

**SUNDAY
01 DEC**

WORKSHOPS

08:00 to 09:00 Registration

MORNING (09:00 to 12:30) :

- SAFIRE for Service Providers, Guy Halse & Donald Coetzee, TENET/SAFIRE.

FULL DAY (09:00 to 17:00):

- CHPC User Tutorials: (1) Induction, Andrew Gill & Kevin Colville, CHPC; (2) PBS Pro for Users, Nkwe Monama & Zama Mtshali, CHPC; and (3) Practical HPC, Krishna Govender & Andrew Gill, CHPC.
- SIG: Security by Design and flaws in IoT Architectures, Meshack Ndala & Zintle Sanda (convenors), CHPC.
- SIG: Weather and Climate Modelling, Mary-Jane Bopape (convenor), SAWS, Fabio Porto (convenor), LNCC - DEXL (Brazil), Victor Stepanenko (convenor), MSU
- From A to AI with Intel, Walter Riviera, Intel
- Schrödinger Materials Science Suite, Caroline Krauter, Schrödinger
- Receptor based virtual screening, molecular docking and molecular dynamics to explore promising molecules, Tahir Pillay, UP, and Ataul Islam, University of Manchester
- Machine Learning and Applications Part 1, Deepak Kar and Bruce Mellado, Wits University

10:30 to 11:00 Break

12:30 to 13:30 LUNCH

15:00 to 15:30 Break

08:00	REGISTRATION		
	OPENING KEYNOTE: Chair: <i>Dr Samuel Mabakane</i> , CHPC. (OR Tambo Hall)		
09:00 - 09:45	Welcome: Dr Happy Sithole, Centre Manager: NICIS DSI Opening Address: Dr Phil Mjwara, Director-General: Department of Science and Innovation		
09:45	Digital Transformation: Issues of the Public Service, <i>Mr Mandla Ngcobo</i> , Government CIO: Department of Public Service and Administration		
10:30	BREAK		
	VENUE: CAPE TOWN HPC Storage and IO	VENUE: KING SHAKA HPC Applications	VENUE: OR TAMBO HALL 2 School Learners
11:00	High Performance Data Access: the Hermes approach, <i>Xian-He Sun</i> MeerKAT archive and data access, <i>Martin Slabber</i> Updating the Outdated Storage Paradigm to Handle Complex Computational Workloads, <i>Craig Bungay</i>	Journey to the Compute: a researcher's perspective of using applications on high performance computers, Blake Joyce HPC for Medical Interventional Planning Applications, <i>Malebogo Ngoepe</i> Next Generation Sequencing: where big data and HPC meet, <i>Brigitte Glanzmann</i> Field-induced exotic electronic phases in spin-filter tunnel junctions, <i>Aniekan Ukpong</i>	SCRATCH programming, CHPC Security and Social Media, SANReN Your Data, DIRISA
12:30	LUNCH		

	VENUE: CAPE TOWN HPC Storage and IO	VENUE: KING SHAKA HPC Applications	VENUE: HEATHROW Quantum Computing
13:30	<p>Designing Reusable Composable Components for the (HPC) I/O Stack, <i>Ali Butt</i></p> <p>PETSc: High-Performance Software Library for Engineering and Science Simulation, <i>Hong Zhang</i></p> <p>NEXTGenIO: exploring the potential of non-volatile memory in HPC, <i>David Homan</i></p>	<p>Research highlights from the Molecular Bio-computations and Drug Design Research Group at UKZN, <i>Mahmoud Soliman</i></p> <p>Computational Fluid Dynamics: from solar thermal receivers and collectors to sub-antarctic island wind simulation, <i>Ken Craig</i></p> <p>Predicting Thermodynamic Properties of Ionic Liquids — from Molecular Simulation to Machine Learning, <i>Gerhard Venter</i></p> <p>Interaction between <i>S. mansoni</i> Universal stress G4LZ13 protein and selected poly-phenols: a bioinformatics investigation, <i>Abidemi Paul Kappo</i></p>	<p>Please see online timetable for details</p>
15:00	BREAK		
	VENDOR CROSSFIRE: Coordinator: <i>Dan Olds</i> . (OR Tambo Hall)		
15:30	INTEL • ALTAIR • BOSTON • AMD • DELL • SCHRÖDINGER • MELLANOX		
17:00	POSTER PRESENTATIONS Convenor: Dr Daniel Moeketsi, CHPC (OR Tambo Foyer)		
18:00	Intel KEYNOTE: Chair: <i>Dr Happy Sithole</i> , NICIS. (OR Tambo Hall)		
19:00	INTEL BRAAI (BIRCHWOOD BOMA)		

