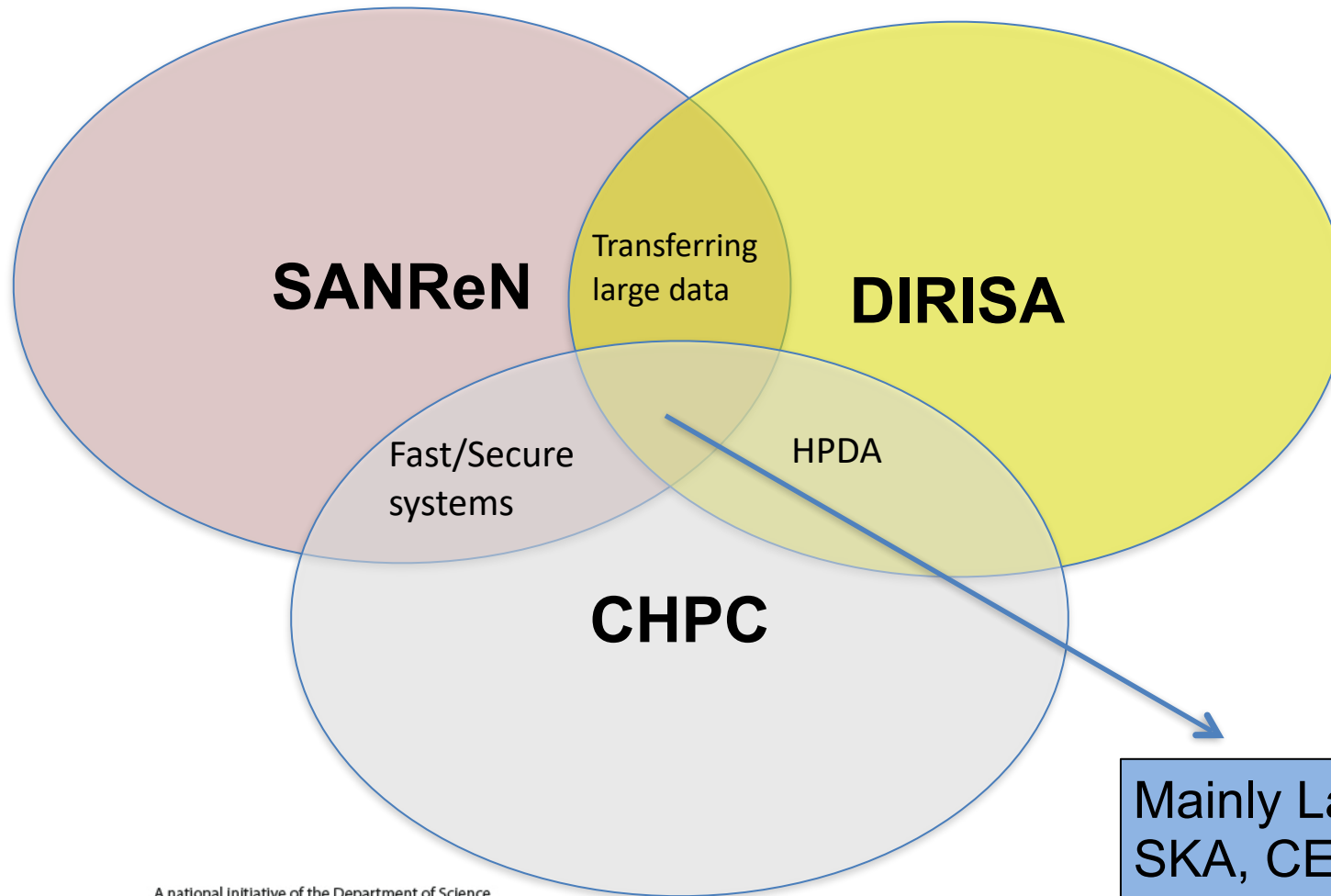
25 September 2023

A national initiative of the Department of Science and Innovation and implemented by the CSIR



science & innovation
Department
Science and Innovation
REPUBLIC OF SOUTH AFRICA





- Common services between any two entities of NICIS
- Intersection of the three entities most crucial, as defines the success of overall NICIS.
- Development of cross-cutting skills internally and within the community

Mainly Large Scale Science projects:
SKA, CERN, 4IR, SADC C.I. Framework,
Climate Change (e.g. IPCC)

A national Initiative of the Department of Science
and Innovation and Implemented by the CSIR

