



# Centre for High Performance Computing 2020 National Conference

## Monday 30 November 2020

### HPC Applications: 1 (14:00-15:00)

-Conveners: Chair: Daniel Moeketsi

time	[id] title	presenter
14:00	[128] A Spatial Model for Covid-19	Dr KIMMIE, Zaid
14:30	[87] A new view of the centre of our galaxy with MeerKAT	Dr HEYWOOD, Ian

### HPC Applications: 2 (15:15-16:15)

-Conveners: Chair: Charles Crosby

time	[id] title	presenter
15:15	[83] Simulation of atmospheric composition and air quality on the CHPC	Prof. GARLAND, Rebecca
15:45	[108] Epsilon Aerospace Computational Mechanics	Mr MTHEMBU, Ndumiso

## Tuesday 01 December 2020

### HPC Applications (11:00-12:00)

-Conveners: Chair: Andrew Gill

time	[id] title	presenter
11:00	[113] Electron density in uncovering reaction mechanism	Prof. CUKROWSKI, Ignacy
11:30	[58] HPC as an Enabler for Growth in Computational Fluid Dynamics Research	Dr BHAMJEE, Muaaz

### HPC Applications (12:15-13:15)

-Conveners: Chair: Zintle Sanda

time	[id] title	presenter
12:15	[148] Development and application of climate models over Africa using the CHPC	Prof. ABIODUN, Babatunde
12:45	[39] Interfacial and Morphological phase transitions in Polymeric Materials	Prof. PELLICANE, Giuseppe

### HPC Applications (14:00-15:00)

-Conveners: Chair: Inus Scheepers

time	[id] title	presenter
14:00	[146] High-performance computing in the era of genomics	Dr EMAMI-KHOYI, Arsalan
14:30	[45] Toward the development of an efficient and scalable computational fluid dynamics solver for mesoscale phase separation problems	Dr REYNOLDS, Quinn

### HPC Applications (15:15-16:15)

-Conveners: Chair: Nkwe Monama

time	[id] title	presenter
15:15	[99] Cooperation between computational modelling and experimental characterization of materials	Dr MODIBA, Rose
15:45	[114] Dealing with the MeerKAT Data Deluge: Risk for the Data Centre, Reward for the Scientist	Dr FRANK, Bradley

# Wednesday 02 December 2020

## HPC Applications (11:00-12:00)

-Conveners: Chair: Charles Crosby

time	[id] title	presenter
11:00	[74] Foodborne disease surveillance using next-generation sequencing	Dr PIERNEEF, Rian
11:30	[106] A multi-physics framework for modelling coupled heterogeneous transport and reaction kinetics	Dr OXTOPY, Oliver

## HPC Applications (12:15-13:15)

-Conveners: Chair: Anton Lopis

time	[id] title	presenter
12:15	[125] Novel Peptides as Potent Inhibitors of SARS-CoV-2 that work by Two distinct mechanisms: Molecular Docking and Dynamics Approach	Dr KIRURI, Lucy
12:45	[1] Machine learning-based prediction of phases in high-entropy alloys	Prof. MACHAKA, Ronald

## HPC Applications (14:00-15:00)

-Conveners: Chair: Krishna Govender

time	[id] title	presenter
14:00	[82] Large Scale Computations in Data Science	Dr BAH, Bubacarr
14:30	[100] Rational design of Sn(IV) porphyrins for photodynamic therapy: progress to date and future perspectives	Prof. MACK, John

## HPC Applications (15:15-16:15)

-Conveners: Chair: Benjamin Barsch

time	[id] title	presenter
15:15	[92] An ab initio high performance computing approach to time-dependent cosmic-ray modulation	Mr MOLOTO, Katlego
15:45	[101] Lung Health Screening by Automatic Cough Analysis with Applications to Tuberculosis and COVID-19	Dr PAHAR, Madhurananda