Centre for High Performance Computing 2019 National Conference

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Birchwood

Book of Abstracts

Contents

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A Comparative Study of Cubic and B-Spline Interpolation Methods

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Numerical methods are essential in many scientific applications for their ability to make discrete data sets continuous. Interpolation is one commonly used method, which helps one to predict the value of any point between two adjacent data points of a data set. Furthermore, polynomial interpolation with a sufficiently high degree can make the data set differentiable. One consequence of using high-degree polynomials is the oscillation towards the endpoints, also known as Runge's Phenomenon[1] Cubic spline interpolation overcomes this problem by connecting data points in a piece-wise fashion. However, its complex formulation requires nested iterations in higher dimensions, which is time-consuming. In addition, the calculations have to be repeated for computing each partial derivative at the data point, leading to further slowdown. The B-spline interpolation is an alternative representation of the cubic spline method, where a spline at a point could be expressed as the linear combination of piecewise basis functions[2]. It was proposed that implementing this new formulation can accelerate many scientific computing operations involving interpolation[3].

Numerical interpolation was implemented in free energy methods for many purposes, from calculating intermediate energy states to deriving forces from free energy surfaces. The results of these calculations can provide insight into reaction mechanisms and their thermodynamic properties. The free energy methods include biased flat histogram methods, which are especially promising due to their ability to accurately construct free energy profiles at the rarely-visited regions of reaction spaces. Free Energies from Adaptive Reaction Coordinates (FEARCF)[4] that was developed by Professor Kevin J. Naidoo has many advantages over the other flat histogram methods. FEARCF uses cubic spline interpolation to derive biasing forces from the free energy surface, driving the reaction towards regions with higher energy. A major drawback of the method is the slowdown experienced in higher dimensions due to the complicated nature of the cubic spline routine. If the routine is replaced by a more straightforward B-spline interpolation, sampling and generating free energy surfaces can be accelerated.

The study aims to perform a detailed comparison between the cubic spline interpolation and B-spline interpolation methods. At first, data sets of analytic functions were used to compute the percentage errors of both methods by taking the functions themselves as reference. The performances of the two methods were evaluated at the endpoints, inflections points and regions with a steep gradient. Both methods generated identically approximated values with a percentage error below 1%, although they both performed poorly at the endpoints and the points of inflection. Increasing the number of interpolation knots reduced the errors, however, it caused overfitting in the other regions. In addition, cubic spline suffered from a drastic slowdown in higher dimensions with up to 103 in 3D and 105 in 4D interpolations. The same results applied to the classical molecular dynamics simulations with FEARCF with a speed-up of up to 103 when B-spline interpolation was implemented. To conclude, the B-spline interpolation method can enhance the efficiency of the free energy calculations where cubic spline interpolation is the currently-used method.

Supported Student:

Travel & Accom.

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A Computational Fluid Dynamics Approach to Selecting a Concentrating Solar Thermal Plant Location around a Ferromanganese Smelter

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Abstract for poster proposal, see PDF attached.

Supported Student:

Accommodation Only

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A DFT study of methoxy substituted alpha,beta-symmetrical ketones supported by experimental methods

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Density functional theory (DFT/B3LYP) calculations on a series of six methoxy substituted symmetrical dibenzylideneacetone analogues have been performed to determine the effects of solvent polarity and substituents on their stability. Conformational and molecular geometry analysis indicates that the trans-trans conformer of the studied compounds is the most stable one and this is supported by experimental 1H NMR results. The calculated molecular geometry parameters are in agreement with X-ray crystallographic data. The IR, UV-vis absorption and NMR (1H and 13C) spectra of the compounds were theoretically obtained and compared with the experimental ones. Various theoretical molecular parameters like dipole moment, frontier molecular orbital (FMO) energy, lifetime of the first excited state (τ), global chemical reactivity descriptors, natural bond orbital analysis and ΔEHOMO-LUMO gap are presented at the same level of theory. Good correlations were obtained between the calculated and experimental data. It was found that addition of electron-donating substituents and increasing solvent polarity greatly affects the stability of the present compounds. Inspection of the FMOs revealed the n □ □* nature of the lowest-lying transition and also predicted their photoinstability under UV illumination.

Supported Student:

No

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A comparison of the chemical reactivity properties of bioactive flavonols: A Computational nutraceutics approach

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In 1989, Dr. Stephen Defelice introduced the definition of nutraceutical [1] as any substance that is a food or part of a food and provides medical or health benefits, including the prevention and treatment of diseases [2]. The term 'Computational Nutraceutics' was coined in 2013 as a new concept for predicting the molecular structure, spectroscopy, and chemical reactivity of bioactive compounds using computational chemistry. [3] Flavonoids are phenolic compounds that occur in food either as free monomers (quercetin, catechin) or oligomers (procyanidins), or they are bound to saccharides as glycosides. In addition to their antioxidant properties, flavonoids have been reported to exhibit other multiple biological effects such as antiviral, antibacterial, anti-inflammatory, vasodilatory, anticancer and anti-ischemic. In this study the focus is the chemical reactivity properties of 3 bioactive flavonols (morin, myricetin and quercetin). The molecular geometry and the electronic properties such as the frontier molecular orbitals (Figure 1), ionization potential and electron affinity were calculated to get an insight of the molecular properties. The molecular electrostatic potential (MEP) was determined to examine their electrophilic or nucleophilic reactivity. The chemical reactivity descriptors such as the chemical potential, electronegativity, global hardness, electrophilicity index, and global softness was also determined.

Supported Student:

Travel & Accom.

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A first-principles study of Half-Heusler Intermetallic Compound MgAgAs with composite 2D-TiC/Mo2TiC material

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A theoretical study conducted to give a more elaborate investigation of the electronic and optical properties as well as the role of the heterostructures in Thermoelectric energy generation which is still deficient.

1. The electronic properties (density of state, band structures and charge carrier mobility)
2. work functions
3. Heat transfer simulations
4. optical property (absorption coefficient) are also considered in this study

Supported Student:

Waive Fees Only

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A molecular dynamic simulation studies of structural and mechanical properties on B19 TiPd-Pt shape memory alloys

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TiPd alloys have been suggested for commercial applications with a great potential due to their high strength and good corrosion resistance. High temperature structural and mechanical properties of B19 TiPdPt alloys are important for actuators applications, which are not well understood currently. The semi-empirical embedded atom method interatomic potentials incorporated in the LAMMPS code are employed to investigate the temperature dependence of the B19 TiPdPt structures. The lattice expansion, and elastic properties were calculated to determine the transformation and stability at varied temperature range. We found that binary TiPd alloy display possible transformation from B19 to B2 at 1447 K. At 6.25 at. % Pt, the temperature variation of the lattice parameters for the B19 phase transforms to B2 phase at approximately 1371 K which is indicated by the a/b ratio of 1.451. The elastic constants and shear modulus decrease with an increase in temperature. The temperature dependence of Pugh (Bulk to Shear ratio) and Poisson‘s ratio are studied and ductility is improved with an increase in Pt content. It was found that the addition of Pt results in higher transformation temperature of the TiPd shape memory alloy. Our theoretical results highlight the suitability of this method in predicting temperature dependent properties of TiPdPt alloys and show ability in selecting and designing desired actuators for aerospace application.

HPC content
Structural properties and Molecular dynamics calculations of the B19 TiPd-Pt alloys were achieved by utilizing various codes in the Medea environment at the CHPC.
The structural properties were achieved by utilizing the VASP code, LAMMPS code was utilized to study the temperature dependence, mechanical properties and phase transformation of the structures.
Application code: VASP, LAMMPS
Problem size: 16-2048 atoms
Core count: 48
Computational challenges: no challenges experienced so far.

Supported Student:

Waive Fees Only

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A survey of selected pathogenic bacteria in chickens from rural households in Limpopo province.

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A survey of selected pathogenic bacteria in chickens from rural households in Limpopo province
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Salmonella and Escherichia coli are major pathogens responsible for economic loss to the poultry industry. This study was designed to determine the prevalence of these pathogens in household raised chickens and study their virulence and antibiotic profiles. For this purpose, 40 chickens were purchased from families in the Capricorn district and sacrificed for sampling. Tissues were cultured on different bacteriological media followed by biotyping using matrix-assisted laser desorption ionization-time of flight (MALDI-TOF). Disk diffusion test was performed to determine the antibiotic susceptibility profiles of these bacteria. Out of a total of 160 tissue samples from the chickens, E. coli and Salmonella were found in these tissues and further investigated the pathogenic E. coli using Polymerase Chain Reaction (PCR). The invA gene, a confirmatory gene of Salmonella was detected in all the Salmonella isolates. The study revealed that there is a high prevalence of Salmonella and pathogenic E. coli in these chickens. Therefore, further studies on identification at species level are highly recommended to provide management and sanitation practices to lower this prevalence. The antimicrobial susceptibly data generated from this study can be a valuable reference to veterinarians for treating bacterial diseases in poultry.