08:00	REGISTRATION		
	KEYNOTES: Chair: <i>Mr Leon Staphorst</i> , Director: SANReN (OR Tambo Hall)		
09:00	eInfrastructures as enablers for global science and education, <i>Dr Josva Kleist, NORDUnet</i>		
09:45	Scientific Applications on Heterogeneous Architectures - Data Analytics and the Intersection of HPC and Edge Computing, <i>Prof. Michela Taufer, U. Tennessee Knoxville</i>		
10:30	BREAK		
	VENUE: CAPE TOWN HPC Technology	VENUE: KING SHAKA HPC Applications	VENUE: HEATHROW SA NREN
11:00	<p>Parallel and Distributed Search Algorithms, <i>Cornelia Inggs</i></p> <p>Machine Learning approaches for HPC, <i>Peter Braam</i></p> <p>Evaluating the Compressibility of Elevation Data using Space- Filling Curves, <i>Conrad Haupt</i></p>	<p>Design of selective reagents and functional materials: A theoretical and experimental approach, <i>Zenixole Tshentu</i></p> <p>SAVIME - Simulation Analysis and Visualization in-Memory, <i>Fabio Porto</i></p> <p>Advancing the understanding of interactions between plasma arcs and power electronics with HPC, <i>Quinn Reynolds</i></p> <p>Convective scale modelling on the CHPC: ICON vs COSMO, <i>Patience Mulovhedzi</i></p>	<p>Cloud Computing a Solution to Internet Services Downtime at Namibian Institutions of Higher Learning, <i>Shadreck Chitauro</i></p> <p>BRICS programme on "Cybersecurity: Software and Data Security", <i>Joey Jansen van Vuuren</i></p> <p>Brainstorming on a Guiding Policy Framework towards Ethical Conundrums around Artificial Intelligence of Things (AIoT), <i>Attlee Munyaradzi Gamundani</i></p> <p>SANReN Data Transfer Pilot, <i>Kassandra Pillay</i></p>
12:30	LUNCH		

	VENUE: CAPE TOWN HPC Technology: Vendors	VENUE: KING SHAKA HPC Applications	VENUE: HEATHROW BoF: HPC Ecosystems & System Administration
13:30	<p>Distribute AI workload on HPC with Intel, <i>Walter Riviera</i>, Intel</p> <p>Secure and Dynamic HPC Cloud Bursting into Public Clouds, <i>Ian Littlewood</i>, Altair</p> <p>TBA, <i>Yael Birk Hoter-Ishay</i>, Mellanox</p>	<p>The research benefits of improving equity, diversity and inclusion, <i>Toni Collis</i></p> <p>Benchmarking off-the-shelf radio astronomy software on Lengau, <i>Sean February</i></p> <p>BIOPERIANT12, a regional high-resolution model configuration towards developing the South African VrESM Earth System Model, <i>Nicolette Chang</i></p> <p>The Adoption of Deep Learning in Weather Forecast, <i>Yania Molina Souto</i></p>	<p>Please see online timetable for details</p>
15:00	BREAK		
15:30	BOF: WOMEN IN HPC Coordinator: Dr Khomotso Maenetja, University of Limpopo <i>(Auditorium)</i>		

17:00–18:00

POSTER PRESENTATIONS

Convenor: Dr Daniel Moeketsi, CHPC

(OR Tambo Foyer)