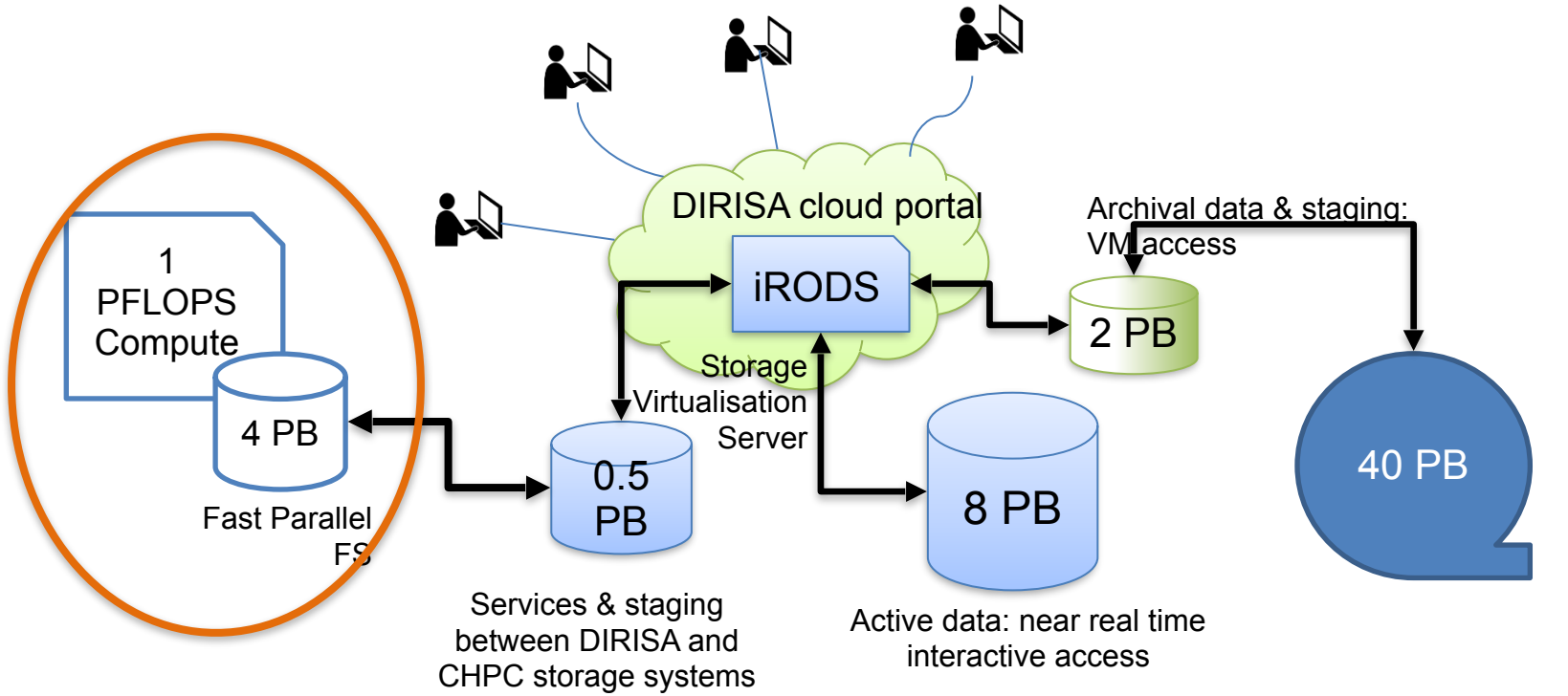


Strategic Objectives

- SO1** • Sustain a **world class** and relevant **national integrated cyberinfrastructure system** for Science and Technology
- SO2** • Enable and promote **eScience** in South Africa.
- SO3** • Position South Africa to take part in, host and **lead large scale global research and science projects** (e.g. SKA and CERN experiments).
- SO4** • Provide **thought leadership** to South Africa's evolving cyberinfrastructure strategy and activities, and facilitate the uptake of advanced cyberinfrastructure.
- SO5** • Foster the development of **human capacity in cyberinfrastructure and its application**, and contribute to the transformation of this sector.

A national Initiative of the Department of Science and Innovation and implemented by the CSIR

