

High Performance Computing Impact

Happy Sithole
NICIS, South Africa
23 September 2024

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



Introduction to CHPC



Digital Research Infrastructure: HPC Systems

- ❑ Lengau cluster since **7 March 2017** (First phase June 2016)
- ❑ Africa's first Petascale system \Rightarrow **1.029 PFlops = 1 029 TFlops**

(121st on Top500* – June 2016)

(127th on Top 500* – June 2017)

Lengau (HPC Cluster)

- 1386 nodes
- 32 832 cores
- 30 V100 GPUs
- 56Gbps IB interconnect
- 4PB Lustre storage
- ~1Pflop/s HPL



Deployed in 2016/17
Debut at 121 on Top500

Special Nodes

- 5 High memory nodes
- 30 GPU nodes

Future: New HPC Cluster at the CHPC

- ❑ HPE/Intel Emerald Rapids 4PF HPC Cluster
- ❑ Cluster Commissioning: Nov/Dec 2024 (estimation...)
- ❑ Some details of the new HPC system:
 - **512 EMR Compute Nodes with 2*8593Q 2.2GHz 64-cores 385W**
 - **Compute Interconnect Network : NDR200**
 - **Administration network : 10GbE**
 - **Layout : 10 racks : 9*800 + 1*600 = 7,800mm**
 - 8 racks for compute nodes (800mm)
 - 1 rack for service nodes (600mm)
 - 1 rack for interconnect (800mm)
 - **Estimated Utilization Power Consumption for the solution : 690KW**

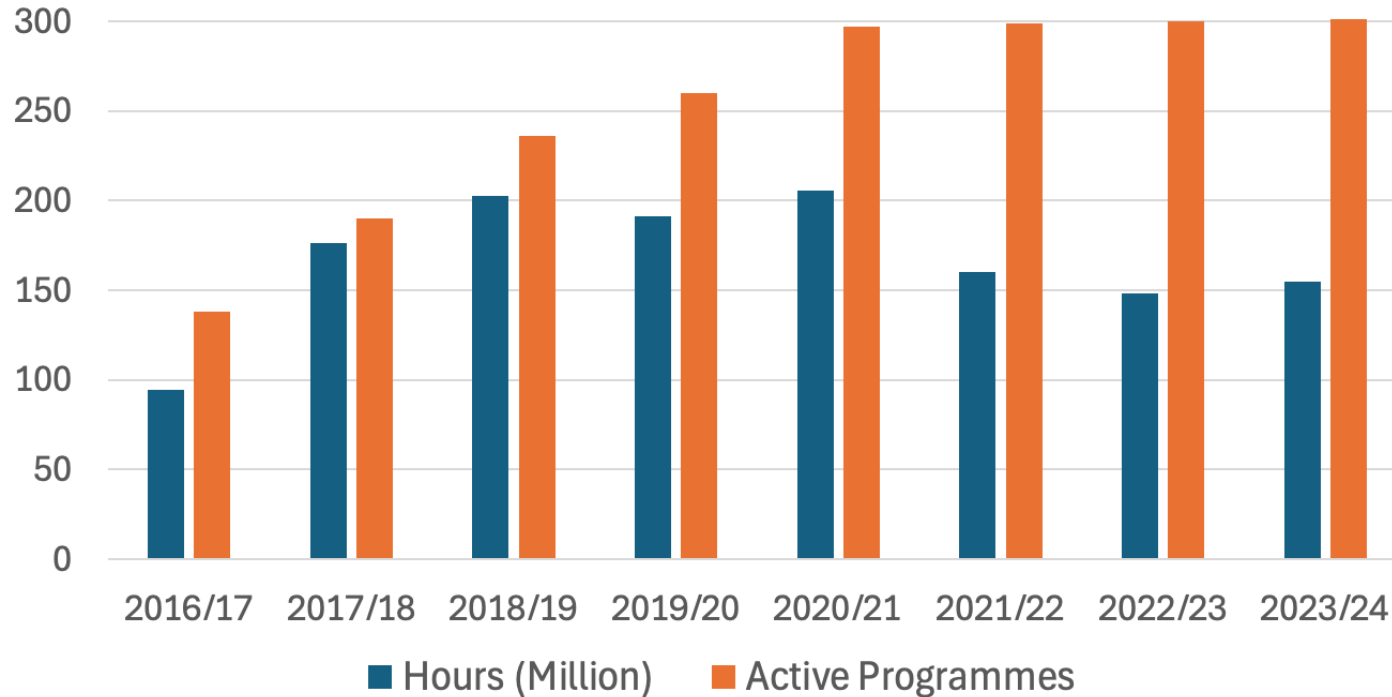
CHPC Lengau Cluster Usage

(Status: 15 Aug 2024)

	All Time	6 Months
❑ Total Active* Research Programmes	573	257
❑ Total Core Hours Used (Million)	1311	79
❑ Total Active Users	2540	882