Supported Student:

Waive Fees Only

Workshop / 25

Accelerated free energy calculations using open-source tools

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We will use open-source free energy tools and the Galaxy Platform (BRIDGE) to calculate absolute and relative free energies of protein-ligand binding. Setting up free energy molecular simulations, using scripts, the Linux command line and using HPC resources can be complex. Further not all steps are repeatable. With the Galaxy Project platform, BRIDGE and Galaxy Comp Chem we aim to provide a web application to assist researchers in conducting repeatable computer simulations and analysis using curated workflows.

Supported Student:

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Accelerating Automated Machine Learning Frameworks With GPU Algorithms

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The popularity of machine learning (ML) has led to a vast amount of approaches to learning a model. Techniques such as support vector machines (SVMs), random forests (RFs), K-nearest neighbours (KNN) and stochastic gradient descent (SGD), all requiring their own set of hyperparameters to be chosen before learning, gives a large search space of approaches. Automated machine learning (AutoML) is a method for choosing the best ML algorithm and corresponding hyperparameters for a given dataset without human intervention. This is important for both ML experts and non-experts alike. For example, a medical researcher using machine learning on their dataset may not be familiar with less popular techniques that may in fact be the best approach for them. For ML experts, AutoML shifts the focus of the researcher to the feature engineering aspect of the ML pipeline, rather

than spending a large amount of time trying to find the best algorithm or hyperparameters for a given dataset. Although there have been many advances in solving the search space problem, all approaches must still test a number of different methods first before deciding which best suits the given dataset. This task is computationally expensive and so any improvement in efficiency is valued. Research in parallelised graphics processing unit (GPU)-based versions of ML algorithms shows significant performance improvements over serial or CPU-based implementations. In this work, we explore approaches to GPU-based versions of ML algorithms and integrate them in an AutoML framework. The research question is therefore whether implementing GPU-based ML algorithms in an AutoML platform will improve the performance and efficiency of that platform.

HPC Aspects of This Research

We implement the MIT ATM automated machine learning framework on an HPC cluster,
where each node consists of 1 GPU.

In particular:

- We introduce a method for running ATM on a multi-node cluster, through a command line interface.
  We note that the current ATM documentation does not describe such a method. Furthermore, the use of the word 'cluster' in the current ATM documentation refers to a cluster of 'workers'; multiple processes on a single machine, as opposed to multiple processes on multiple machines.
- We implement state of the art GPU machine learning algorithms/libraries to replace the current serial algorithms.
- We demonstrate how to write a custom CUDA machine learning classifier and integrate it into the ATM framework.

These concepts can be extended to other AutoML frameworks.

The ATM framework relies on each node having access to the dataset from a centralised location. To this end, the Model Database Hub (where the dataset resides along with classifier results) is mounted on an NFS server.

The cluster used is the Wits Mathematical Sciences Cluster. The system has the following partitions:
batch: For general purpose use. Up to 60 nodes each with an i7 7700 CPU, GTX1060 6GB GPU, and 16GB of RAM. ha: For high priority runs when you anticipate load shedding may affect your work. Up to 10 nodes each with an i7 7700 CPU, GTX1060 6GB GPU, and 16GB of RAM.
* biggpu: For jobs requiring more that 8GB of GPU RAM. Up to 3 nodes, two with a GTX1080, and one with a GTX1080ti.

Various configurations/ partitions are used in our experiments.
Our experiments will conclude on the 14th of October 2019. During that time,
we will be testing different datasets of various sizes. Will choose results from a dataset that best show the performance differences for large input sizes.

Due to the complexity of the AutoML framework, we choose to limit the scope of this work to a single GPU per compute node. Thus each Classifier* running on a node in the cluster is limited to using a single GPU.
Future work would include the use of multiple GPUs used to run a single Classifier instance, as well as using MPI and CUDA-aware MPI implementations of the ML algorithms.

* In the ATM framework, a Classifier represents a single train/test run using a method (e.g SVM, KNN, RF etc.) and a set of hyperparameters with a particular dataset.

Supported Student:

Waive Fees Only

SIG Poster / 63

Adsorption of hydroxide, water and modified collectors on sperrylite (100) surface

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Organic collectors plays an important role in the recovery of platinum group minerals (PGMs) via flotation process. Sperrylite (PtAs2), is the world most common PGM and is abundant in the Platreef bushveld complex of South Africa. This mineral has been reported to be hard to float and requires detailed understanding and design of new collectors to improve its recovery. In this study we employed the Vienna Ab-initio Simulation Package (VASP) at Lengau cluster and the surface systems contained more than 120 atoms. We utilised 72 cores and the structures were converged after ten days. We investigated the interaction of hydroxide (OH-), water (H2O) and collectors at different adsorption sites on the most stable (100) surface of PtAs2. The OH- adsorption on As-top site was more exothermic (−406.31 kJ/mol), suggesting preferential adsorption on As atoms than on Pt atoms. The H2O adsorption on Pt-top site was more exothermic (−82.95 kJ/mol), suggesting that it preferred to adsorb on Pt atoms than on As atoms. The case of collectors, we have tested three modified collectors (3-thio-butyl-dithiocarbamate (3-TBDTC), butyl-carbonotrithioate (BCTT) and N-Butyl-1,3-diethylamide (NBDEA)). We observed that the adsorption of 3-TBDTC was much stronger on As-bridging (−164.63 kJ/mol). The NBDEA was found to be less exothermic with adsorption energy of −64.96 kJ/mol on As atom. The BCTT was stronger when bridging on Pt and As atoms with adsorption energy of −110.62 kJ/mol. These showed that 3-TBDTC has good collecting ability than the BCTT and NBDEA collectors. These findings pave a way for design of new collectors that can improve the recovery of hard to float PtAs2 mineral and other arsenide mineral.

HPC Applications / 77

Advancing the understanding of interactions between plasma arcs and power electronics with high performance computing

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Direct-current (DC) arc furnaces account for a significant proportion of installed pyrometallurgical capacity worldwide. Their applications include steel recycling as well as smelting of various materials such as ferrochromium, ferronickel, ilmenite, and others. In order to provide power to such furnaces, alternating current from the grid or other generation sources must be converted into DC by rectification. At industrial scales the rectifier unit is often the single largest capital cost item, and any errors in its specification can result in the entire plant operating inefficiently (or not at all).

In this presentation, computational plasma arc models developed in OpenFOAM® are coupled with circuit simulations of solid-state furnace rectifiers in order to gain insight into the complex interactions between the rectifier's design parameters and the behaviour of the arc. Such approaches provide a first step toward true virtual prototyping and digital twin modelling for the electrical design and optimisation of DC arc furnaces.

High performance computing is a critical enabling tool in such studies, and various aspects of this – including solver performance scaling analysis, software automation, and use of methodologies from other HPC fields – will be touched on during the presentation.

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An Irreversible Inhibitor of HSP72 that Unpredictably Targets Lysine-56 –A molecular insight

Authors: Aimen Aljoundi[1] ; Mahmoud Soliman[2]

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HSP72, a stress-inducing molecular chaperone, is a significant therapeutic target in oncology, but it has proved particularly difficult to inhibit this protein with small molecules owing to competition with the high affinity and abundance of its endogenous nucleotide substrates. Recently, unexpectedly 8-N –benzyladenosine inhibit the HSP 72 by targeting the lysin 56 instead of cyst 17. This prompted us to investigate the dynamic behind this novel drug combination. To get insight into the observed un expected interaction, molecular dynamics simulations have been employed to investigate the inhibitory mechanism as well as the structural dynamics that characterize this effect. Structural dynamic analyses indicate that the lysine bound complex has shown a more compact and stable protein conformation compared to cysteine bound complex. In addition, binding free energy calculation suggest that van der Waals energy interactions were observed to be the main energy component driving this unanticipated effect. Furthermore, per-residue energy decomposition analysis identified Tyr 40, Glu 267, and Thr 264 as key residues that contribute largely to this unpredicted effect. The findings highlighted in this study provide a molecular understanding of the dynamics and mechanisms that mediate the new drug design paradigm for HSP72 chemical probes in oncology treatment.

Supported Student:

Travel & Accom.

SIG Poster / 117

Anion receptor design for the development of $[PtCl6]2^-$ selective reagents

Author: Cyprian Moyo[1]

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The word document has the full version of the Abstract, and is attached under the attachments section.

The ever-increasing demand for Platinum Group Metals (PGM's), coupled with their low natural abundance and complex processes required for their extraction has rendered this rare group of metals as the most sought after in the advent of the 21st century. Consequently, there is an increasing need to engineer new reagents with molecular functionalities that offer high selectivity and loading capacities. This will enable more efficient recovery of PGM chlorido species from feed solutions derived from mineral ores, and also secondary sources such as spent catalytic converters. The innovation of the aforesaid reagents undoubtedly requires a design strategy that considers both the electronic and stereochemical requirements of the target anion. Herein, a two-fold anion receptor design method for developing highly selective reagents for $[PtCl6]2^-$ in HCl medium is reported (Figure 1).