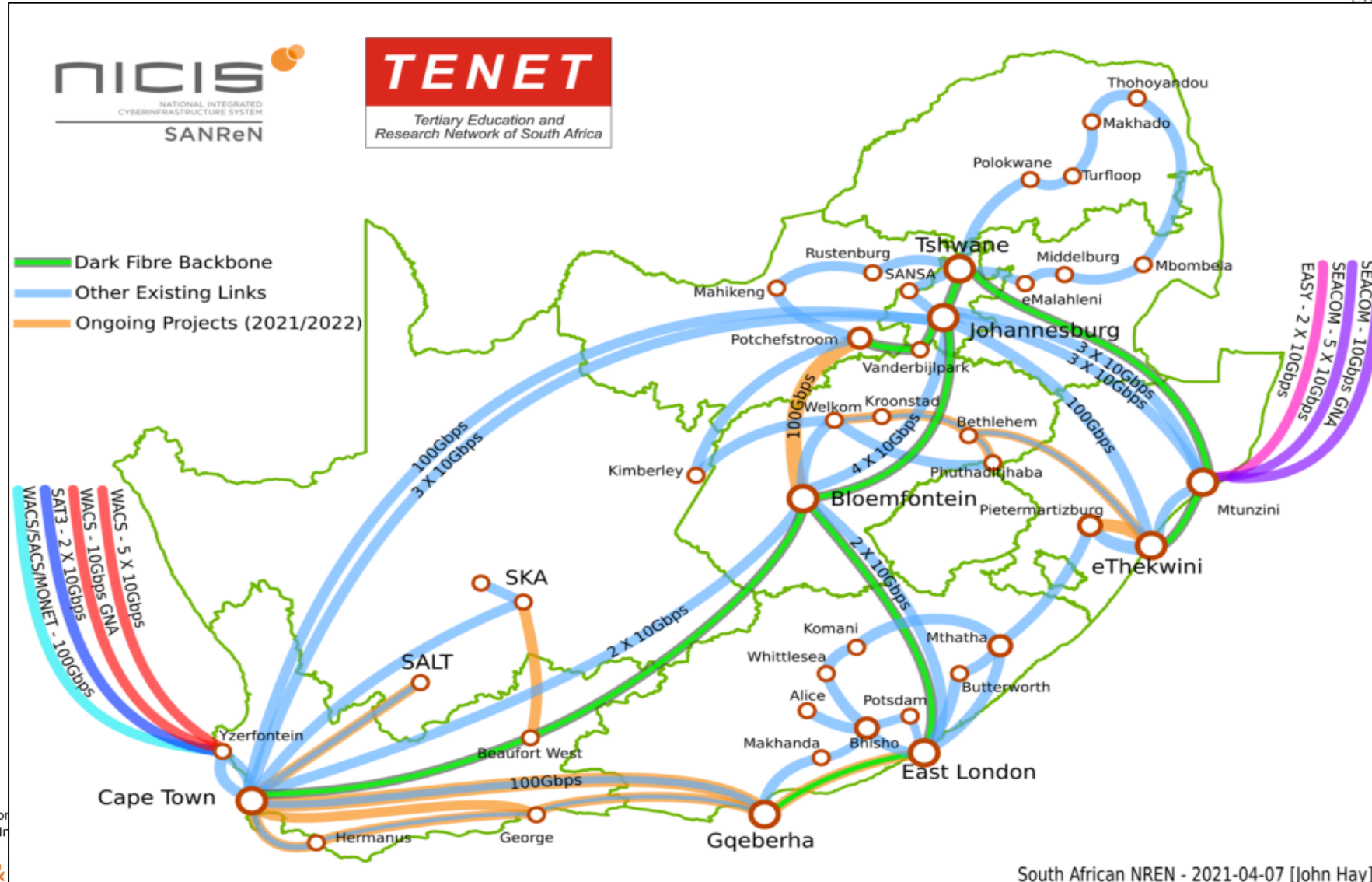




- Open (FAIR) Data & Open Science
- Federated locally and globally (“One-stop-shop” catalogue)
- Certified as Trusted Repository
- Linked to funder systems
- Suite of services for RDM and data intensive analytics

A national Initiative of the Department of Science and Innovation and implemented by the CSIR

Network Infrastructure



A nation and In

South African NREN - 2021-04-07 [John Hay]

NICIS Platforms



- **Lengau = “Cheetah”**
- **Installed 2015 with 1.6 PFLOP performance**
- **1 345 Nodes of INTEL processors**
- **Rear-door water cooling system**
- **7 Petabytes of Lustre storage**
- **Close to 100% utilisation**



- **GPU Cluster with 9 Nodes each with 4 NVIDIA – V100 processors.**
- **Mainly used for Machine Learning, Artificial Intelligence and Materials Science applications.**



- **OpenStack Cloud named SEBOWA**
- **52 Nodes with INTEL processors**
- **Installed in March 2020**
- **Used for many applications including COVID-19 Data Services**



- **CERN Tier-2 Grid facility**
- **Supports ALICE and ATLAS experiments**

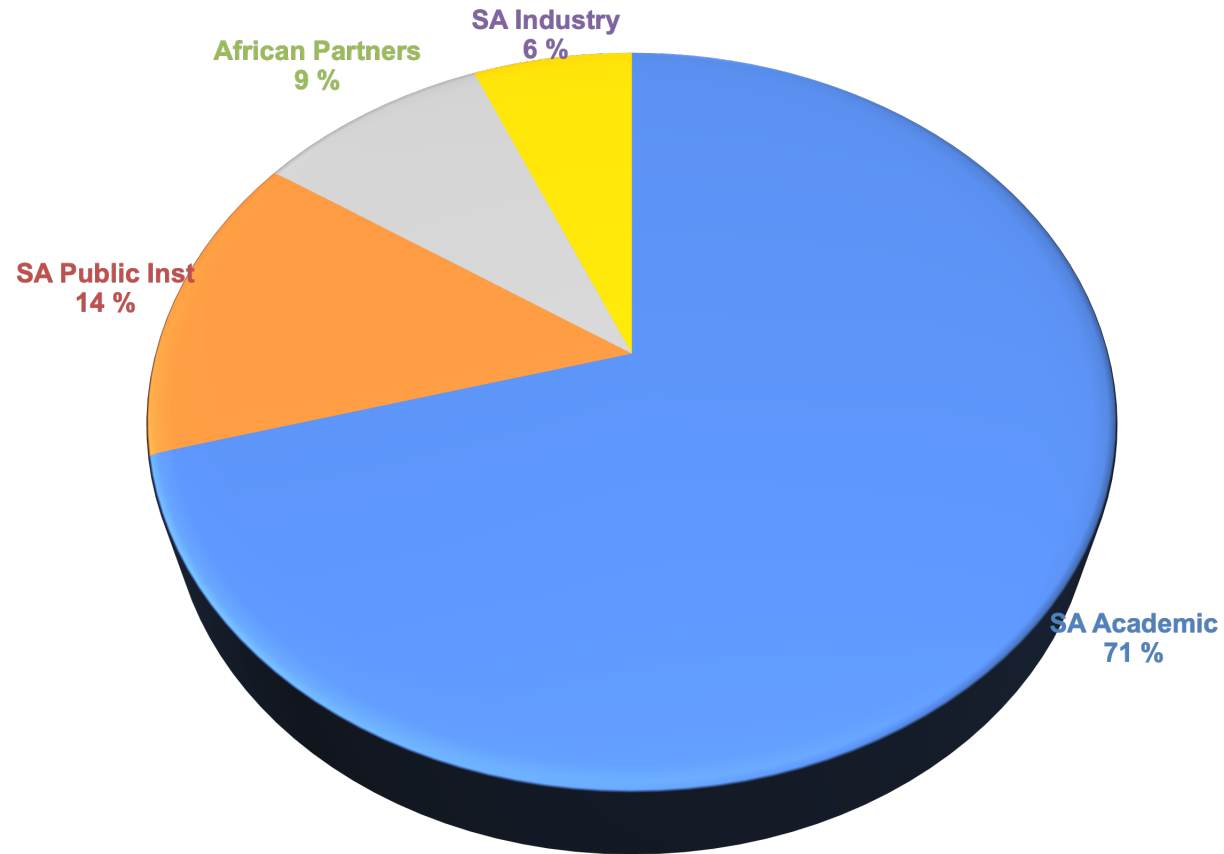
of the Department of Science
and implemented by the CSIR