** Active refers to usage of more >1000 core hours*

CHPC Cluster Usage: *Past 8 Years Trend*

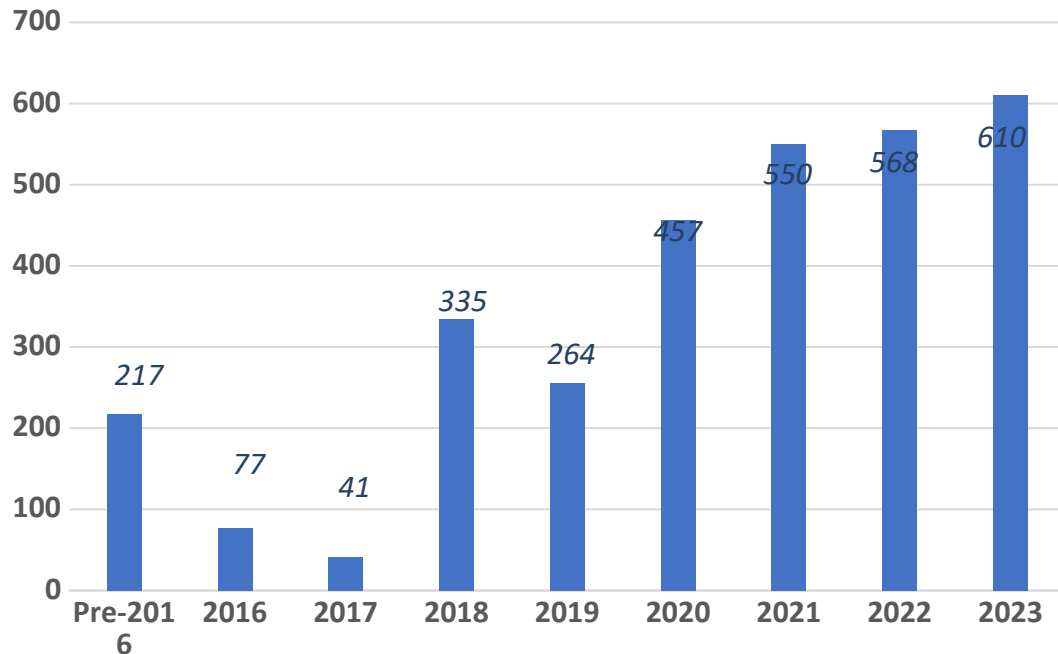


** Active refers to usage of more >1000 core hours*

CHPC User Research Outputs: 2007-2023

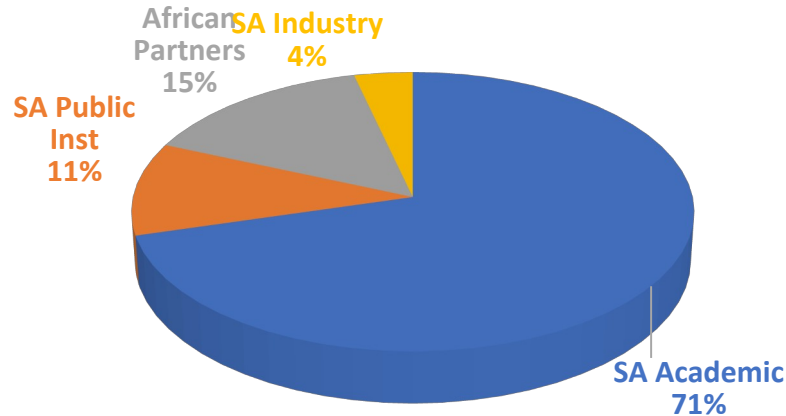
Total Research Outputs Count Per Calendar*

Year



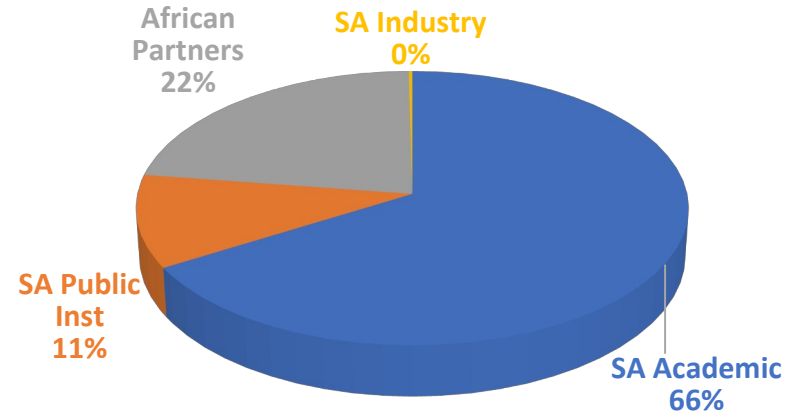
Total Number of
Research Outputs*:
3111

CHPC User Categories **Total Active* Programmes** Past 6 Months *(until 15 Aug 2024)*



Active Programmes

Total: 269



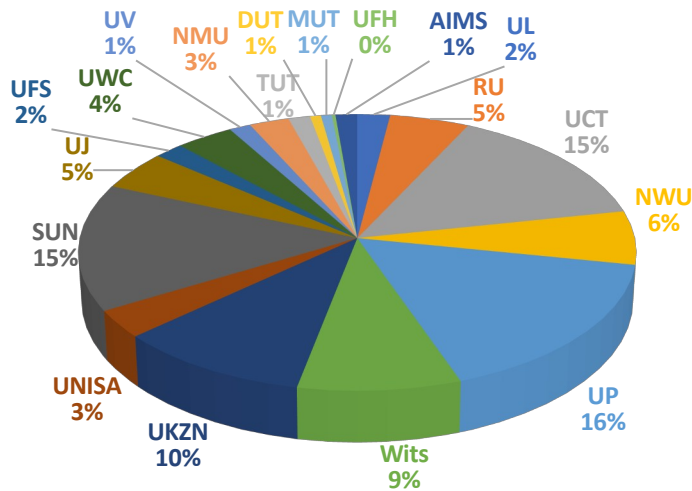
Hours Used (Million)

Total: 109 million

**Active refers to at least 1000 compute hours used over the relevant period.*

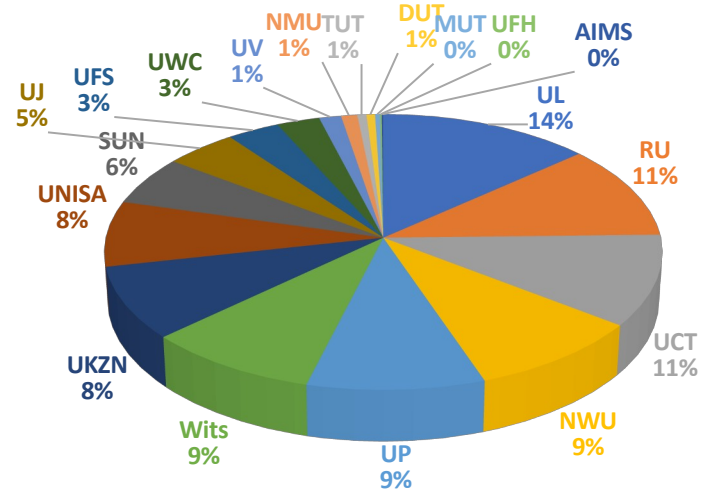
CHPC Use: SA Universities **Total Active* Programmes**

Lengau All Time (Jun 2016 – 15 Aug 2024)



Active Programmes

Total: 431



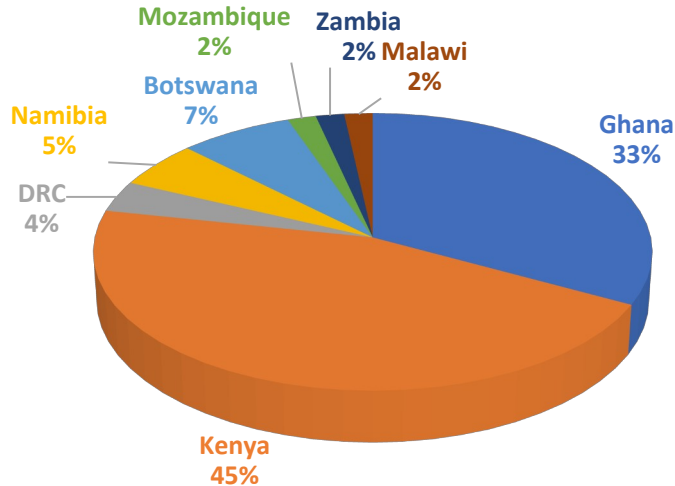
Hours Used (Million)

Total: 1097 million

*Active refers to at least 1000 compute hours used over the relevant period.