Through a combination of theory, molecular modelling techniques and crystallography (see below), we were able to prove that derivatization of the protonated form of triethylenetetramine,

([TETAH4]4+), by R groups offers greater complementarity to $[PtCl6]2^-$ (lower ΔUreorg) and hence higher binding energies to the anion in silico.

DIRISA / 213

Application of Ontology Engineering in Data Intensive Research

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Theme/Focus Area: Harnessing the Power of Data Intensive Research for 4IR

Abstract:

Data is used on a daily basis to enable the functioning of organizations and the execution of pertinent tasks and projects. With this in mind, technological trends play a vital role in how it is generated, retrieved and processed to add value. The prevalence of the 4IR which has resulted in the vast and rapid generation of data across various channels and platforms. This has in turn necessitated a need for the revisiting and or development of tools and methodologies that can foster the effective management and processing of said data.

In comes a miraculous "solution" in the form of ontologies, which bear gifts in the form of the following (to name a few):

- Semantics (improves a system's efficiency of reasoning-makes domain assumptions explicit)
- Information extraction
- Domain conceptualization/modelling
- Knowledge discovery
- Knowledge representation and packaging
- Adapting to user preferences
- Mitigation of information overload

The application of Ontology Engineering in data intensive research has the potential of harnessing fruitful research outputs if applied effectively. This will required having a comprehensive understanding of the underlying needs and requirements of the research that will be undertook by experts. This will in turn guide the overall project through ensuring that all tasks and activities executed are aligned with the vision of the project. Seeing that one of the underlying objectives of the 4IR entails the use of machines to facilitate and automate tasks performed by humans; the use of ontologies in conjunction with data intensive research will enable effective and efficient decision-making through the provision of the retrieval and representation of relevant/applicable sources of data and information.

This presentation seeks to address the manner in which the notion of Ontology Engineering can be applied to aid many of the current methodologies applied to facilitate data intensive research in the era of the 4IR.

Keywords: Ontology, Information Management, Information Retrieval, Information Extraction, Decision Support, Data, Information, Ontology Engineering, Knowledge Management

Supported Student:

HPC Applications / 169

BIOPERIANT12, a regional high-resolution model configuration towards developing the South African VrESM Earth System Model

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In understanding and predicting a changing global climate system, the representation of ocean-biogeochemistry processes in the Southern Ocean is particularly important because of the key role it plays in global carbon-climate feedbacks. To date, Earth System Models (ESMs) do not adequately resolve important ocean dynamics (e.g., mesoscale processes), features that are critical in Southern Ocean heat and CO2 fluxes and storage. Therefore high resolution ocean biogeochemical models provide essential constraints to the medium resolution (100km) global ESMs.

The South African ESM, VrESM, comprises of globally coupled atmosphere, ocean, ice, land-surface, atmospheric-chemistry, and ocean-biogeochemistry models. Building and running the ESM is therefore a huge task: both scientifically and computationally. Several numerical models, each discretized on a global grid need to be integrated in space and time, while additionally passing information to each other. As part of a multi-institution and multi-year goal of building South Africa's first Earth System Model, which will be run at the CHPC, we have been developing the ocean-biogeochemistry component of the VrESM (PISCES-SOCCO). BIOPERIANT12 is a critical platform in this development.

We present the NEMO v3.4 regional model configuration BIOPERIANT12, our most computationally-challenging model to date and run on CHPC's Lengau cluster. BIOPERIANT12 simulates ocean, ice, biogeochemistry of the circumpolar Southern Ocean (south of 30°S) from 1989 to 2009, prescribed by ERA-interim atmospheric forcing. BIOPERIANT12 is high resolution at a mesoscale-resolving 8 km in the horizontal and in the vertical: ranges from 6 m resolution at the surface to 250 m at the ocean bottom over 46 vertical levels.

In addition to the technical aspect of developing the PISCES-SOCCO source code for VrESM, we have to configure VrESM for an improved representation of the Southern Ocean. BIOPERIANT12, thus serves in multiple ways: (1) as a comparison for ocean biogeochemistry in the ESM, (2) as a large test case for ocean-biogeochemical evaluation metrics for the ESM, (3) as an experimental platform for understanding processes which influence atmosphere-ocean carbon exchange in the Southern Ocean, which additionally helps improve the ESM. We discuss PISCES-SOCCO development progress as well as the building and evaluation of BIOPERIANT12.

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BRICS meeting on HPC in climate and weather simulations

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A closed session for South Africa, Brazil and Russia representatives for discussion of joint activities in the area of weather and climate modelling based on first principles, machine learning and using HPC hybrid architectures, especially GPUs.

SA NREN / 215

BRICS programme on "Cybersecurity: Software and Data Security"

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he BRICS Network University (BRICS NU) is a network of 60 universities, 12 each from the five BRICS countries. The BRICS NU is aimed at developing partnerships and exchange programmes in six thematic areas (ITGs) determined by the BRICS Ministries responsible for education. This project forms part of the University Capacity Development Programme (UCDP), an umbrella imitative developed and implemented by the South African Department of Higher Education and Training to build capacity in South African universities in three key areas: student success, staff development and programme/curriculum development. The BRICS NU ITG on Computer Science and Information Security (CSIS) representatives from the BRICS countries, agreed that CSIS ITG will focus on developing a BRICS Masters programme on ìCybersecurity: Software and Data Security. The presentation will include the proposed content, development and implementation plan of the BRICS Masters Programme.

Supported Student:

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BRIDGE: Biomolecular Reaction & Interaction Dynamics Global Environment

Author: Tharindu Senapathi[None]

Co-authors: Chris Barnett [1] ; Kevin J. Naidoo [1]

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The pathway from genomics through proteomics and onto a molecular description of biochemical processes make the discovery of drugs and biomaterials possible. A research framework common to genomics and proteomics is needed to conduct biomolecular simulations that will connect biological data to the dynamic molecular mechanisms of enzymes and proteins. Novice biomolecular modelers are faced with the daunting task of complex setups and a myriad of possible choices preventing their use of molecular simulations and their ability to conduct reliable and reproducible computations that can be shared with collaborators and verified for procedural accuracy.
In this presentation, we follow from the previous work where the *Dynamics* facility of the BRIDGE[1] computational dashboard developed on the Galaxy platform[2] that makes possible fundamental molecular dynamics, analysis and analytics of biomolecules. Here we introduce the Free Energy suite of functions that makes the up the *Interaction* facility in BRIDGE. We illustrate the binding free energy calculations carried out on a set of sialyltransferase inhibitors and show how BRIDGE facilitates Drug Discovery programmes for skilled and less skilled computational scientists. These simulations can be scaled over multiple CPU's. Absolute free energy calculations scaled best using GPU's.

1. Senapathi, T.; Bray, S.; Barnett, C. B. J. B. Biomolecular Reaction & Interaction Dynamics Global Environment (BRIDGE). 2019.
2. Afgan, E.; Baker, D.; Batut, B.; Van Den Beek, M.; Bouvier, D.; Čech, M.; Chilton, J.; Clements, D.; Coraor, N.; Grüning, B. A. J. N. a. r. The Galaxy platform for accessible, reproducible and collaborative biomedical analyses: 2018 update. 2018

Supported Student:

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HPC Applications / 168

Benchmarking off-the-shelf radio astronomy software on Lengau

Author: Sean February[1]

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MeerKAT, one of the world's most powerful radio telescopes in operation today, is producing science-ready data into the now public-facing archive at a steady rate. In this talk, we will assess the performance of off-the-shelf tools for post-processing and imaging MeerKAT data on Lengau.