Research in Technology



- Evaluate technology for HPC and cloud
- Investigate and develop technology to improve HPC systems
- Provide a consulting service for HPC and cloud technology
- Collaborate with users with special applications to drive efficiency
- Operate experimental systems

User Categories

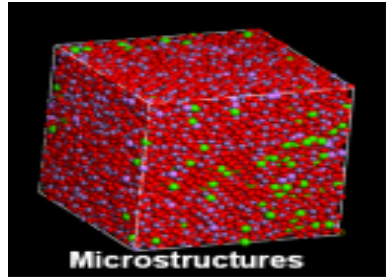


A national initiative of the Department of Science and Innovation and implemented by the CSIR



HPC Applications: Materials

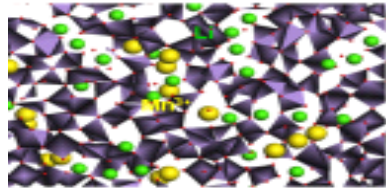
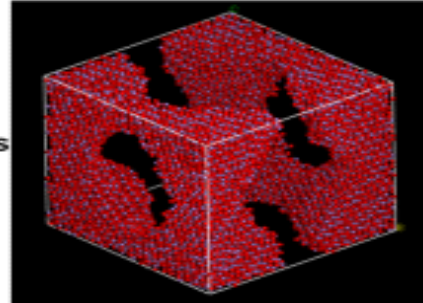
Materials Science / Chemistry / Health



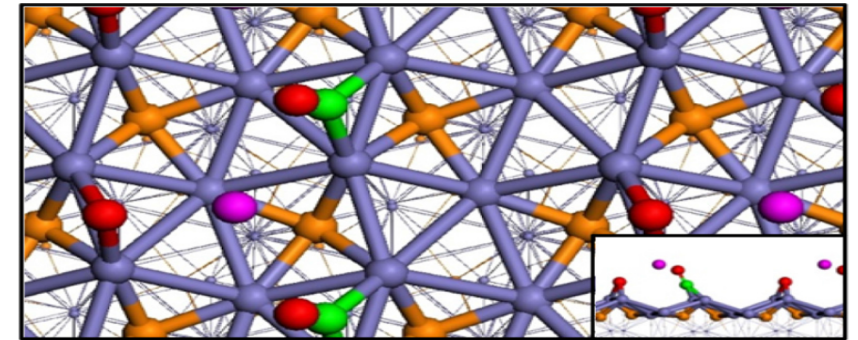
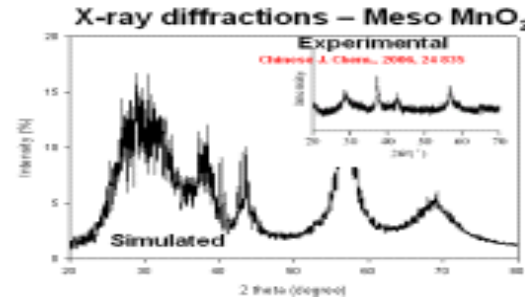
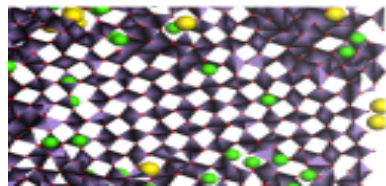
Amorphisation Recrystallisation Grown MnO₂

Lithiated MnO₂
Li_{0.1}MnO₂

Meso-porous



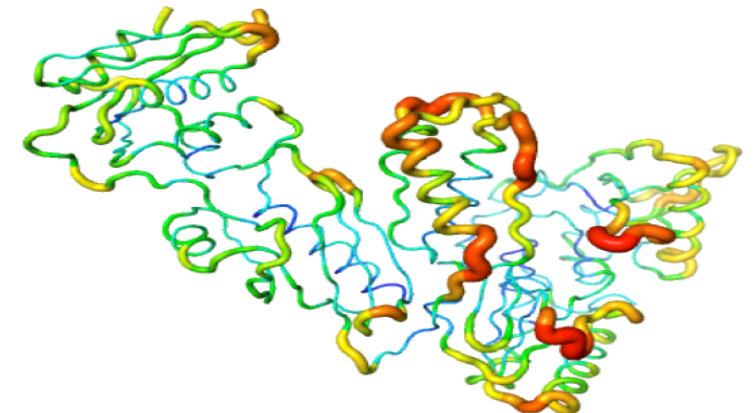
Mn⁴⁺



Computational Catalysis
(Comp Chem / Materials Science)