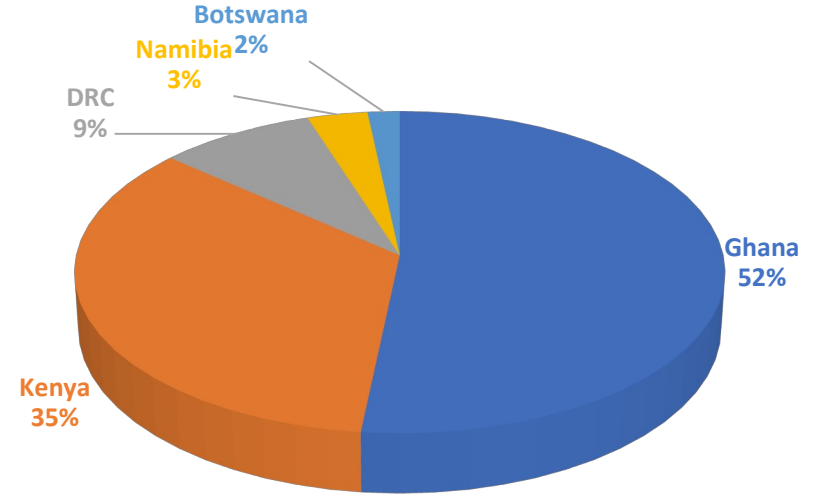
CHPC Use: African Partners **Total Active* Programmes**

Lengau All Time (Jun 2016 – 15 Aug 2024)



Active Programmes

Total: 55



Hours Used (Million)

Total: 174 million

**Active refers to at least 1000 compute hours used over the relevant period.*

CHPC Use: Industry **Total Active*** Programmes

(Full Lengau

Lifetime

Apr 2016 - 15 Aug

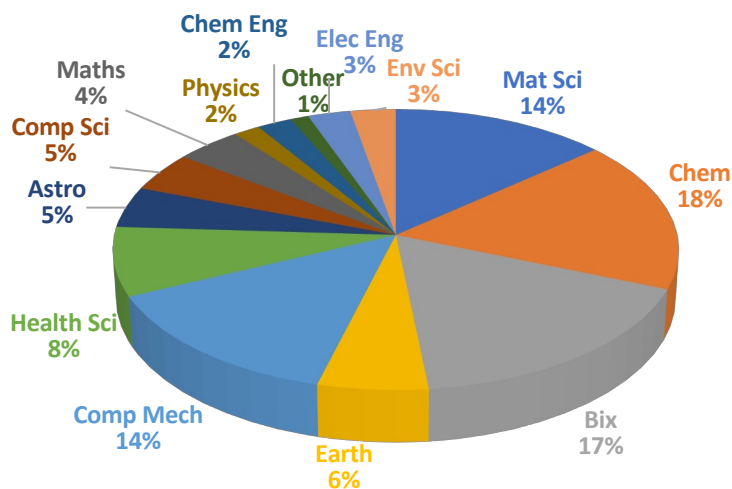
2024)

**Active refers to at least 1000 compute hours used over the relevant period.*

Company	#Hours (Millions) (All Time)	%	Company	#Hours (Millions) (All Time)	%
Johnson Matthey	5923194	46.0	Ex Mente	40489	0.3
eScience	2331554	18.1	Venter Consulting Engineers	38051	0.3
De Beers Marine	897643	7.0	IGS	34538	0.3
Aerotherm	801332	6.2	Structa Konsult	31444	0.2
Hatch	509937	4.0	Howden South Africa	26865	0.2
Cauchy Consult	431948	3.4	PABT	23800	0.2
Inqaba Biotec	315584	2.5	Eskom	21745	0.2
Epsilon Engineering	229477	1.8	Cinnamon Teal Aerospace	19542	0.2
Starke Ayres	226635	1.8	Zutari	17957	0.1
Qfinsoft	175820	1.4	Multotec	17463	0.1
BBE Consulting	168401	1.3	FTT Technology, Namibia	13383	0.1
Zutari	145217	1.1	Biomine Health	10992	0.1
Kapa Biosystems	133260	1.0	Rotech Systems	8585	0.1
Mamadi & Company SA	112318	0.9	Sebenzana Consulting	8101	0.1
Aim Technologies	110390	0.9	Knight Piv©sold Consulting	6946	0.1
Greenplan	86715	0.7	EnFloTech	4296	0.0
SMEC	81803	0.6	EMSS Consulting	2453	0.0
GLPS	75071	0.6	Nanodyn	1748	0.0
Agriprotein	70780	0.6	Altair Engineering Ltd	1351	0.0
Mintek	40648	0.3	TOTAL	13197478	100.0

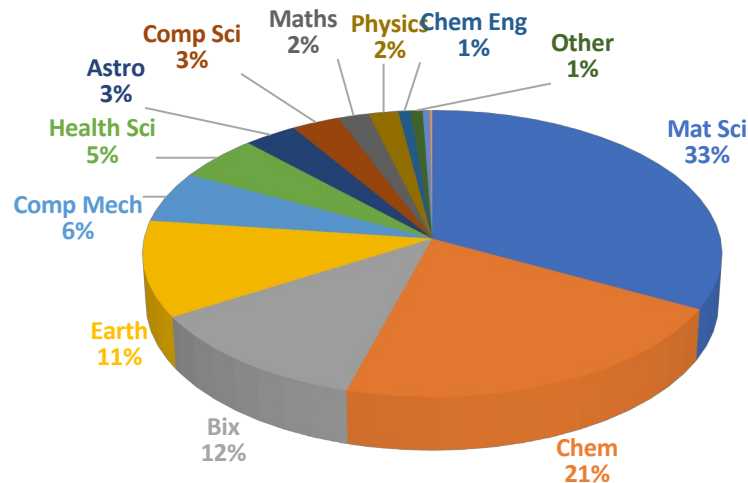
CHPC Use: Disciplines **Total Active* Programmes**

Lengau All Time (Jun 2016 – 15 Aug 2024)



Active Programmes

Total: 606



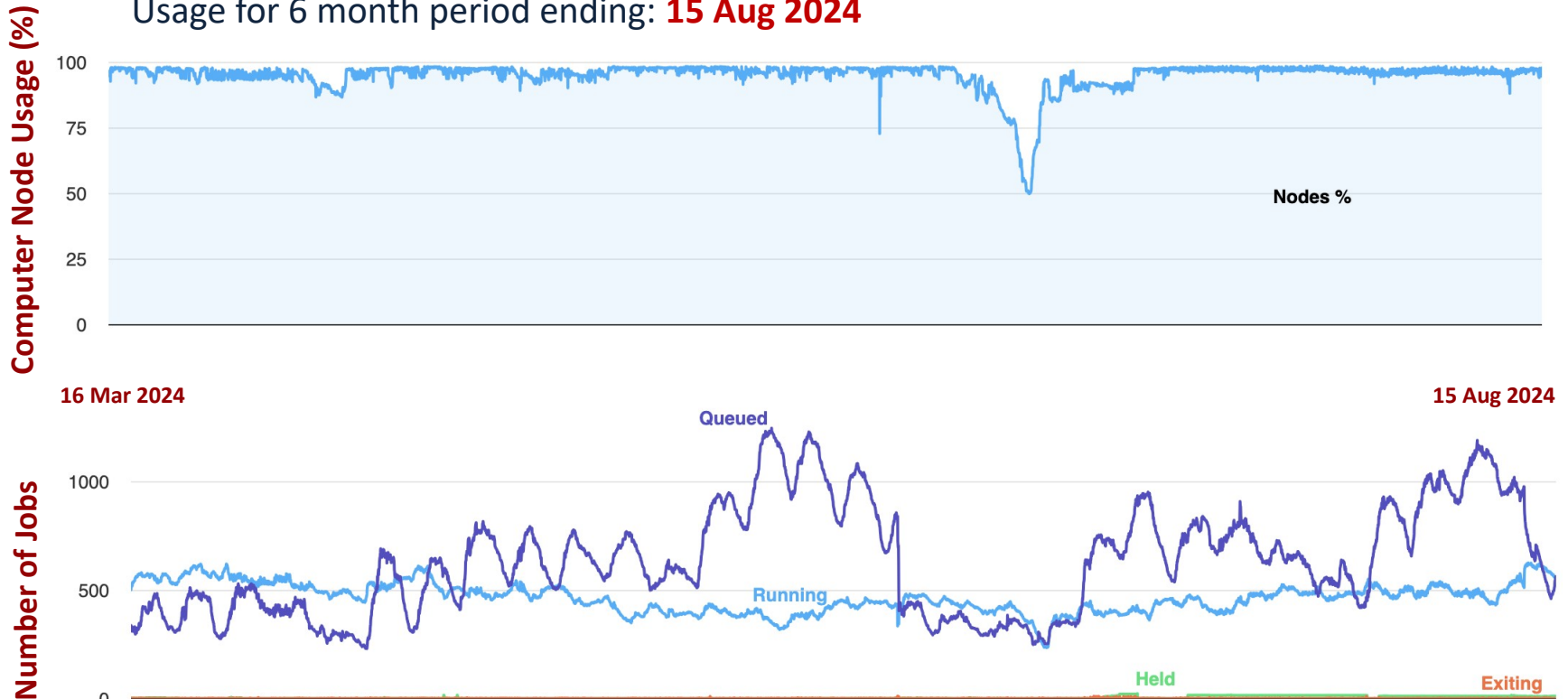
Hours Used (Million)

