

Centre for High Performance Computing 2022 National Conference

Wednesday 30 November 2022

HPC Applications: 1 - ICC-L-Amethyst - Amethyst Room (10:15-11:15)

-Conveners: Chair: Dr Kingsley Obodo

time	[id] title	presenter
10:15	[101] Molecular simulations for material optimization	Prof. CARBONE, Paola
10:45	[102] CHPC's biotech industry support - From luxury to necessity	Dr GANESAN, Hamilton

HPC Applications: 2 - ICC-L-Amethyst - Amethyst Room (11:45-12:45)

-Conveners: Chair: Dr Quinn Reynolds

time	[id] title	presenter
11:45	[114] Climate modelling and seasonal climate forecasting at CSIR using the CHPC cluster	Dr SIYAKATSHANA, Njabulo
12:15	[103] Uncovering new possibilities in Engineering with High-Performance Computing (HPC)	Mr MARÉ, Charl

HPC Applications: 3 - ICC-L-Amethyst - Amethyst Room (13:45-14:45)

-Conveners: Chair: Prof Paola Carbone

time	[id] title	presenter
13:45	[112] The use of Cheminformatics in understanding the molecular mechanisms of South African Phytochemicals in the treatment of metabolic diseases	Dr RAMHARACK, Pritika
14:15	[42] Simulation of mesoscale convective systems with the Conformal Cubic Atmospheric Model on the CHPC	Mrs MULOVEDZI, Patience

Thursday 01 December 2022

HPC Applications: 3 - ICC-L-Amethyst - Amethyst Room (13:45-14:45)

-Conveners: Chair: Prof Cornie van Sittert

time	[id] title	presenter
13:45	[109] Evaluating the mycobacterial proteostasis system as a drug target in tuberculosis	Prof. EDKINS, Adrienne
14:15	[100] Computational Modelling using high performance computing for materials prediction and design	OBODO, Kingsley

HPC Applications: 4 - ICC-L-Amethyst - Amethyst Room (15:15-16:15)

-Conveners: Chair: Dr Madison Lasich

time	[id] title	presenter
15:15	[97] Heat Transfer in Greenhouses	Dr KRUGER, Sunita
15:45	[99] Using AI to perceive humans	Prof. VAN DER HAAR, Dustin

Friday 02 December 2022

HPC Applications: 5 - ICC-L-Amethyst - Amethyst Room (10:15-11:30)

-Conveners: Chair: Dr Thobani Gambu

time	[id] title	presenter
10:15	[136] Density functional studies of protonated and alkali metal (Li, Na and K) incorporated T-doped 2D zeolite model (T= B, Ga)	Prof. CHETTY, Nithaya
10:35	[7] HPC and Chemical Engineering Thermodynamics at MUT	Dr LASICH, Madison
10:55	[135] Application of high-performance computing at the Council for Geoscience	Dr SAKALA, Emmanuel
11:15	[132] Q&A	

HPC Applications: 6 - ICC-L-Amethyst - Amethyst Room (12:00-13:00)

-Conveners: Chair: Prof Hasani Chauke

time	[id] title	presenter
12:00	[84] Application of computational genomics in poultry and ruminant health improvement	Prof. ADELEKE, Matthew A.
12:30	[95] Exploiting a Tripartite Alliance of Computational Chemistry, Cheminformatics and Machine Learning for Computer-Aided Catalyst Discovery	Dr ADEYINKA, Adedapo

HPC Applications: 7 - ICC-L-Amethyst - Amethyst Room (14:00-15:00)

-Conveners: Chair: Prof Adrienne Edkins

time	[id] title	presenter
14:00	[38] Investigating chaos through computing: Condensates, plasma, astronomy, biology and beyond	Dr HILLEBRAND, Malcolm
14:30	[91] Understanding the catalytic activity of molybdenum carbide surfaces: what we can learn from surface-mobility of reaction intermediates	Dr GAMBU, Thobani