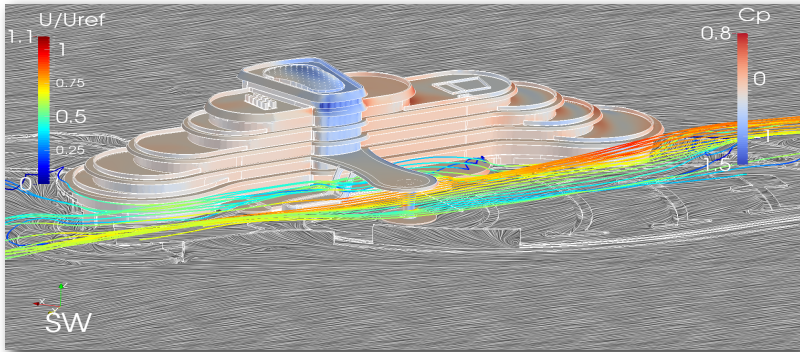
**Energy Storage – Battery
Development**
(Materials Science)

**Drug-Design Molecular
Modelling**
(Computational Chemistry)

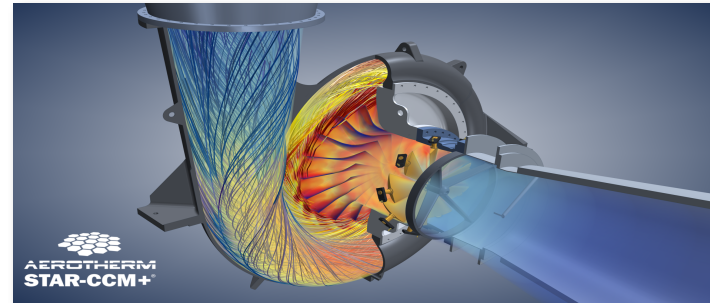


HPC Applications: Engineering

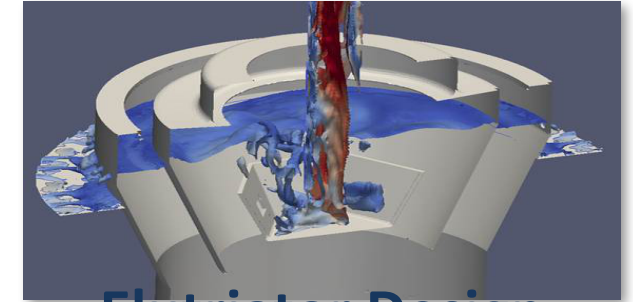
Computational Mechanics / Engineering



Building aerodynamics
(ECI-JV)

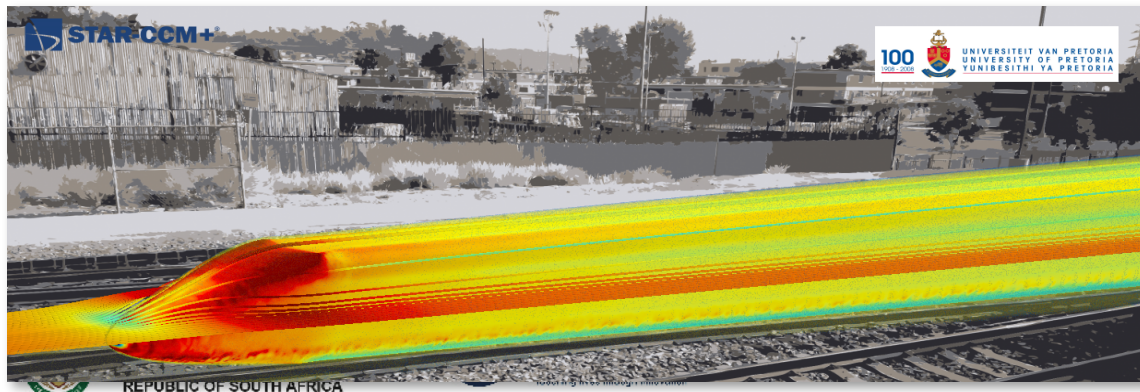


Centrifugal Steam Compressor
(Aerotherm)



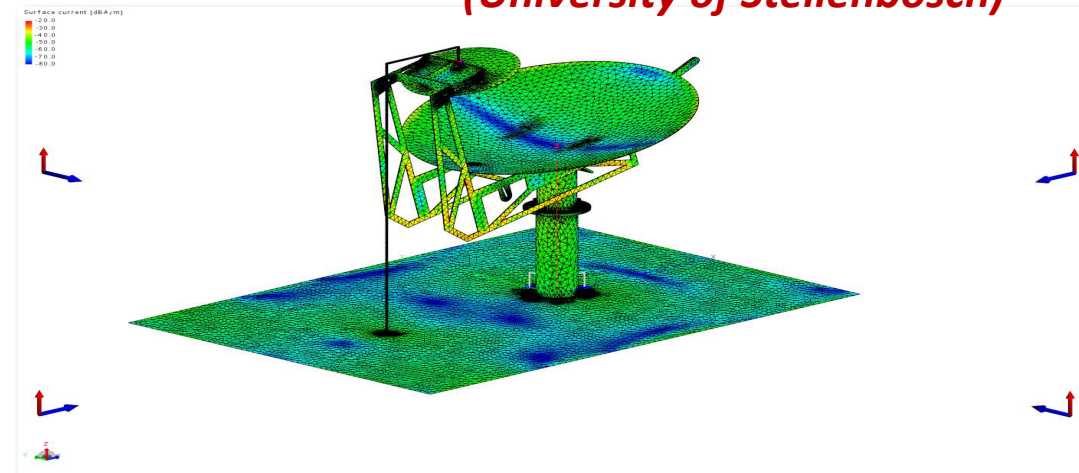
Elutriator Design
(De Beers Marine)