Total: 1419 million

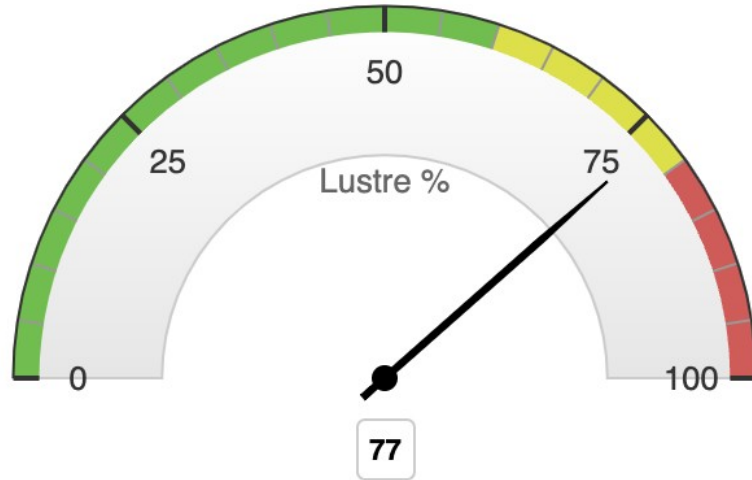
*Active refers to at least 1000 compute hours used over the relevant period.

CHPC Lengau Usage (Past 6 Months): CPU Cluster

Usage for 6 month period ending: **15 Aug 2024**



CHPC Lengau: Lustre Storage (Total Capacity: 4 PB)



Status on:

15 Aug 2024

User Data Categories on Lustre:

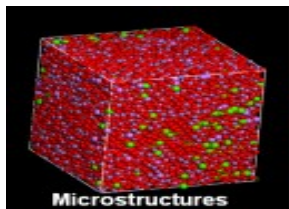
- Individual** User Directories (± 2 PB)
- Shared** Directories (± 1 PB)

Management of data according to Lustre Policy...

Execution of deletion scripts...

**Significant Storage Resources now available
from DIRISA...**

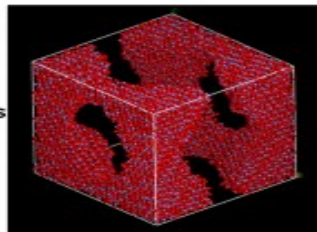
Materials Science / Chemistry / Health



Amorphisation Recrystallisation Grown MnO_2

Lithiated MnO_2
 $\text{Li}_{0.1}\text{MnO}_2$

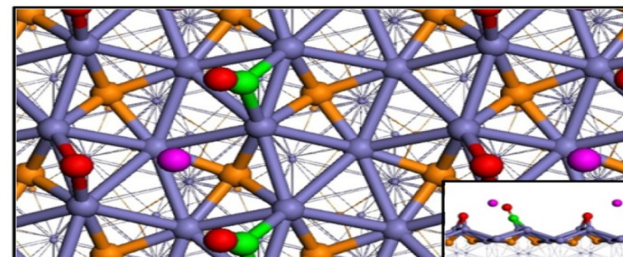
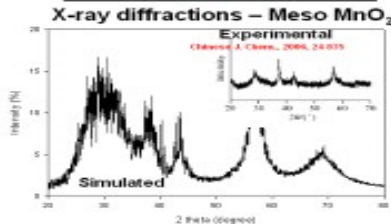
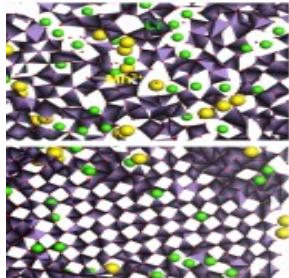
Meso-porous



Amorphous
 $\text{Li}_{0.1}\text{MnO}_2$

Mn^{3+}

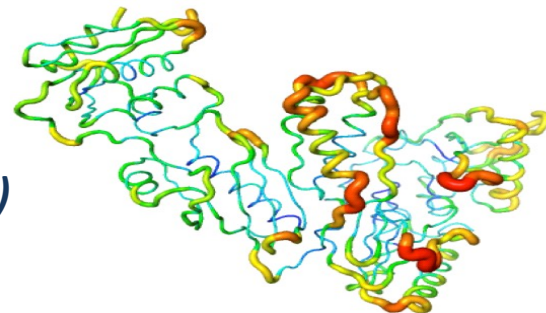
Recrystallised
 $\text{Li}_{0.1}\text{MnO}_2$



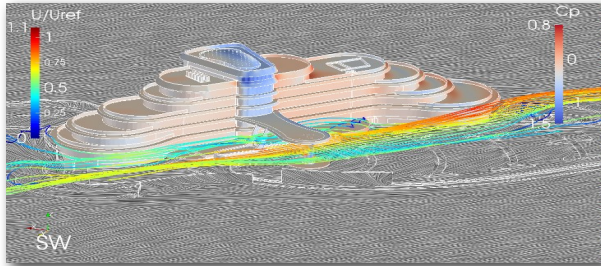
Computational Catalysis
(Comp Chem / Materials Science)

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

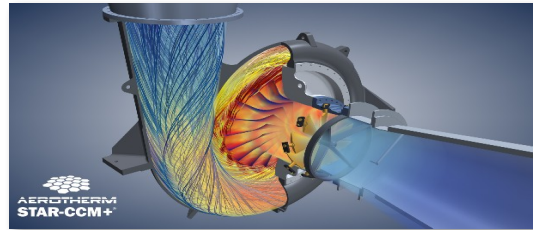
**Drug-Design Molecular
Modelling**
(Computational Chemistry)