SIG Poster / 52

Biosensing of DNA damage in Alzheimer's disease by Computational and Experimental methods

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DNA damage plays a pivotal role in the pathogenesis of Alzheimer's disease (AD) therefore, an innovative ss-DNA/dopamine/TiO2/FTO electrode strategy was developed to detect the genotoxicity upon photocatalytic reactions. This study involves a computational and electrochemical investigation towards the direct measurement of DNA damage. Computational chemistry was useful to resolve the intricate chemistry problems behind electrode constructions. The computational protocols were simultaneously carried out comprising of density functional theory (DFT) calculations, Metropolis Monte Carlo (MC) adsorption studies, and molecular dynamics (MD) simulations. The DFT calculations elucidated the structural, electronics, and optical properties of the electrode components resulting in a good agreement with the experimental parameters. The MC simulations carried out using simulated annealing predicted the adsorption process within layer-by-layer electrode as well generating reliable inputs prior to MD simulations. A 100 ns MD simulations were performed using a canonical ensemble provided information on the thermodynamics parameters such as total energy, temperature and potential energy profiles, including radius of gyrations and atomic density profiles. Binding energies calculated from the MD trajectories revealed increasing interaction energies for the layer-by-layer electrode, in agreement with the experimental characterization studies. Experimentally, the ss-DNA was electronically linked to TiO2/FTO surface through dopamine as a molecular anchor. Electrochemical measurements using cyclic voltammetry and electrochemical impedance spectroscopy were employed to characterize the electrode modifications. The square

wave voltammetry was subsequently used to measure the DNA damage and the ability of antioxidant treatment using ascorbic acid (AA). The presence of AA significantly protected the DNA from the damage, and therefore used as a potential treatment in AD. The electrochemical characterizations were in a good agreement with the theoretical investigations (i.e. HOMO-LUMO DFT levels and binding energies). In addition, guanine residues predicted by DFT as the most reactive sites of the ss-DNA involved in the genotoxic reactions. Overall, the theoretical studies successfully validated the experimental study as well as providing the molecular basis of interaction phenomena towards electrode constructions. Our results highlight the potential application of this methodology to screen the genotoxicity in Alzheimer's, suggesting the important role of theoretical studies to predict the molecular interaction and validation of the DNA-based sensors and bioelectronics.

SA NREN / 162

Brainstorming on a Guiding Policy Framework towards Ethical Conundrums around Artificial Intelligence of Things (AIoT)

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The convergence of Artificial Intelligence and the Internet of Things (IoT) gave birth to the now Artificial Intelligence of Things (AIoT). These innovative initiatives have both envisaged benefits and concerns. Among the grey areas around these emerging technologies is how to regulate and address ethical issues that may arise as a result of their adoption and use thereof. This research will advocate a guiding framework for policy makers, to aid in the decision-making processes on ethical issues that may be raised regarding AIoT. The research findings will help the public, private, and civic sectors to understand the myriad issues around AIoT and guiding procedures which they can employ to navigate such issues in all-inclusive and democratic governance. There are long-standing developmental issues in the field of ICTs and sustainable development in most of the developing countries, and such issues are creating a rift between governments and the private sector as they lament the speed at which technology is advancing and the slow pace at which laws are enacted. The exponential growth of technology demands the need to foster cross-pollination of ideas through NRENs between policy makers and academics, so as to bridge the gap between law formulation and technological advancements. This research will focus on future considerations of AIoT policy implementations in five southern African countries as per the demarcation of UN's territories namely: - Botswana, Lesotho, Namibia, South Africa, and Eswatini. The selection is mainly informed on the basis that, the countries are already sharing a common interest that involves guiding principles – SACU and also purposely sampled by the size of the region. On the other hand, the selection of Southern African countries will be opportune as all of them have the potential to navigate the emergence of new technologies and incorporate such in their policy and frameworks as they push towards realizing their respective NDPs and SDGs. The fact that most of these countries have recently or are about to host their elections within this year, may help in following the policy implementations and adjustments if any by their respective governments. The role that multilateral organizations such as the UN can play in supporting such policies with particular focus on AIoT, which could be triangulated to other developing countries.

SIG Poster / 60

CF3-pyridinyl substitution on anti-malarial therapeutics: Probing differential ligand binding and dynamical inhibitory effects of a novel triazolopyrimidine-based inhibitor on Plasmodium falciparum Dihydroorotate dehydrogenase

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The quest for reliable Dihydroorotate dehydrogenase (DHODH) inhibitors has engendered the discovery of potential therapeutic compounds at different stages of clinical trials. Although promising, high attrition rates and unfavorable bioactivities have limited their drug developmental progress. A recent structural modification of DSM265, a triazolopyrimidine-based inhibitor, yielded DSM421, derived by the substitution of the SF5-aniline group on DSM265 with a CF3-pyridinyl moiety. Consequently, DSM421 exhibited improved pharmacological and pharmacokinetics attributes relative to DSM265. The improved bioactivity mediated by the CF3-pyridinyl group leaves us with a curiosity to investigate underlying ligand-binding mechanisms and dynamics using computational methods. Presented in this study are insights that clearly explain the effects of structural SF5-aniline → CF3-pyridinyl modifications on pfDHODH inhibition. Findings showed that the CF3-pyridinyl group induced an optimal and stabilized positioning of DSM421 within the binding pocket, allowing for steady and strong intermolecular interactions which favored its stronger binding affinity as estimated and correlated with bioactivity data. These interactions consequently induced a pronounced stabilization of the structural conformation of pfDHODH by restricting residue motions, which possibly underpinned its enhanced inhibitory activity relative to DSM265. Active site interactions of the CF3-pyrinidyl group with residues Ser236, Ile237, and Phe188 characterized by strong π-π stacking and halogen interactions also stabilized its positioning which altogether accounted for its enhanced inhibitory prowess towards pfDHODH. On the contrary, fewer and weaker interactions characterized DSM265 binding which could explain its relatively lower binding affinity. Findings will facilitate the design of novel pfDHODH inhibitors with enhanced properties.

Workshop 1 CHPC Users Guide / 46

CHPC Induction Tutorial

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A brief introduction to using the CHPC cluster for new users. This tutorial covers:

- connecting
- transferring files
- Lustre
- PBSPro
- writing job scripts
- job submission and control
- monitoring running jobs

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CHPC Industry Forum

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The CHPC Industry Forum is focused on engagement with the current and prospective non-academic user base of the CHPC. During the session feedback from existing industry users will be provided, an update will be given on the status of CHPC support to this user category, as well as open discussion on the opportunities and challenges for HPC support to this sector. The session is open for any interested delegate to attend.

SIG Poster / **144**

COMPUTATIONAL MODELLING STUDY ON PHASE STABILITY OF TiO₂ and MnO₂

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Energy is the basis of societies' welfare, economic and development. Population growth, industrial development, and economic growth lead to increased energy demand. Due to their high energy and long cycling life, lithium-ion batteries have held a significant share of the energy storage market for portable electronics and electric vehicles. However, with the rapid development of renewable energy plants, there is an urgent demand for energy storage systems with exceptionally good cycling performance, high safety and low cost. Discovering materials to improve the safety and power density of existing Li-ion batteries is important, here we consider a study on TiO2 and MnO2. In the current work we present a comparative study on structural, mechanical, vibrational and electronic properties of TiO2 and MnO2 investigated using ab initio method within density functional theory. Lattice parameters for the materials are in good agreement with experimental values to 5%. The heats of formations suggest that the structures are stable with negative values. Elastic properties indicates that the structures are mechanically stable due to positive elastic constant and satisfying necessary mechanical stability criteria condition for tetragonal structure. UNCLE code and Monte Carlo simulation was used to determine 36 phases of mixed Ti-MnO2 system.
Keywords: Energy storage, Lithium-battery, ab initio, Phase stability

BoF / **154**

Ceph and other large data storage systems

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A round table to share experiences, lessons learned and many of the other issues specific to large storage systems.

For anyone that's involved or interested in the design, testing and management of a large software defined data storage system.

Each attendee will be given 5 minutes (or more) to introduce themselves, and their current storage implementation (if applicable).

After the introduction, the agenda for the remaining time will be drawn up. Suggested topics for the agenda: a comparative analysis of storage software implementations (positives and negatives); a list of common issues agnostic to implementation, like configuration management, cluster monitoring, benchmarking tools and hardware specifications.

SIG Poster / **9**

Chemical Reactivity Properties of Bioactive Pentacyclic Triterpenoic Acids by Conceptual DFT

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See attached word document.

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Chemistry, Material science and Health science

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SIG: technical presentations in Chemistry, Material science and Health science

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Climate Research for Development - modelling and applications

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In this BoF closed session, weather scientists and application specialists from six SADC countries contributing to the Climate Research for Development (CR4D) fellowship will discuss the way forward in the improvement of numerical models presented during the weather and climate modelling SIG. Further, there will be short presentations on the development of products for different sectors and discussions around the development of products for the agriculture, hydrology, health, energy and disaster risk reduction sectors in the SADC region. This discussion/workshop forms part of the CR4D deliverable.

SA NREN / 228

Cloud Computing a Solution to Internet Services Downtime at Namibian Institutions of Higher Learning

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E-learning has been adopted by many institutions as a means by which to foster an effective teaching and learning environment. Namibian institutions of higher learning have not been left behind and are also using e-learning systems. Use of e-learning brings about many benefits like that of students being able to access learning material anywhere and anytime but implementation of e-learning has its own drawbacks of which cloud computing could be the answer. Furthermore, higher learning institutions run their own IT systems and buy their own IT infrastructure which has implications on the overall institutions' budgets. Data on issues with overall IT operations not just for e-learning systems was obtained from a case site at one of the Namibian institutions of higher learning. The study showed that the institutions' IT systems have problems that cloud computing could be able to solve.