High-speed Train Design *(UP):*



Radio-Astronomy Dish Design

(University of Stellenbosch)

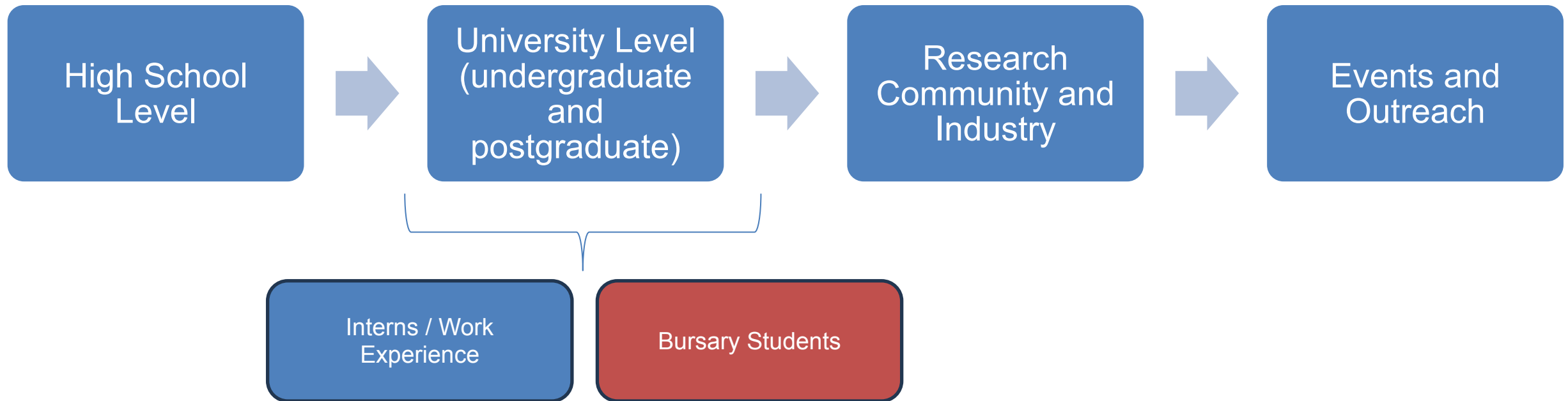


HPC Applications: Astronomy

- **Testing and Evaluation** of compute, network and data infrastructures
- Data Transfer Node (**DTN/Globus**) Setup
- Active **Research Programme** at CHPC (Software Requirements, Benchmarking Imaging Pipelines, etc.)
- Physical **Hosting of MeerKAT Data Servers**
 - Peraplex Data Storage Pods (20 PB)
 - IBM Tape Library (>20 PB)



NICIS HCD Pipeline



A national initiative of the Department of Science and Innovation and implemented by the CSIR

High School Level

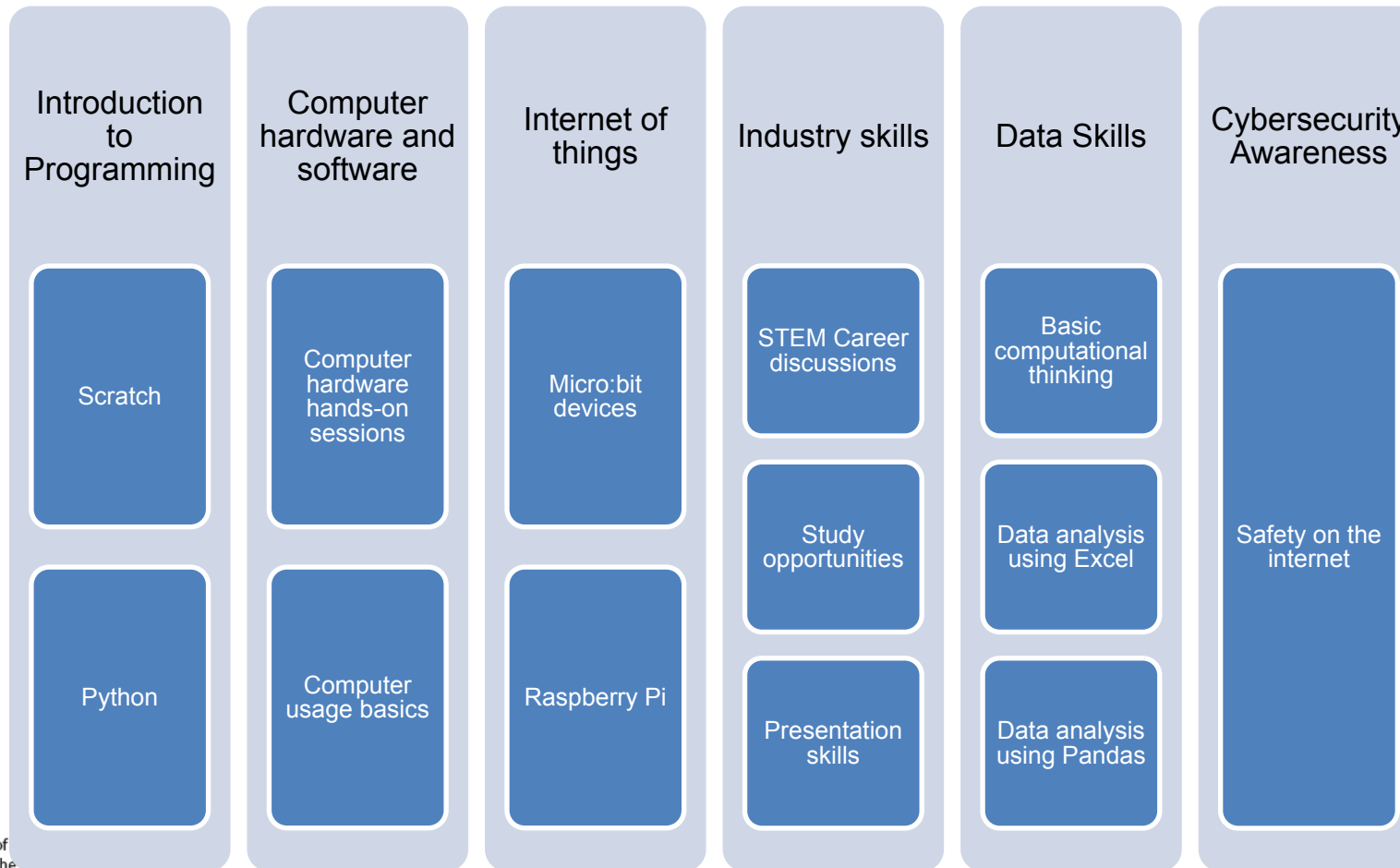
- DIRISA Coding School
 - Introducing python programming and data science concepts to high school learners
- CHPC Learn how to code
 - Introducing scratch programming to high school learners



