

Centre for High Performance Computing 2025 National Conference

Monday 01 December 2025

HPC Applications: 1 - BICC.G-C1 - C1 Tsitsikamma (11:15-12:45)

-Conveners: Chair: Prof Lyudmila Moskaleva

time	[id] title	presenter
11:15	[194] Simulating Potential Impacts of Solar Radiation Modification on African Climate	Prof. ABIODUN*, Babatunde
11:35	[145] Drug Design, Resistance and Metabolisms through CHPC	Prof. TASTAN BISHOP*, Ozlem
11:55	[177] Molecular Modelling in Research: From Basic Research Methods to Advanced Research	Dr GUMEDE*, Njabulo
12:15	[58] Elevating Material Simulations with Open Source – From Consumer to Contributor	Dr WARMBIER, Robert
12:35	[208] Q&A	Q&A

HPC Applications: 2 - BICC.G-C1 - C1 Tsitsikamma (13:30-15:00)

-Conveners: Chair: Prof Ozlem Tastan Bishop

time	[id] title	presenter
13:30	[127] The Impact and Benefits of Partnering for Operational Weather Forecast Continuity	Ms LANDMAN*, Stephanie
13:50	[143] Computational modelling of functional materials and chemical reactivity using molecular dynamics, DFT and wave-function-based approaches	Prof. MOSKALEVA*, Lyudmila
14:10	[178] Unravelling plant-biotic/abiotic stress using computational biology and bioinformatics tools.	Dr RAUWANE*, Molemi
14:30	[64] Fitting Classical Forcefields Programmatically for Application in Molecular Dynamics Simulations	Dr KGATWANE, Kenneth
14:50	[211] Q&A	Q&A

Tuesday 02 December 2025

HPC Applications: 3 - BICC.G-C1 - C1 Tsitsikamma (11:00-12:30)

-Conveners: Chair: Prof Regina Maphanga

time	[id] title	presenter
11:00	[139] Turbomachinery Modelling on the CHPC	Prof. VAN DER SPUY*, Johan
11:20	[22] High Resolution Modelling of Tropical Cyclone Characteristics using the Lengau Cluster	Dr STEINKOPF, Jessica
11:40	[108] Density functional theory of thermoelectric properties of graphene	Dr RAMOSHABA, Moshibudi
12:00	[118] Multiscale modelling of chemical systems on HPC and quantum computers	Prof. KEAL, Thomas
12:20	[213] Q&A	Q&A

HPC Applications: 4 - BICC.G-C1 - C1 Tsitsikamma (13:30-15:00)

-Conveners: Chair: Dr Njabulo Gumede

time	[id] title	presenter
13:30	[140] Engineering Strategies for Perovskites Materials	Prof. MAPHANGA*, Regina
13:50	[141] Cosmology with radio telescopes: finding a needle in the datastack	Prof. SANTOS*, Mario
14:10	[116] 1KSA - Decoding South Africa's Biodiversity	Dr SWART, Patricia
14:30	[25] HPC in all the right places – accelerating modelling workflows in metallurgical engineering applications	Dr REYNOLDS, Quinn
14:50	[226] Q&A	Q&A

HPC Applications: Users BoF - BICC.G-C1 - C1 Tsitsikamma (15:30-17:00)

-Conveners: Chair: Dr Werner Janse Van Rensburg

time	[id] title	presenter
15:30	[149] CHPC Users BoF	Dr JANSE VAN RENSBURG, Werner
16:30	[138] Computational Chemistry and Material Science Special Interest Group (SIG)	GOVENDER, Krishna

Wednesday 03 December 2025

HPC Applications - BICC.G-C1 - C1 Tsitsikamma (11:00-12:30)

-Conveners: Chair: Dr Ndanduleni Lethole

time	[id] title	presenter
11:00	[144] HPC Applications Enabling Catalysis Design for Ammonia Decomposition to Produce Hydrogen	Ms MOTSA*, Nomcebo
11:20	[136] Computational Insights into Wind Patterns and Albatross Mortality	Ms SCHOOMBIE*, Janine
11:40	[111] Acceleration of Electronic Structure Codes on Heterogeneous Hardware	Dr PULIGHEDDU, Marcello
12:00	[56] Rational design of porphyrin and BODIPY analogues for biomedical applications: further progress and future perspectives	Prof. MACK, John
12:20	[236] Q&A	Q&A

HPC Applications - BICC.G-C1 - C1 Tsitsikamma (13:30-15:00)

-Conveners: Chair: Ms Nomcebo Motsa

time	[id] title	presenter
13:30	[179] Exploration of future magnetic and cathode materials through computer-based simulations.	Dr LETHOLE*, Ndanduleni
13:50	[99] Architectural Variations of Li ₂ MnO ₃ -Li _{0.69} MnO ₂ Core-Shell Cathodes During the Cycling Process	Prof. LEDWABA, Raesibe
14:10	[52] Computational challenges of running kilometer-scale Earth System Models in a developing country	Mr MOALUSI, Tumelo
14:30	[109] Developing a Sustainable and Performant GPU Implementation of Plane-Wave DFT	Mr SMITH, Matthew
14:50	[148] Q&A	Q&A

HPC Applications: Women in HPC BoF - BICC.G-C1 - C1 Tsitsikamma (15:30-16:30)

-Conveners: Chair: Prof Khomotso Maenetja

time	[id] title	presenter
15:30	[131] Women in HPC BoF	Prof. MAENETJA, Khomotso