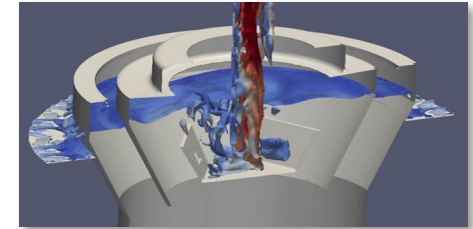
Computational Mechanics / Engineering



Building aerodynamics
(ECI-JV)

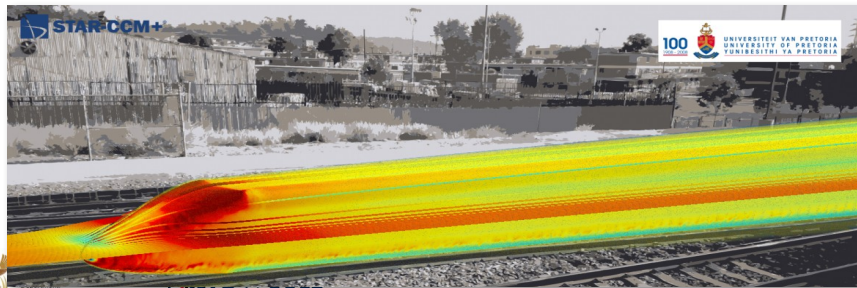


Centrifugal Steam Compressor
(Aerotherm)

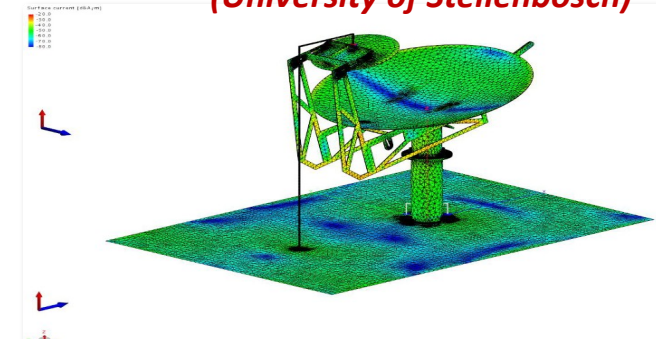


Elutriator Design
(De Beers Marine)

High-speed Train Design *(UP)*:



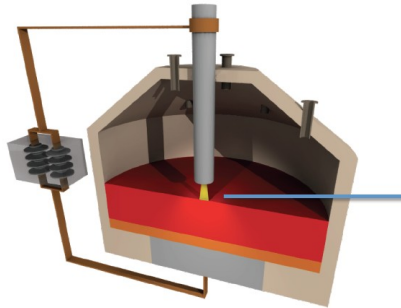
Radio-Astronomy Dish Design *(University of Stellenbosch)*



CASE STUDY

Mintek: Pyrometallurgy

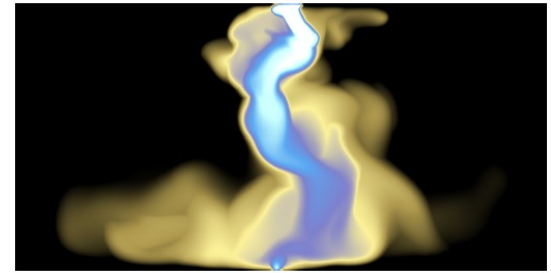
- ❑ DC Furnace **Plasma Arc electric smelting** simulations
- ❑ **CFD** and Magnetohydrodynamics (**MHD**) simulations
- ❑ Resulted in **patent** for Mintek on **arc detection technology**
- ❑ **Fully dependent** on **CHPC** for HPC resource requirements



Cross-section of DC Furnace
Showing Plasma Arc (photo)



Photographic Image



Simulated

Courtesy: Dr Quinn Reynolds (Mintek)

CASE STUDY

De Beers Marine: Diamond Mining

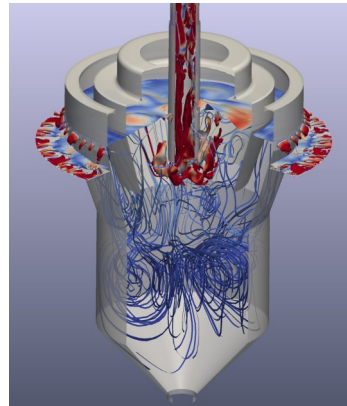
- ❑ Mining of **diamonds from seabed** west coast of SA and Namibia
- ❑ Advanced **technologies** required **for seperation** of diamonds by wet screening, grinding and deagglomeration
- ❑ Dependent on CHPC for **CFD** evaluations of **dewatering** sub-system **designs**
- ❑ Resulted in effective **decision making** for technology implementations

DE BEERS
GROUP OF COMPANIES



© Shane Branquinho
MarineTraffic.com

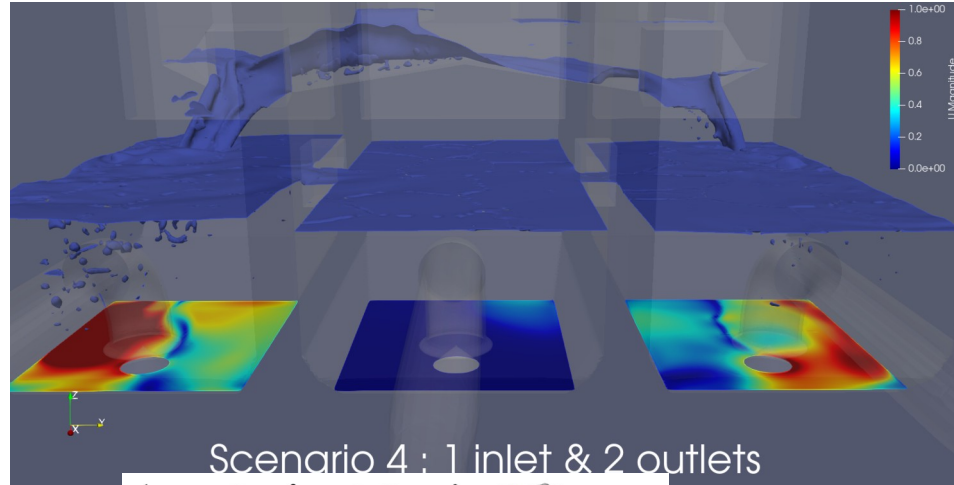
SS Nujoma – Mining Vessel



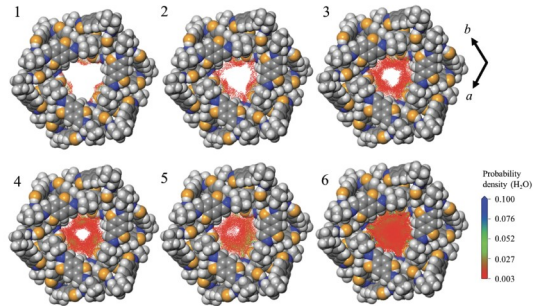
**Courtesy: Mr Imraan Parker
(De Beers Marine)**

HPC Applications

CFD simulation of sewage pumping station of City of Cape Town. In-house consultancy work by NICIS Engineers



Scenario 4 : 1 inlet & 2 outlets



Water harvesting from the atmosphere searching for materials that release water at near room temperatures done by Stellenbosch University: Publication in Nature

HPC Utilisation in Agriculture

Journal in animal production with impact on genomic sequencing of Nguni and Bonsmara crossbreeds at ARC Unit in Irene Pretoria

Home ▶ All Journals ▶ Journal of Biomolecular Structure and Dynamics ▶ List of Issues ▶ Latest Articles ▶ Molecular modeling and simulation studie ...