A national initiative of the Department of Science and Innovation and implemented by the CSIR



High School Level



A national Initiative of the Department of
and Innovation and Implemented by the



University Level

- CHPC Student Cluster Competition (SCC)
 - Promote and develop HPC skills in undergraduate students
- DIRISA Student Datathon Challenge (SDC)
 - Promote data skills and problem solving through technology.
- SANReN Cybersecurity Challenge (CSC)
 - Promote interest in Cybersecurity
- Annual competitions have selection, national and international rounds
- Participation across all provinces and universities in South Africa and also includes SADC region



University Level

Student Cluster Competition

Build super-computer

Reproducibility challenge

Test benchmarks

Apply optimization techniques

Cybersecurity Challenge

Capture the Flag

Attack and Defend teams

Social engineering attacks

Hacking challenge

Student Datathon Challenge

Data Exploration Modelling and Visualisation

Artificial Intelligence, Machine Learning and Natural Language Processing

Problem solving using data and technology

Conducting research and producing poster / abstract

A national Initiative of the Department of Science and Innovation and implemented by the CSIR



University Level

- CHPC Monthly Coding Challenges
 - Learning continuation after coding summer school.
- DIRISA Datathon Training
 - Continued training programme linked to the Datathon Challenge
- National E-Science Postgraduate Teaching and Training Platform (NEPTTP)
 - Develop human capital skills to conduct cutting-edge research in the field of e-Science i.e. South African Research Infrastructure Roadmap (SARIR), the Square Kilometre Array (SKA) etc.
- SANReN Guest Lectures and Training
 - Presentations on cybersecurity awareness and training focusing on network security and social engineering at SU / Android security and pen testing at RU
 - Postgraduate Modules at UWC (Information security risks / Mobile security forensics)

A national initiative of the Department of Science
and Innovation and implemented by the CSIR



Research Community and Industry

NICIS
NATIONAL INTEGRATED
CYBERINFRASTRUCTURE SYSTEM

- SANReN TRANSITS Training
 - Computer Security and Incident Response Team (CSIRT) personnel training. Expertise in operational, organisational, legal and technical areas.
- CHPC-NITheCS-ICTP (International Centre for Theoretical Physics) Training
 - HPC for sustainable development
- CHPC-NITheCS Coding Summer School
 - Train researchers in various domains on fundamentals of python, bash, data science, HPC and computational sciences.
- HPC Ecosystems Training
 - System administrators, OpenHPC. Africa wide.
- SIGHPC Education Global Seminar Series

A national initiative of the Department of Science
and Innovation and implemented by the CSIR



science & innovation
Department
Science and Innovation
REPUBLIC OF SOUTH AFRICA



Research Community and Industry

- DSI Hardware and Coding Workshops
 - Train representatives from all provinces on robotics and coding
- BRICS Future Skills Challenge
 - Multi-day online skills Olympics across BRICS nations focused on solving real world problems in specific future skills area.
 - SANReN Cybersecurity expert – Dr Heloise Meyer.
- CHPC Winter School
 - Practical HPC course and Parallel Programming. Intermediate course on using HPC cluster and parallel programming.
- CHPC Induction Course
 - Self-study online course to introduce the CHPC cluster and functions