Keywords: Cloud computing, e-learning, education, downtime

Supported Student:

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Comparison between thermodynamic stable Pt0.5Ni0.5 bimetallic alloy surfaces and a Pt (111) surface

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One of the biggest problems we face today is global warming. Global warming is the result of amongst other things pollution due to the use of fossil fuels. Too decrease the pollution clean, sustainable, alternative energy sources are needed. One such clean, sustainable, alternative energy source is the splitting of water into hydrogen and oxygen. The water splitting reaction consists out of two half reactions, namely the electro-catalytic oxygen evolution reaction (OER) and the electro-catalytic hydrogen evolution reaction (HER).1 However, the OER reaction is hindered by the large overpotential of 1.23V. At present the electro-catalyst used for the OER reaction is platinum (Pt). However, Pt is a rare and expensive resource. For this reason an alternative electrode material is needed. Such alternative electrode materials are Pt alloys. These alloys have been investigated for the oxygen reduction reaction (ORR) and a record low overpotential of 0.69 V was obtained with PtNi nanoparticles. Making PtNi nanoparticles a highly active electrocatalyst for the ORR reaction. On the other hand, Ni-containing materials such as oxides and hydroxide have shown excellent performance for the OER reaction.2,3 This implies that a combination of Pt and Ni in an alloy could have great potential as a bifunctional electrocatalyst for both the ORR and OER reactions. Therefore, the relationship between the equilibrium composition of the two metals, the distribution of the metal atoms and the electronic structure in PtxNi1-x alloys were investigated.4 In the study4 thermodynamically stable bulk structures and an optimal ratio of Pt0.5Ni0.5 were obtained, as shown in Figure 1.(attached document)

In this investigation, using DFT calculations implemented in the Materials Studio 2016 software,5 surface and adsorption properties were investigated on the thermodynamically stable Pt0.5Ni0.5 alloy and a Pt(111) surface. The Pt0.5Ni0.5 alloy surface was cleaved at five fractional top positions (0, 0.5, 1.0, 1.5 and 2). Five different surface terminations were obtained for the Pt0.5Ni0.5 surface (Figure 2,attached document) so that the surface arrangement varied for each of the surface terminations. Hydrogen adsorption was performed onto these surface terminations on the atop, fcc, hcp and bridge adsorption sites, to obtain information on the influence of nearest neighbours on the electronic and surface properties. According to the surface energy results, the most stable surface termination was that of the 0.5 surface termination, which was also the most stable surface termination after hydrogen was adsorbed onto the fcc adsorption site. Overall, the adsorption energies of the 0.5 surface termination is more stable than those of the pure metal surfaces at a low surface coverage.

Supported Student:

Accommodation Only

HPC Applications / 165

Computational Catalysis @ NWU

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At the North-West University (NWU) interest in incorporating computational chemistry in training and research started in the late 1990. Although there was not much support for this interest in computational chemistry, the need for understanding the chemistry in especially catalysis was identified.

Starting with old discarded computers and the cheapest possible software, the first attempts were made in calculating structures of transition metal complexes used in catalysis research at NWU. Due to the limitation of the resources, only gas phase reactions in homogeneous catalysis could be investigated. As the value of the computational investigations became evident, more resources were acquired.

It was however only in 2002 that support from the Research Focus Area (previously called Separation Technology) at NWU was obtained. Formal training of one staff member and the establishment of a dedicated Laboratory for Applied Molecular Modelling was funded. After careful evaluation of the needs in the research and the abilities of the researchers, it was decided to invest in Accelrys Materials Studio (for research) and Spartan (for training) software. At the same time 10 workstations and a 12 CPU cluster were acquired.

Although this was a major step forward, catalysis research was still limited to gas phase reactions in homogeneous catalysis investigations, with transition state calculations being a challenge. At this stage the CHPC was established. After a short phase of development and streamlining operations and software at CHPC, access to these resources were obtained by NWU researchers.

With the access to CHPC resources, limitations to the type of investigations gradually disappeared. The homogeneous catalysis investigations could be expanded to real system investigation, including solvents. Models could be expanded from explanations of observations to prediction for activity. Heterogeneous catalysis could also be included in research.

Now, computational catalysis research at NWU was ready to investigate real problems and try to find solutions. One such real problem being investigated at NWU is the development of new/alternative catalysts to apply in the generation of alternative and renewable energy.

HPC Applications / 15

Computational Fluid Dynamics: from solar thermal receivers and collectors to sub-antarctic island wind simulation

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The parallel cluster at the CHPC is used to provide speed-up on three fronts in the Computational Fluid Dynamics (CFD) simulations discussed. The first is for optimization of the parameterized geometry of a swirling jet impingement solar thermal receiver where many runs of fairly large Large Eddy Simulation CFD models are required. The second problem that benefits from the massively parallel approach, is that of a transient simulation of the atmospheric boundary layer turbulent flow field around a heliostat with a very small time step, requiring many time steps for a meaningful time series. This simulation is required to determine peak loads and perform the fluid-structure interaction of such a solar collector. The last type is for large models of wind flow over Marion island containing close to hundred million computational cells. These models are used to predict wind patterns that affect plant and bird life, especially as influenced by continued climate change.

HPC Applications / 103

Computational Modelling Study on Stability of Li-S/Se System

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Lithium Sulphur batteries suffers from the low conductivity of S and the solubility of intermediary polysulfide species during cycling. It has been reported that Se and mixed SexSy represent an attractive new class of cathode materials with promising electrochemical performance in reactions with both Li ions. Notably, unlike existing Li/S batteries that only operate at high temperature, these new Se and Li/SexSy electrodes are capable of room temperature cycling. To study large systems and impact of temperature effectively, empirical interatomic potentials of Li2S were derived and validated against available experimental structure and elastic properties. Complex high temperature transformations and melting of Li2S was reproduced, as deuced from molecular dynamics simulations. Li2S was found to withstand high temperatures, up to 1250K each which is a desirable in future advanced battery technologies. Cluster expansion and Monte-Carlo simulations were employed to determine phase changes and high temperature properties of mixed Li2S-Se. The former generated 42 new stable multi-component Li2S-Se structures. Monte Carlo simulations produced thermodynamic properties of Li2S-Se system for the entire range of Se concentrations obtained from cluster expansion and it demonstrated that Li2S-Se is a phase separating system at 0K but changes to mixed system at approximately 350K.

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Computational and metagenomics analyses of Toxoplasma in raw food, livestock, companion animals and the environment

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Globally, Toxoplasmosis infections are widespread as one of most common diseases of humans and animals. Toxoplasmosis is caused by a protozoan parasite known as Toxoplasma gondii. Infections in animals results in miscarriages, whereas, infections in pregnant women cause mental retardation and blindness in children, in addition to ocular problems in immunocompetent individuals, such as people with acquired immunodeficiency syndrome (AIDS). Some of the high-risk food products are contaminated meat, unpasteurized milk, fresh plant products such as vegetables and water. Faecal samples of companion animals, majorly from the cat family could transmit the infection to human beings. The first broad objective of this study is to carry out computational genome-wide identification of heat shock proteins and antigens in the Toxoplasma genome. Heat shock proteins (HSP) regulate key signal transduction events in many organisms and perform critical functions in growth, development, and virulence in many parasitic protozoa including T. gondii. Data mining of publicly available shotgun metagenome sequences will be carried out for ccomputational genome-wide survey of heat shock proteins and antigens with the aim of ultimately developing effective vaccine against T. gondii. Computationally, we will characterise physiochemical properties of the heat shock proteins and antigens, perform multiple sequence alignment, determine and estimate evolutionary trace analysis. Secondly, it is to detect different variants of Toxoplasma in terms of virulence, pathogenicity and genomic diversity to understand the genetic architecture, course and transmission routes of toxoplasmosis in human food chain, animals and environment in KwaZulu-Natal using metagenomics analysis. Tissue samples will be collected from raw food of animal and plant origin, and faecal samples from animals and soil samples. Samples will be processed, and DNA extracted and further prepared for genomics analysis. We will determine the species composition of the samples, perform statistical analysis using R and Python to estimate abundance, richness, Simpson and Shannon index and diversity of the species. Beta diversity will be computed using distance metrices generated from unweighted UniFrac analysis, principal coordinates analysis (PCoA) and non-metric multidimensional scaling (NMDS). Analysis of variance will be used to compare univariate analysis of alpha diversity measures.

Supported Student:

Travel & Accom.