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- 1. Introduction
- 2. Materials and methods
- 3. Results
- 4. Discussions
- Conclusion
- Future perspectives
- Supplemental material**
- Acknowledgements
- Disclosure statement
- Additional information

Supplemental Material

Acknowledgments

We also thank the South African Bioinformatics Institute (SANBI), UWC for the training in molecular modeling, docking, interaction analysis and molecular dynamic simulation for DRM. The FP7 WeNMR (project# 261572), H2020 West-Life (project# 675858) and the EOSC-hub (project# 777536) European e-Infrastructure projects are acknowledged for the use of their web portals, which make use of the EGI infrastructure with the dedicated support of CESNET-MetaCloud, INFN-PADOVA, NCG-INGRID-PT, TW-NCHC, SURFsara and NIKHEF and the additional support of the national GRID Initiatives of Belgium, France, Italy, Germany, the Netherlands, Poland, Portugal, Spain, UK, Taiwan and the US Open Science Grid. RC contributed to the first draft of the manuscript and the development of the study protocol. The authors would like to acknowledge the CHPC for the use of their resources to perform the molecular dynamic studies and the National Integrated Cyber infrastructure system.

Disclosure statement

No potential conflict of interest was reported by the author(s).

Related research

People also read Recommended articles Cited by

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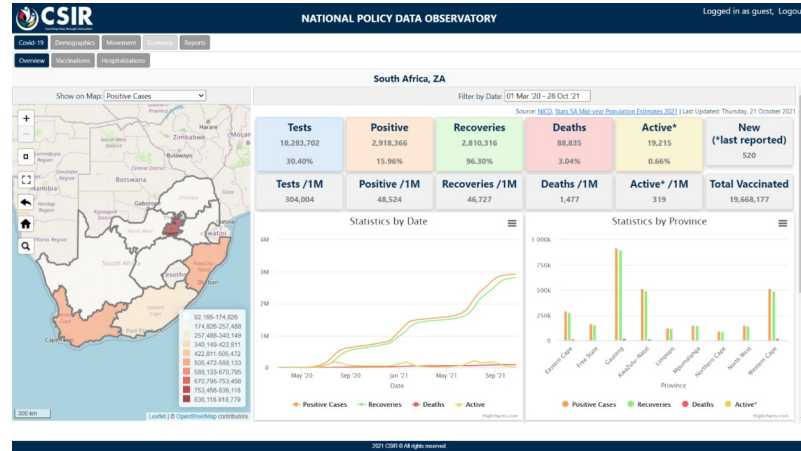
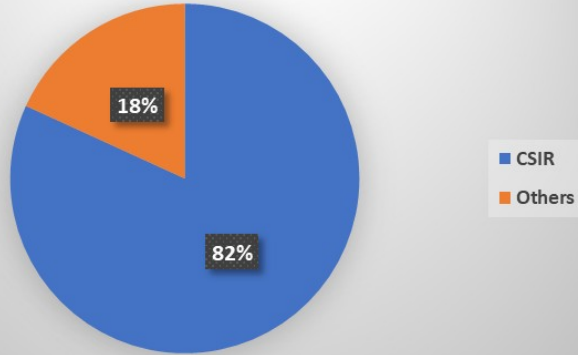
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Abdelmoujoud Faris et al.
Journal of Biomolecular Structure and Dynamics
Published online: 7 Dec 2023

Network pharmacology combined with molecular docking and experimental verification to elucidate functional mechanism of Fufang Zhenzhu Tiaozhi against type 2 di... >

Bo Li et al.
Journal of Biomolecular Structure and Dynamics

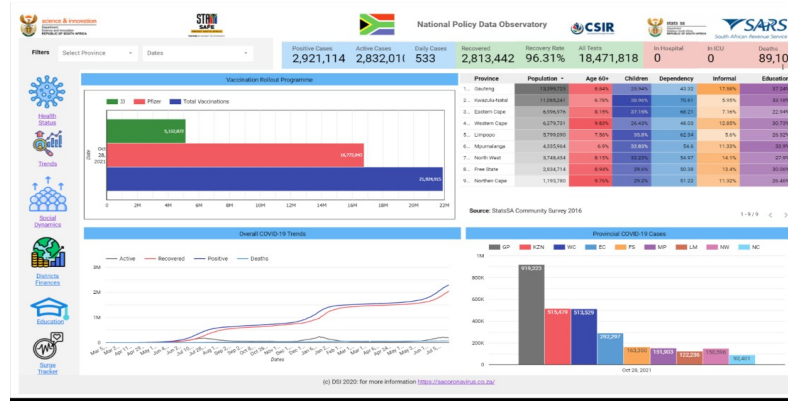
Sebowa Cloud Projects



NATIONAL POLICY DATA OBSERVATORY

Hosted on Sebowa and the data is also used for other several projects:

- NPDO dashboard - contains Covid-19, Demographic, Mobility, Financial, Report data and more.
- Goggle studio dashboard – contains Covid-19 data analysis, insights and more.
- SA's development Indicators dashboard (**New**) - tracking of South Africa's Development Indicators published by the Department of Planning, Monitoring & Evaluation on an annual basis.
- CSIR Logistics observatory platform (**New**)



Vaccine certificate systems portal

- ❑ The Vaccine certificate system portal allows vaccinated South Africans to access and download their digital Covid-19 vaccination certificates
- ❑ This project is hosted on NICIS cloud, and it runs highly scalable virtual infrastructure required to handle the extremely high load, where millions of South Africans access this portal on daily basis.

South African COVID-19 Vaccine Certificate System



health

Department:
Health
REPUBLIC OF SOUTH AFRICA

This is the official South African COVID-19 Vaccine Certificate System Portal

- Verification of the Vaccine Certificate feature is optimized for mobile devices.
- Only people who are COVID-19 vaccinated can retrieve their COVID-19 Vaccine Digital Certificate.
- If you have updated any of your personal details on EVDS, you will need to re-download your certificate.
- **The QR Code generated is not intended to be readable by the general public**, it is meant to be used by entities requiring to verify the certificate's validity, using a Vaccine Certificate System inbuilt QR scanner.
- If the certificate you have downloaded has 'version 1' on it, **please re-download a new certificate (version 2)**.