08:00	REGISTRATION		
	KEYNOTES: Chair: <i>Dr Anwar Vahed</i> , Director: DIRISA (OR Tambo Hall 2)		
09:00	DALI: A Data life cycle instrument for management and sharing of data: Towards the reproducibility and data reuse of scientific research, <i>Prof. Hakizumwami Birali Runesha, University of Chicago</i>		
09:45	Eliminating Weapons of Math Destruction: Next-Generation Arithmetic, <i>Prof. John Gustafson, National University of Singapore</i>		
10:30	BREAK		
	VENUE: CAPE TOWN BoF: HPC Education	VENUE: KING SHAKA HPC Applications	VENUE: HEATHROW DIRISA
11:00	Please see online timetable for details.	High throughput in silico screening for tailored catalytic reactivity and selectivity, <i>Caroline M. Krauter</i> Smoke and ventilation simulation using the CHPC, <i>Kenneth Allen</i> In-silico investigations of metal coordinating enzymes: From Biofuel production to Antimicrobial drug resistance, <i>Vuyani Moses</i> Use of high-throughput sequencing to uncover resistance mechanisms in sugarcane, <i>Robyn Jacob</i>	More than meets the eye: Towards an Artificial Intelligence Observatory, <i>Matias Carrasco Kind</i> EOS storage system, <i>Sean Murray</i> The Capture, Storage and Consumption of the MeerKAT Radio Telescope's Sensor Data, <i>Suleiman Hoosen</i> Federating the Ilifu Cloud, <i>Rob Simmonds</i>
12:30	LUNCH		

	<p>VENUE: CAPE TOWN HPC Technology: Vendors</p>	<p>VENUE: KING SHAKA HPC Applications</p>	<p>VENUE: HEATHROW DIRISA</p>
13:30	<p>AMD EPYC – Delivering the Future of HPC, Matt Foley, AMD</p> <p>Clouds and HPC– Can They Work Together?, David Power, Boston Limited</p> <p>HPE in Supercomputing, Marco Vieira, Hewlett Packard Enterprise</p>	<p>Computational Catalysis @ NWU, Cornie van Sittert</p> <p>Speech data harvesting and factorized deep neural network development for the low-resource indigenous languages of South Africa, Jaco Badenhorst</p> <p>Computational Modelling Study on Stability of Li-S/Se System, Cliffon Masedi</p> <p>Finite volume modelling of dense granular flow in rotary kilns, Alfred Bogaers</p>	<p>Developing infrastructure for federated data analysis for protected human data, Nicola Mulder</p> <p>Developments Around Data in Botswana to support 4iR preparedness, Research, Innovation in a Developing Country, Tshiamo Motshegwa</p> <p>Evolution of a South African eResearch support service, Dale Peters</p> <p>Cyber Security Threats – Is Our Research Data Safe? Isak van der Walt</p>
15:00	BREAK		
15:30	<p>BOF:CHPC Pls and Users (Auditorium) Coordinator: Dr Werner Janse Van Rensburg, CHPC</p>		<p>BOF: CEPH (Heathrow) Coordinator: Mr Isak van der Walt, U.of Pretoria</p>
17:00	INTERMISSION		
18:00	<p>THE FUTURE OF COMPUTING WILL BE NON-VON NEUMANN, <i>Prof. Thomas Sterling, Indiana University</i> Chair: Dr Happy Sithole, Centre Manager: NICIS (OR Tambo Hall 2)</p>		
19:00	PRIZE-GIVING DINNER (Serengeti Lapa)		

THURSDAY
05 DEC

WORKSHOPS

08:00 to 09:00 Registration

FULL DAY (09:00 to 17:00) :

- SIG: CHPC Industry Forum, Werner Janse Van Rensburg, CHPC
- SIG: Chemistry, Material science and Health science, Cornie van Sittert, North-West University, Jeanet Conradie, University of Free State and Marilé Landman, University of Pretoria
- Accelerated free energy calculations using open-source tools: Galaxy Project platform, BRIDGE and Galaxy Comp. Chem., Kevin J. Naidoo, Chris Barnett, and Tharindu Senapathi, University of Cape Town
- NVIDIA Deep Learning Institute (DLI) Deep Learning Fundamentals, Krishna Mouli, Boston Limited
- HPC on OpenStack, David Power, Boston Limited
- iRODS core competencies, capabilities, patterns and use cases, Claude Fortune, DIRISA
- Simplifying Research Data Management with Globus, Vas Vasiliadis, University of Chicago
- Machine Learning and applications Part 2, Deepak Kar and Bruce Mellado, Wits University
- SIG: NICIS Cyber Security Engagement, NICIS

AFTERNOON (13:30 to 17:00) :

- ~~Tuning and optimisation of parallel programs on the CHPC's Lengau cluster, Samuel Mabakane, CHPC.~~

10:30 to 11:00 Break

12:30 to 13:30 LUNCH

15:00 to 15:30 Break