1

Computational determination of skin sensitizing potency of 1,4-benzoquinone derivatives

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The aim of this research on skin sensitizing species is to develop an alternative method to animal-based methods for assessing the allergenic potency of chemicals. Among these chemicals, benzoquinone and its derivatives are categorized as extreme skin sensitizers. Typically, these sensitizers bind to proteins in the skin. Therefore, in this work, the reaction of benzoquinone derivatives (BQD) with nitrobenzenethiol (NBT), as a surrogate for protein haptenation, was investigated. The intra-fragment, inter-fragment and atomic properties of the products of the reaction of 4-nitrobenzenethiol (NBT) with three different 1,4-benzoquinone derivatives (BQD) were studied. The use of global electronic reactivity indices was employed on eleven benzoquinone derivatives. The computed reaction rate constants favour the synthesis of compound (NBT-BQ), while compound (NBT-2,5DBQ) is the least favourable. A hyperchromic shift to higher absorbance in terms of the molar absorptivity was observed from and their $\pi \longrightarrow \pi^*$ excitation transition was found to be HOMO-1 to LUMO, which is

predominantly intra-fragment within the atoms of NBT in the three compounds of BQD. The n ⟶ π * electronic transition, that is, the HOMO to LUMO transition, involves the inter-fragment electron excitation from fragment BQD to NBT. The resonance electron delocalization within the fragment BQD plays a more significant role in the stability compared with the fragment NBT. According to the global electrophilicity scale, all the BQDs investigated here are categorized as strong electrophiles. The reactivity of BQDs containing electron-donating groups is lower and are more stable than BQ while BQDs containing an electron-withdrawing substituents were predicted to be more reactive. BQDs can be arranged in decreasing order of 2,5-DCBQ > 2,6-DCBQ > CBQ > DBRBQ > BQ > MBQ > tBBQ > 2,6-DBQ > DMBQ > 2,5-DBQ > HBQ.

Keywords: Electronic transition, global reactivity indices, rate constants, skin sensitization, , charge transfer, anisotropic and isotropic hyperfine function, Fukui indices

Supported Student:

Travel & Accom.

SIG Poster / 155

Computational investigation of the binding characteristics of β-amyloid fibrils

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Timely and accurate diagnosis of Alzheimer's disease (AD) remains a major challenge in the medical arena. β-amyloid (Aβ) imaging techniques such as positron emission tomography and single photon emission computed tomography require the use of an imaging probe. To date, only flutemetamol, florbetaben and florbetapir have been approved for clinical use as imaging probes. Design of imaging probes requires a detailed understanding of disease mechanism(s) and receptor-ligand interaction. In this study, molecular docking, molecular dynamics and binding free energies were used to investigate the multiple binding sites exhibited by β-amyloid fibrils. Protein atomic models 2BEG, 5KK3, 2M4J, 2LMN, 5OQV, 2NAO, 2MVX and 2MXU (protein databank codes) were used to investigate the nature and location of binding sites and binding profiles of selected molecules with known affinities. Although amyloid fibrils are known to have multiple binding sites, we demonstrated that model 2MXU possesses one druggable site which can bind with common scaffolds currently being used in the imaging of amyloid fibrils. Models 2NAO, 5KK3 and 2M4J revealed that even though multiple sites may be available in some fibrils, the entire protein may not have a druggable site. Molecular dynamics revealed atomic model 2MXU to be less flexible in comparison to 2BEG. The outcomes of this investigation can be translated to assist in designing novel molecules that can be used for brain imaging in Alzheimer's disease.

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Computational study of β-MnO₂ as cathode material for lithium ion batteries using DFTB technique.

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Lithium manganates (LiMn2O4 or LiMnO2) are considered as a cathode material for lithium batteries, because they have tunnels which allow smooth diffusion of lithium ion. LiMnO2 became of major interest, simply because manganese is not only relatively inexpensive but also the desired properties for the electrode. One of the major demands is to modify and strengthen the structural stability of MnO¬2 in order to prevent rapid capacity fading during cycling. Dmol3, is a density functional theory-based program which is used to find the parameters for ferromagnetic MnO2. After successfully parameterizing MnO2, the lattice parameters were comparable with previously calculated DFT calculations reported in literature. Density functional tight binding (DFTB) was employed to investigate the electronic properties of MnO2 such as density of states (DOS) and band structures in order to validate the parameters derived using DFTB. The DOS were calculated to check the nature of MnO2. The electronic band structures calculated indicates the absence of a gap at Fermi level, thus MnO2 is a metallic. The electronic properties calculations were running in parallel on 16 of 3600 cores using CHPC with memory usage of 2048 MB. These findings are important in preserving the crystal structure of MnO2 and the maintenance of capacity during cycling.

Supported Student:

Waive Fees Only

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Computer simulations of Na0.22TiO2 nanospheres at increased temperature as anode electrode material for Na-ion batteries.

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Generated nanosphere-architectured TiO2 1 are promising as anode electrode materials for sodium rechargeable batteries due to their capacity to host more sodium ions and to withstand high simulations temperatures. In these study, recrystallisation synthesis of nanosphere Na0.22TiO2 (17172 atoms) structure was simulated from an amorphous precursor by running large scale molecular dynamics (MD) method through DL_POLY_2 [2] with a constant simulation time step of 0.003 ps and 192 nodes to predict structural stability. Recrystallisation synthesis, was then proceeded by the cooling process towards 0 K, the cooled nanosphere Na0.22TiO2 structure was then heated to 2000 K with temperature intervals of 100 K using ensemble NVT Nosé-Hoover. The calculated Ti-O pair correlation was evaluated by their Radial Distribution Functions (RDF's), where the extent of crystallisation was confirmed during cooling synthesis. The simulated X-ray diffraction (XRDs) spectra agrees well with the experimental XRD's [2] and the modelled microstructural defects, which all exhibited peak domains and patterns of both rutile and brookite polymorphic phases at high temperatures, thus confirmed structural stability. These results provides new insights on nanosphere Li0.22TiO2 architectured structures to be an excellent candidate as anode materials for sodium ions batteries (NaIB), due to its ability to store larger amounts of Na+ ions and can withstands high temperatures conditions.

Keywords: Computer Simulations, Recrystallisation, NaxTiO2 Nanosphere, Na ion batteries

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Supported Student:

Travel & Accom.

HPC Applications / 82

Convective scale modelling on the CHPC: ICON vs COSMO models

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The South African Weather Service has recently embarked on a business case to address its computational needs. Part of this was to identify the most suitable convective scale Numerical Weather Prediction (NWP) model for the Southern African region. The Unified model (UM), the main model run by SAWS for operational purposes, the Weather Research and Forecasting (WRF) Model and the Consortium for Small-scale Modeling (COSMO) model were used for the study. A number of weather parameters were selected for the study, and results generally showed that the three models are comparable. However, with much model development taking place around the world, the COSMO will soon be replaced by the Icosahedral Non-hydrostatic (ICON) model. It, therefore, makes sense to conduct the same study for the ICON as for the COSMO in order to investigate whether the new model is an improvement of the former one. Simulations for both the COSMO and ICON are run on the CHPC.

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Creating an HPC Culture with Love, Shoestring, and Duct Tape

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HPC in its modern form within the Mathematical Sciences at the University of the Witwatersrand can trace its roots back to 2004. We share a manager's perspective of what was required to create a self-sustaining culture of HPC within our laboratories, with access to little resources or institutional buy-in.

Supported Student:

No

DIRISA / 210

Cybers Security Threats – Is Our Research Data Safe?

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In a world where more and more people are connected every day, new systems pop up and access can be gained from any device anywhere, we need to ask if the data that we are working

on (viewing, editing and manipulating) is original and safe? The value of data as an asset is increasing as well as the potential threat in its transformative and informative power. The concept and roll out of Institutional Repositories (IR) and Institutional Data Repositories (IDR) is fairly mainstream in South Africa, hosting large valuable and often invaluable sets of data. In a connected world, cyber threats are real and have to date caused harm to many organisations. Is our data really safe and trustworthy in South Africa? South Africa has seen a dramatic increase in the amount of cyber-attacks in 2019, with as much as a 22% increase in malware attacks compared to 2018 alone. Malware attacks only form part of an array of cyber threats that are carried out on a daily basis. In short, the answer is that no system is 100% safe against cyber attacks, there are however systems and processes in place to increase and safeguard our data.

Today's cybercriminal strategies target every link in the attack chain to gain access to resources and data, exploiting them relentlessly. Holding data for ransom, modifying data, defacing of data and selling of data are some of the perils that more and more organisations are facing when breached. The key to safeguarding data is to ensure that policies, systems and procedures are put in place to deal with the various links in the attack chain. This presentation will focus on what is happening on an international and national level with regards to cyber security threats and how it affects our research data. The presentation will also highlight the attack chain and what can be done at the various linkages to make systems and organizations more secure.