GET MY VACCINE CERTIFICATE

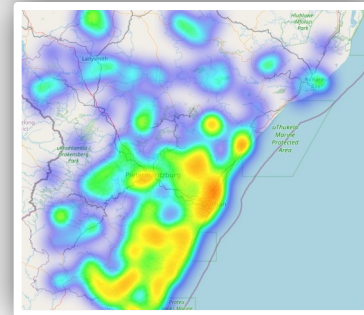
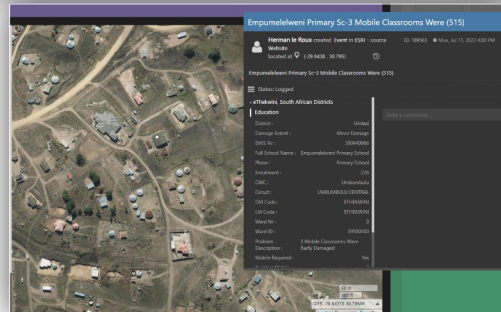
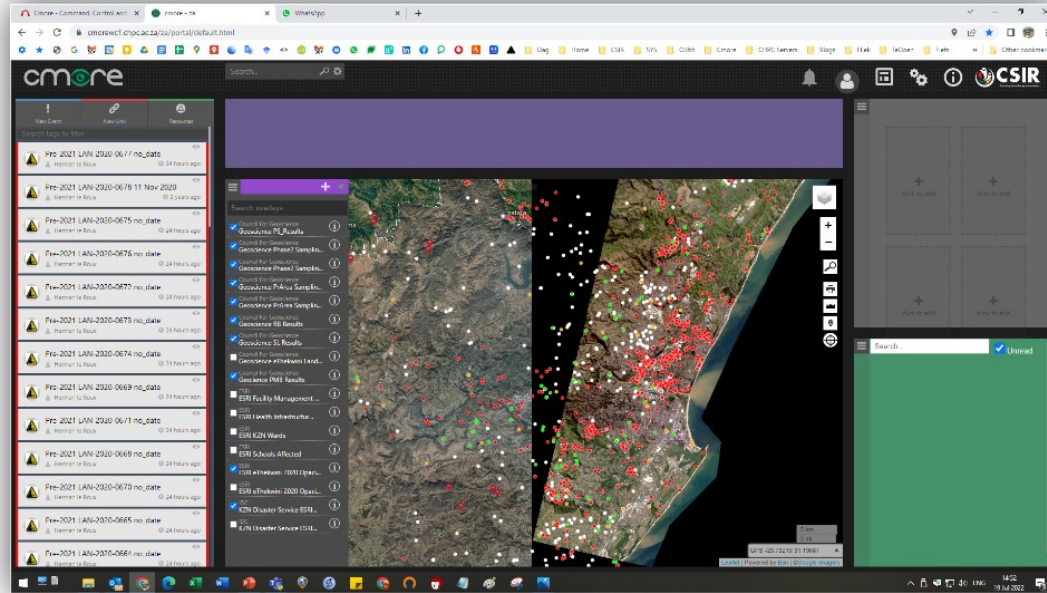
VERIFY A VACCINE CERTIFICATE

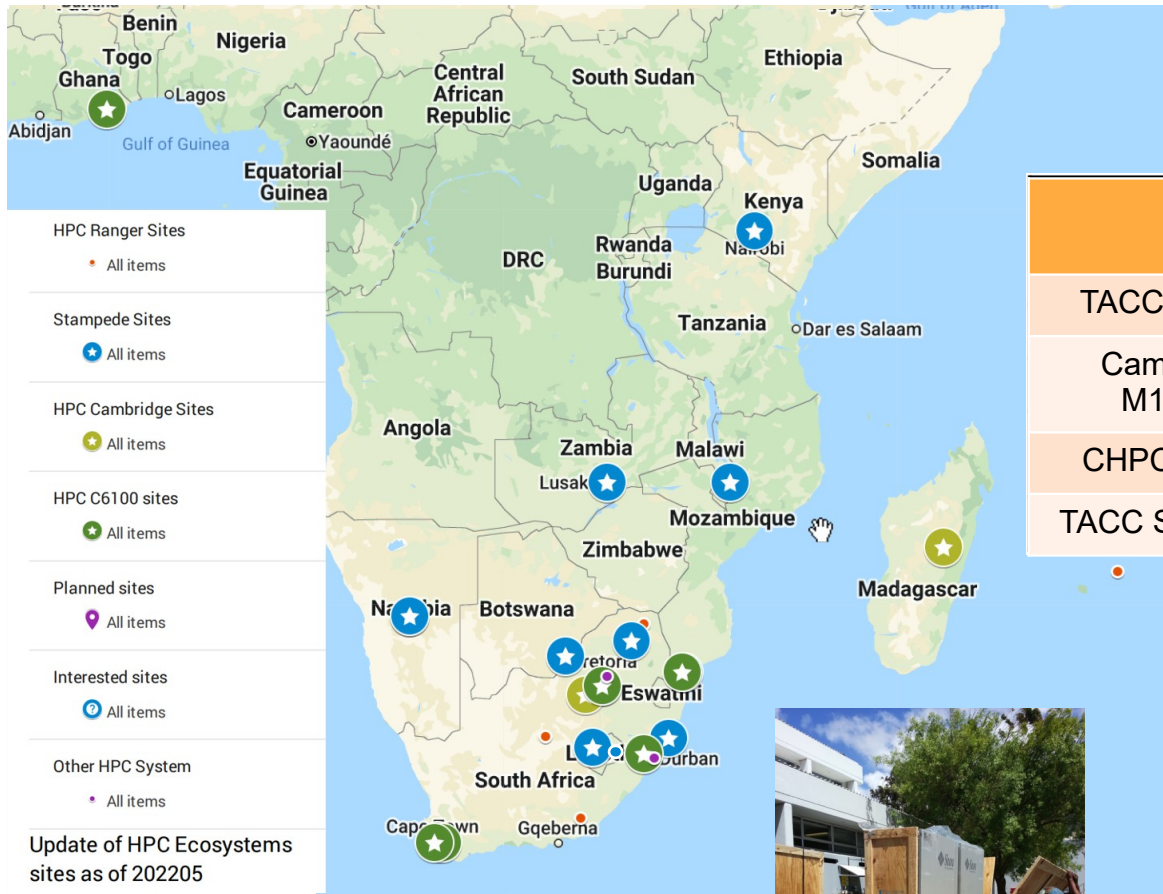
A national initiative of the Department of Science and Innovation and implemented by the CSIR

CMORE Project: Support to IDC/PICC on KZN Flood Data Integration

Integration of data points and GIS overlays into a single view from various data owners

- KZN Office of the Premier
- Council for Geoscience
- Microsoft
- SANSA
- SANRAL
- ESKOM
- SAWS
- CSIR

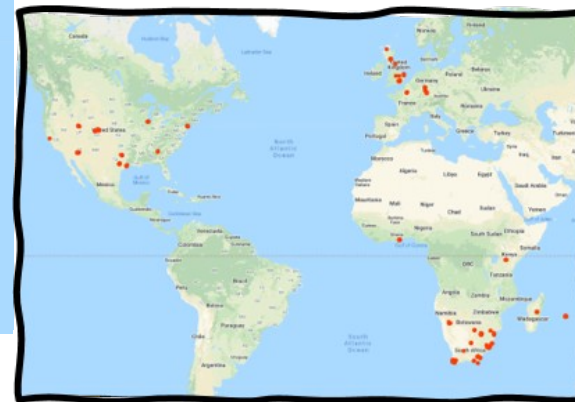




	GLOBAL (17)	LOCAL (~17)
TACC Ranger	5	6
Cambridge M1000e	1	1
CHPC C6100	2	5
TACC Stampede	9	3 (+2)