A national initiative of the Department of Science
and Innovation and implemented by the CSIR



science & innovation
Department
Science and Innovation
REPUBLIC OF SOUTH AFRICA



Events and Outreach

- NICIS National Conference
- DIRISA National Research Data Workshop
- SANReN ZA-REN Week
- Attending various expo's:
 - World Science Forum
 - Working World Expo 2023 / World of Work Week
 - International Super Computing Conference (ISC) 2023, HPC 2023
 - International Data Week (IDW) 2023
 - CSIR-NICIS Nelson Mandela Day Outreach
 - National Science Week



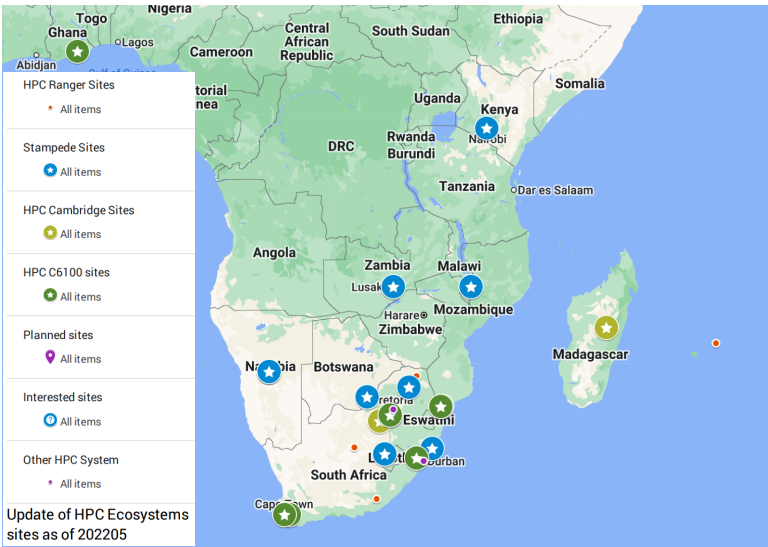
A national initiative of the Department of Science
and Innovation and implemented by the CSIR



science & innovation
Department
Science and Innovation
REPUBLIC OF SOUTH AFRICA

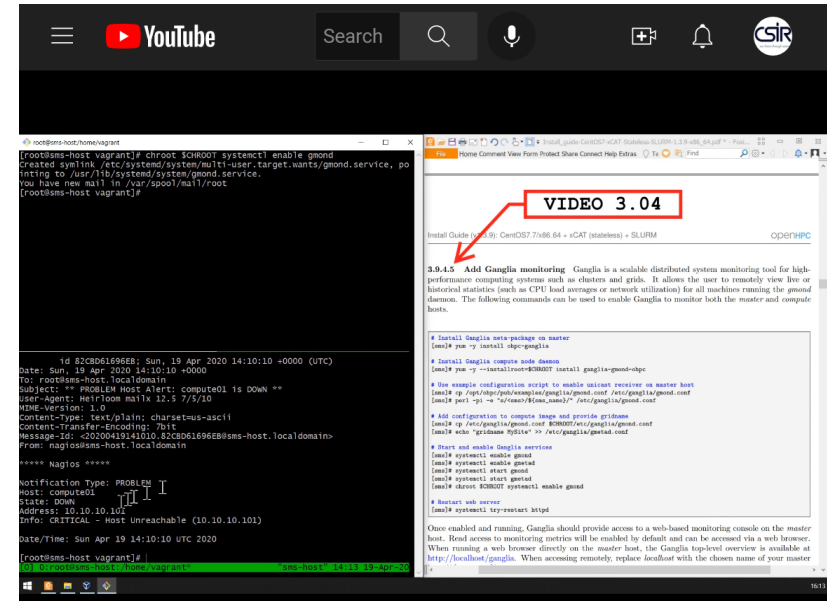


35 systems in 12 countries.
Trained 400+ HPC SysAdmins.



- UFH
- UL
- UniVen
- UNMW- Mahikeng
- Sol Plaatjie
- UKZN
- US
- Wits
- UniZulu
- DUT
- UM
- SMU

Online OpenHPC Virtual Training Lab



VIDEO 3.04

```
[root@ms-host vagrant]# chroot /sbin/systemd enable gmond
Created symlink /etc/systemd/system/multi-user.target.wants/gmond.service, pointing to /usr/lib/systemd/system/gmond.service.
You have new mail in /var/spool/mail/root.
[root@ms-host vagrant]#
```

```
1d 82CB061696E8: Sun, 19 Apr 2020 14:10:10 +0000 (UTC)
Date: Sun, 19 Apr 2020 14:10:10 +0000
To: root@ms-host.localdomain
Subject: ** PROBLEM Host Alert: compute01 is DOWN **
User-Agent: NetFlow n2lix 12.5 7/5/10
MIME-Version: 1.0
Content-Type: text/plain; charset=us-ascii
Content-Transfer-Encoding: 7bit
Message-ID: <20200419141010.82CB061696E8@ms-host.localdomain>
From: nagios@ms-host.localdomain

***** Nagios *****

Notification Type: PROBLEM
Host: compute01
State: DOWN
Address: 10.10.10.102
Info: CRITICAL - Host unreachable (10.10.10.10)

Date/Time: Sun Apr 19 14:10:10 UTC 2020

[root@ms-host vagrant]#
```

Website: www.nicis.ac.za

A national initiative of the Department of Science
and Innovation and implemented by the CSIR



science & innovation
Department
Science and Innovation
REPUBLIC OF SOUTH AFRICA