Supported Student:

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DFT modelling of interactions in cobalt-based catalyst for FTS

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The Fischer-Tropsch (FT) process can be described as a combination of reactions that convert syngas, with CO and H_2 as primary content, into long chain hydrocarbons (Syncrude) to be refined into transportation fuels, lubricants and other petrochemicals. Among the commercially implemented catalysts, cobalt is considered as a successful candidate for catalysing FTS reactions towards long chain hydrocarbons (C_5+) due to its high activity and longer lifespan. To further drive the selectivity towards the longer chain hydrocarbons, Manganese (Mn)-based promoters have been considered for the cobalt catalyst system. This is because Mn promotion increases the amount of adsorbed CO with weakened C-O bonds. So far, studies have shown that Mn exists in the oxidic form as MnO_x whereby the promoter element as Mn^2+, facilitates the cleavage of the C-O bond through Lewis acid-base interactions. To address the validation of the mechanism behind the promotional effects and expand on theoretical work on Mn promotion, a suitable catalyst-promoter model needs to be devised. This project, therefore, deals with determining the likely oxidic form of the promoter considered as MnOx ligands using Density Functional Theory (DFT). Models of the Co/MnO_x systems will be generated using Material Studio for the Co (100) and Co (111) surfaces and validated using geometric optimization and thermodynamic calculations. The electronic effects of the valid ligands on CO, will be assessed through co-adsorption models whereby the position of the d-band centre of the promoted catalyst system will be compared to equivalent unpromoted catalyst system through density of state (DOS) plots. DFT calculations will be performed on the CHPC Lengau cluster using Vienna Ab-Initio Simulation Package (VASP). To maximize calculation efficiency in terms of computational resources used, optimization of the input tags such as parallelization and mixing tags for CPU-based runs, will be performed based on the calculation type.

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DFT study of the mechanisms and kinetics of nickel oxidation

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Like most transition metals, nickel has found wide spread use as a catalyst in processes such as steam reforming, methanation and fat hardening. During these processes, nickel catalysts may be deactivated due to sulphur poisoning, carbon deposition, sintering or oxidation. For instance, Matsumura and Nakamori 1 reported that the activity of nickel catalysts mounted on a variety of supports decreased during steam reforming due to the oxidation of the catalysts.

To improve our understanding on the effects and the possible prevention of nickel oxidation in industrial processes, it is necessary to investigate the mechanism of the oxidation process. Various mechanisms of nickel oxidation have been proposed. Garruchet et al. [2] suggested a vacancy - mediated mechanism, whereas Megchiche et al. [3] suggested interstitial diffusion of oxygen in the nickel lattice.

The relation between nickel surfaces morphology and nickel oxidation has not been covered extensively. In this study, we focus on the transport of atomic oxygen through various nickel surfaces in the presence and absence of vacancies in order to gain insight in the initial steps in the oxidation of metallic nickel. This study investigates a variety of nickel surfaces in terms of surface energy, chemisorption energy of oxygen on nickel surfaces and activation energy for diffusion using DFT methods. Successively, the knowledge on nickel surfaces will aid in the evaluation of the mechanisms and kinetics of oxidation of nickel.

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SIG Poster / **132**

DFTB study of Li_xTiO₂ with trigonal bipyramid structures: an insight into lithium-ion battery anode materials

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In lithium-ion battery, graphite is a widely used anode material, but it has some disadvantages as compare to TiO2 nanoparticles anode such as electrical disconnection, structural deformation, and initial loss of capacity. The choice of the anode material is very important for an effective development of a high energy density batteries and the use of high capacity electrode materials (anode & cathode) is an essential factor.
The computational simulation calculations have been performed at CHPC (Lengau) for our systems using 48 cores. The TiO2 trigonal bipyramid (TB) structures anode is a material that conducts electric current and they do not expand to more than 5% their original volume during charging and shrink

again during discharge. Given these exciting properties, it becomes necessary not only to synthesize such solid-state and molecular systems but also to model their properties at an appropriate size and time scale. In this work we study TiO2 polymorphs (bulk and nanospheres) in an effort to understand how the DFTB+ potentials influence structural parameters and electronic properties. Our structural and electronics parameters are in good agreement with the experimental results.

SIG Poster / 4

Deciphering the "elixir of life": Dynamic perspectives into the allosteric modulation of mitochondrial ATP synthase by J147, a novel drug in the treatment of Alzheimer's disease

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The discovery of J147 represented a significant milestone in the treatment of age-related disorders, which was further augmented by the recent identification of mitochondrial ATP synthase as the therapeutic target. However, the underlying molecular events associated with the modulatory activity of J147 has remained unresolved till date. Herein, we present, for the first time, a dynamical approach to investigate the allosteric regulation of mATP synthase by J147, using a reliable human αγβ protein model. The highlight of our findings is the existence of the J147-bound protein in distinct structural associations at different MD simulation periods coupled with concurrent open ↔ close transitions of the β catalytic and α allosteric (ATP5A) sites as defined by Cα distances (d), TriCα (Θ) and dihedral (ϕ) angular parameters. Firstly, there was an initial pairing of the αγ subunits away from the β subunit followed by the formation of the 'non-catalytic' αβ pair at a distance from the γ subunit. Interestingly, J147-induced structural arrangements were accompanied by the systematic transition of the β catalytic site from a closed to an open state while there was a concurrent transition of the allosteric site from an open αE conformation to a closed state. Consequentially, J147 reduced the structural activity of the whole αγβ complex while the unbound system exhibited high atomistic deviations and structural flexibility. Furthermore, J147 exhibited favourable binding at the allosteric site of mATP synthase with considerable electrostatic energy contributions from Gln215, Gly217, Thr219, Asp312, Asp313, Glu371 and Arg406. These findings provide details on the possible effects of J147 on mitochondrial bioenergetics, which could facilitate the structure-based design of novel small-molecule modulators of mATP synthase in the management of Alzheimer's disease and other neurodegenerative disorders.

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Delving into the Characteristic Features of "Menace" Mycobacterium Homologs: A Structural Proteomics Perspective

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The global increase in the morbidity/mortality rate of Mycobacterial infections, predominantly renascent tuberculosis, leprosy, and Buruli ulcers have become worrisome over the years. More challenging is the incidence of resistance mediated by mutant Mycobacterium strains against front-line antitubercular drugs. Homologous to all Mycobacteria species is the GlcNAc-6-phosphate deacetylase (NagA) that catalyzes essential amino sugars synthesis required for cell wall architecture, hence, metamorphosing into a novel pharmacological target for curtailing virulence and drug-resistance. In this study, we employed integrated bioinformatics methods to explore unique features pertinent to Mycobacteria NagA across six (6) most detrimental Mycobacterium species; tuberculosis (Mtb), smegmatis (MS), marinum (MM), ulcerans, microti, and africanum. This approach is essential for multi-targeting and could result in the identification of potential polypharmacological antitubercular compounds. DynaMut and PolyPhen2 were used to analyze the functional impact of non-synonymous single-nucleotide polymorphisms (nsSNPs) found across NagAs. Comparative sequential analyses revealed ≤ 50% of the overall structure, including the catalytic Asp-267 and reactive Cys-131, remained conserved. MS-NagA and MM-NagA possess unique hydrophobic isoleucine (Ile) residues at their active sites in contrast with leucine (Leu) found in other variants. More so, unique to the active sites of the NagA is a 'subunit loop' that covers the active site; probably crucial in binding (entry and exit) mechanisms of targeted NagA inhibitors. Relatively, nsSNP mutations exerted a destabilizing effect on the native NagA conformation. Structural and dynamical insights provided, basically pin-pointed the "Achilles' heel" explorable for the rational drug design of target-specific 'NagA' inhibitors potent against a wide range of mycobacterial diseases.

Keywords: Mycobacterium infections, GlcNAc-6-phosphate deacetylase, peptidoglycan, bioinformatics tools, Molecular dynamics simulations, mutations

Supported Student:

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Denoising Autoencoder Self-Organizing Map

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The Denoising Autoencoder Self-Organizing Map (DASOM) is a combined machine learning method of dimensionality reduction, feature extraction, and clustering1. Deep learning techniques show significant promise in improving the results of various clustering unsupervised learning algorithms, however unsupervised learning requires extremely large data sets in order to obtain accurate results.
The application of this (and many other) machine learning architectures to large data sets requires the use of high performance computing. This scales with the depth of the Denoising Autoencoder and size of the Self-Organizing Map. Whilst the fusion of these two methods is complicated, there exists significant portions of the architecture that can be parallelized.
Two version of the Deep DASOM have been developed: a hybrid shared and distributed memory version and a CUDA C version, the latter showing significant improvements over the former.
This allows for more complex models to be trained, in turn producing better analysis and prediction results.

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Networks 105 (2018) 112–131

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SIG Poster / 58

Density Functional Theory Study for Transition Metal Carbonate (NiCO3, MnCO3 and CoCO3) Precursors for Lithium Ion Batteries

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The abstract is attached as pdf file.

SIG Poster / 36

Density functional modelling of doping strategies to control vacancies in silicon.

