Centre for High Performance Computing 2021 National Conference

Wednesday 01 December 2021

HPC Applications (14:00-15:00)

-Conveners: Chair: Mr Mthetho Sovara (CHPC)

time	[id] title	presenter
14:00	[96] The IPCC Assessment Report Six: modelling contributions from the CHPC	Prof. ENGELBRECHT, Francois
14:30	[132] Computational chemistry and its application in pharmacy and drug development	Prof. RAMASAMI, Ponnadurai

HPC Applications (15:15-16:15)

-Conveners: Chair: Dr Krishna Govender (CHPC)

time	[id] title	presenter
15:15	[105] Surface Enhanced Raman spectroscopy substrates: towards sensitive bio-sensing of infectious diseases	Dr MHLANGA, Nikiwe
15:45	[99] Computational Chemistry within the Laboratory of Applied Molecular Modelling at NWU	Prof. VAN SITTERT, Cornie

Thursday 02 December 2021

HPC Applications (11:00-12:00)

-Conveners: Chair: Mr Nkwe Monama (CHPC)

time	[id] title	presenter
11:00	[36] Agriculture Empowered by SuperComputing	Mr ERDODY, Nicolas
11:30	[28] Investigating the Pressure Effects on Structural Behaviour of Garnet-Type Li7La3Zr2O12 Solid Electrolyte Material: A Classical Molecular Dynamics Study	Prof. LEDWABA, Raesibe Sylvia

HPC Applications (12:15-13:15)

-Conveners: Chair: Dr Charles Crosby (CHPC)

time	[id] title	presenter
12:15	[17] The usefulness of high-performance computing in small scale hydropower technology: Investigating the hydrodynamic effects of hydrokinetic turbines through validated CFD models	Ms NIEBUHR, Chantel
12:45	[75] Application of Computational Alchemy to screen alloys of alumina (Al2O3) as a catalyst support	Dr OUMA, Cecil

HPC Applications (14:00-15:00)

-Conveners: Chair: Mr Inus Scheepers (CHPC)

time	[id] title	presenter
14:00	[129] Infectious disease susceptibility in the context of African genetic diversity	Prof. MÖLLER, Marlo
14:30	[32] Rational design of Sn(IV) porphyrins for photodynamic therapy: further progress and future perspectives	Prof. MACK, John

HPC Applications: BoF: South African Modelling and Simulation Roadmap (15:15-16:15)

-Conveners: Chair: Prof Regina Maphanga (CSIR)

time	[id] title	presenter
15:15	[126] BoF: South African Modelling and Simulation Roadmap	Prof. MAPHANGA, Regina

Friday 03 December 2021

HPC Applications: 6 (12:15-13:15)

-Conveners: Chair: Dr Charles Crosby (CHPC)

time	[id] title	presenter
12:15	[49] Regional and coastal ocean modelling: toward an operational system for well-informed decision making	Dr VEITCH, Jennifer
12:45	[39] Bioinformatics for vegetable breeding at Starke Ayres	Mr MAFIREYI, Godwin

HPC Applications: 7 (14:00-15:00)

-Conveners: Chair: Dr Anton Lopis (CHPC)

time	[id] title	presenter
14:00	[124] Using genome-resolved metagenomics to understand microbial contributions to ecosystem functioning	Prof. MAKHALANYANE, Thulani
14:30	[80] Computational chemistry methods in understanding the properties of porous materials	Prof. ESTERHUYSEN, Catharine

HPC Applications: 8 (15:15-16:15)

-Conveners: Chair: Mr Binjamin Barsch (CHPC)

time	[id] title	presenter
15:15	[98] Improved COVID-19 classification of cough audio	Prof. NIESLER, Thomas
15:45	[25] Understanding metal losses during furnace tapping operations using HPC	Dr REYNOLDS, Quinn