Update of HPC Ecosystems sites as of 202205

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



Solution #4: Virtual Community

Platform	Members	Notes
Google Group	168	~16 countries
HPC Educators Africa COP	13	A 'spin-off' Google Group community was established at the CHPC National Meeting to represent HPC Educators in HPC Ecosystems partner sites.
HPC Ecosystems Slack	178	USA, Europe, Africa community members

Virtual HPC Labs

First:

OpenHPC Virtual HPC Lab

&

OpenHPC Video Tutorials

(available **on-demand**
or
standalone **offline**)

Table 1 – Summary of Formal OpenHPC events (tutorials in red)

Event	Duration in hours	Year & Month	Description <small>Appendix Ref#</small>
SC19	1	2019-11	Birds of a Feather
PEARC19	3.5	2019-07	Tutorial ^{1,2,4}
ISC 2019	1	2019-06	Birds of a Feather
HPCKP'19	0.5	2019-06	Presentation
SC18	1 unknown	2018-11	Birds of a Feather Tutorial
DAAC 2018	unknown	2018-11	Presentation
Open Source Summit 2018	3	2018-08	Tutorial
MVAPICH'18	unknown	2018-08	Presentation
DevConf.CZ 2018	0.25	2018-01	Presentation
SC17	1	2017-11	Birds of a Feather
MVAPICH'17	unknown	2017-08	Presentation
PEARC 17	3.5	2017-07	Tutorial
ISC 2017	1	2017-06	Birds of a Feather
HPCKP 2017	0.5	2017-06	Presentation
SC16	1	2016-11	Birds of a Feather
MVAPICH 2016	unknown	2016-08	Presentation
ISC 2016	1	2016-06	Birds of a Feather
FOSDEM 2016	0.45	2016-01	Presentation

Human Capital Development



Computer Science Post Graduate Research Career Workshop hosted at UP on 16 -17 February 2024



25th Edition of the Working World Exhibition held in Nelson Mandela Bay on 20 – 22 February 2024
Reaching out to 12 963 Gr 11 and 12 Learners



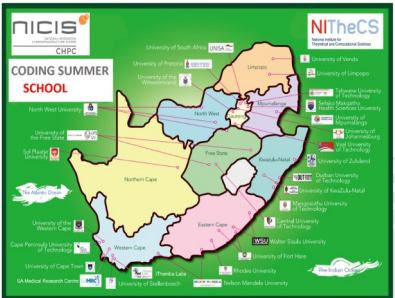
21 Regional representatives for Limpopo and Eastern Cape Provinces attended the Coding Summer School at CHPC on 22 – 26 January 2024



Overview



- Coding Summer School in Numbers**
- 815 participants
 - 30 Venues
 - 6 Month planning
 - 40 Champions
 - 10 Staff & 30 Tutors
- Content**
- Week 1: Python & Bash Intro with Data Science
 - Week 2: ML, Prob & Stats, ODEs, Comp Chem, Bio-informatics



Coding Summer School held from 29 January to 9 February 2024 across 30 venues with 40 Champions and 815 participants

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Special Highlights



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Special Highlights



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HPC Ecosystems Project – DO IT!

<https://hpc-ecosystems.gitlab.io/training/openhpc-101/>

YouTube: 'hpc ecosystems 101 openhpc'

HPC Ecosystems Slack:

<https://tinyurl.com/sighpc-join-ecosystems-slack>

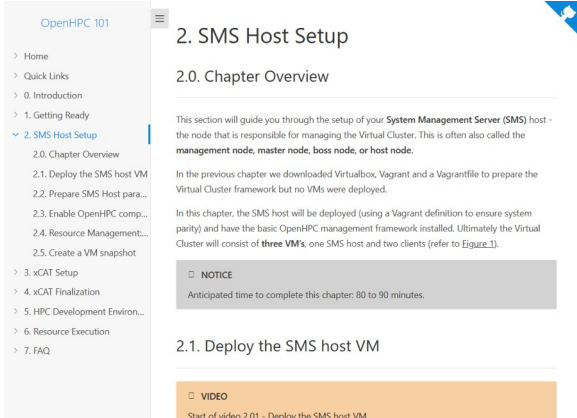
HPC Ecosystems Google Group:

<http://tinyurl.com/SADC-HPC-Apply>

NICIS CHPC Events:

events.chpc.ac.za

A national initiative of the Department of Science and
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OpenHPC 101

- Home
- Quick Links
- 0. Introduction
- 1. Getting Ready
- 2. SMS Host Setup
 - 2.0. Chapter Overview
 - 2.1. Deploy the SMS host VM
 - 2.2. Prepare SMS Host para...
 - 2.3. Enable OpenHPC comp...
 - 2.4. Resource Management...
 - 2.5. Create a VM snapshot
- 3. xCAT Setup
- 4. xCAT Finalization
- 5. HPC Development Environ...
- 6. Resource Execution
- 7. FAQ

2. SMS Host Setup

2.0. Chapter Overview

This section will guide you through the setup of your **System Management Server (SMS)** host - the node that is responsible for managing the Virtual Cluster. This is often also called the **management node, master node, boss node, or host node.**

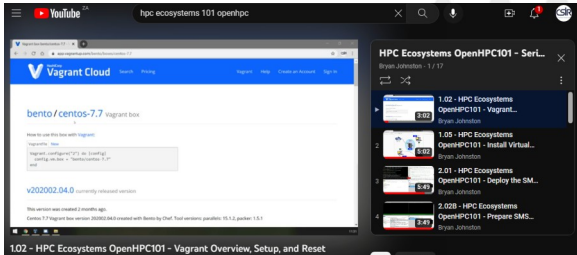
In the previous chapter we downloaded Virtualbox, Vagrant and a Vagrantfile to prepare the Virtual Cluster framework but no VMs were deployed.

In this chapter, the SMS host will be deployed (using a Vagrant definition to ensure system parity) and have the basic OpenHPC management framework installed. Ultimately the Virtual Cluster will consist of **three VMs**, one SMS host and two clients (refer to [Figure 1](#)).

NOTICE
Anticipated time to complete this chapter: 80 to 90 minutes.

2.1. Deploy the SMS host VM

VIDEO
Start of video 2.01 - Deploy the SMS host VM



YouTube: hpc-ecosystems-101-openhpc

Vagrant Cloud

bento/centos-7.7 vagrant-box

How to use this box with Vagrant

```
hostname: sms  
memory: 4096  
vagrant.configure("2") do |config|  
  config.vm.box = "bento/centos-7.7"  
  config.vm.box_url = "https://atlas.hashicorp.com/bento/centos-7.7" />
```

v202002.04.0 Automatically refreshed versions

This version was created 2 months ago

Created 1.7 Vagrant box version: 202002.04.0 created with BoxesByClay. Tool version: parallel_15.1.1, packer_1.5.1

1.02 - HPC Ecosystems OpenHPC101 - Vagrant Overview, Setup, and Reset

1.03 - HPC Ecosystems OpenHPC101 - Install Virtual...

2.01 - HPC Ecosystems OpenHPC101 - Deploy the SM...

2.02B - HPC Ecosystems OpenHPC101 - Prepare SMS...

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