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Density functional theory modelling was used to gain more insights on the interaction of germanium (Ge), tin (Sn) and lead (Pb) dopants with a vacancy. These interactions are often used to control vacancies in silicon in order to avoid the formation of unwanted vacancy complexes. We studied the structure, formation energies, binding energies and the charge state transition energy levels of these defect complexes.

In our research we used Quantum Espresso with the Heyd-Scuseria-Ernzerhof (HSE) hybrid functional to model the defect in a 64-atom supercell. We compare our results with the results of previous calculations using the VASP package using similar parameters.

Quantum confinement effects and finite size corrections were investigated using larger supercells including 216, 512, and 1000 atoms. The results were found to be closer to the previously computed defect level as the supercell size increased. For larger supercells, the band gap predicted by the HSE functional together with the formation energy obtained using the generalised gradient approximation (GGA) was used to plot graphs of formation energy as a function of the Fermi-level in order to determine the charge state transition energy levels. We found that, using the HSE band gaps and by increasing the supercell size, we could use the results of the formation energies calculated using the GGA to accurately predict the defect levels of the defect complexes. We found that Quantum Espresso and VASP gave similar results. We also found that using the GGA functional together with the HSE band gap can accurately predict the defect levels of defect complexes with major saving in computational costs.

HPC Applications / 195

Design of selective reagents and functional materials: A theoretical and experimental approach

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The work illustrates the integration of basic and applied chemistry in the development and application of selective materials for application in desulfurization and denitrogenation of fuel as well as in separation of precious metals. The fuel chemistry study is important from the point of view of the need to drive towards a zero sulfur fuel as mandated by environmental protection agencies in many countries around the world.1 Challenges exist with the current hydrodesulfurization and hydrodenitrogenation processes that are being applied in refineries as they fail to achieve the requisite fuel standards. The second application of functional materials is in separation of important metals. The demand for precious metals is driven by their important applications, and the development of better separating reagents/materials has become important given that the quality of ores is decreasing, and better recovery rates of the metals from secondary sources (such as electronic boards and catalytic converters) will be required in future. This necessitates improvement of the current chemistry in order to process the new feeds.

Experimental and theoretical studies were carried out during the development of the functional chemistry for recognition of target metals and organic compounds. The selective chemistry towards fuel contaminants such as organosulfur and organonitrogen compounds has been developed, and the results are promising as the best material (polymenzimidazole nanofibers) achieve sulfur removal of less than 2 ppm.2 A process involving conversion of sulfur compounds to organosulfones compounds3 has been developed followed by removal of the polar sulfones using selective materials.2 The approach for materials development for metal ions, such as platinum group metals (PGMs), follows the development of reagents that are specific for metal ion chlorido complexes of interest. The innovation of the aforesaid reagents undoubtedly requires a design strategy that considers both the electronic and stereochemical requirements of the target anion. Through a combination of molecular modelling techniques and experimental techniques, we have been able to derive factors that lead to successful separations. Cations as anion receptors specific for [IrCl6]2- and [PtCl6]2^{-} will be presented as well as selective chemistry for orgnosulfur and organonitrogen compounds in fuel. Binding energies and other thermodynamic parameters have been calculated in silico to explain the chemistry involved.

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Supported Student:

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Design, Characterization and in silico studies of 1,3,4-oxadiazole based hybrids as antibreast cancer agents

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emphasized text
Organic synthesis

Spectroscopy
In silico ADME properties prediction
Molecular modelling

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HPC Technology / **14**

Designing Reusable Composable Components for the (HPC) I/O Stack

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The rise of AI/ML in HPC applications is also driving the need for suitable storage abstractions such as the key-value (KV) stores. These abstractions pose new challenges for the HPC I/O stack. Enterprise KV stores are not well suited for HPC applications, and entail customization and cumbersome end-to-end KV design to extract the applications needs. To this end, I will present BESPOKV, an adaptive, extensible, and scale-out KV store framework. BESPOKV decouples the KV store design into the control plane for distributed management and the data plane for local data store. BESPOKV takes as input a single-server KV store, called a datalet, and transparently enables a scalable and fault-tolerant distributed KV store service. The resulting distributed stores are also adaptive to consistency or topology requirement changes and can be easily extended for new types of services. I'll show that BESPOKV-enabled distributed KV stores scale horizontally to a large number of nodes, and performs comparably and sometimes better than the state-of-the-art systems.

DIRISA / **208**

Developing infrastructure for federated data analysis for protected human data

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Datasets of ever increasing size and complexity are being generated in the biomedical field to answer questions about human and animal health. Data on human health have to be managed responsibly to ensure protection of participants in health studies. Additionally, many governments are clamping down on the transfer of datasets out of country borders. In order to respect these concerns while still facilitating ethical and responsible data sharing for analysis, new policies and infrastructure need to be developed. There are several initiatives working in this space, including the Global Alliance for Genomics and Health (GA4GH), which is building standards and tools for sharing of genomic data globally. A new EU funded research project, CINECA (Common Infrastructure for National Cohorts in Europe, Canada, and Africa), is developing infrastructure to implement GA4GH standards to enable the analysis of data across cohorts without the requirement for the transfer of large datasets to third parties. This includes development of security systems for authentication and authorization of researchers, harmonization of data across heterogenous studies, and development of cloud-based tools for federated data analysis within the confines of participant consent. This presentation will describe some of the standards and tools being developed and implemented in the CINECA project.

Supported Student:

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Development of FEARCF library for multi-dimensional free energy simulations on highly parallelized hardware

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Free energy is a critical aspect to understanding chemical reactions as well as molecular structures. For simulations designed to record free energy often the biggest hurdle is adequate sampling. Simulations may be left to run for long enough times, but this becomes resource intensive and some volumes of the reaction space may never be sampled in realistic time frames. Solutions to this problem typically include some means to 'force' the system towards unsampled regions, as well as an ability to combine results from multiple simulations. The FEARCF[1] (Free Energy from Adaptive Reaction Coordinate Forces) method manages to accomplish both of these methods through the use of a biasing potential to find the free energy and the use of WHAM[2] (Weighted Histogram Analysis Method) to combine the histories of multiple simulations into one.

It achieves the first method by deriving a biasing potential from the negative of the recorded probability distribution function (PDF) of the system using the Boltzmann equation that relates probability and energy. The addition of this biasing potential forces the system to move towards region of free energy space that it has not previously sampled since the biasing potential will have a high potential at any previously sampled regions. This biasing force is recalculated after every simulation iteration. The PDF's of multiple repeated simulations are combined using WHAM. The effective utilization of HPC hardware rests on the embarrassingly parallel way in which the PDF's of multiple simulations are generated. For every iteration of the FEARCF run, any number of simultaneous simulations can be run for a set number of steps. This allows for the biasing potential to reach convergence much faster. Once this convergence is reached, the inverse of the biasing potential is equivalent to the free energy.

FEARCF was originally developed for CHARMM but a library has now been developed that can be utilized with any other molecular dynamics software available at HPC centers (See attached figure). The structure of the library is a branching node structure where each node is a defined variable e.g. an atomic position, a vector or plane, and the branches are how each node is calculated using the other nodes. This avoids one having to write out explicitly the calculations of each variable and makes the relaying of information between nodes simple and fast.

All of these advances represent a means to quickly generate free energy information using the speed up capabilities available with HPC architecture.

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DIRISA / **219**

Developments Around Data in Botswana to support 4iR preparedness, Research, Innovation in a Developing Country

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The 3rd Industrial revolution of the 20th Century ushered in the 1st Information Revolution that brought the internet, digitisation, digitilisation and digital transformation and created a basis for knowledge-based economies. It is now widely accepted that the world is experiencing the advent of the 2nd Information revolution that is ushering in a 4th Industrial Revolution - a revolution that is characterised by a fusion of technologies to address current and future human needs. The 4th Industrial revolution is also characterised by large amounts and variety of data – coming from various sources at high frequency – and our ability to analyse them, in real-time and derive information and knowledge for timely decision making. It is anticipated that the 4th Industrial revolution will revolutionise Industry production processes through advanced automation (often referred to Industry 4.0), it also further anticipated that it will revolutionise practice and effectiveness in a variety of areas - health care provision (e.g. personalised medicine), development of Smart Cities , precision agriculture and help address weather and climate change.

There is therefore need for African countries and developing countries to respond to the onset on the 4th Industrial revolution (amidst arguably addressing challenges from previous industrial revolutions still unravelling in the continent) . This will help to bridge the digital divide and help not leave anyone behind – and achieve Africa's vision 2063 – the Africa We Want. It will also help accelerate attainment of Sustainable Development goals through riding on technology advances, efficiency and transparency. There is need for Africa to transform its infrastructure, research & innovation ecosystems, skills and education systems etc – this for 4th Industrial revolution readiness and competitiveness of African economies and Africans in this new dispensation. Africa and African countries need to have tailor made responses to the 4th Industrial revolution and its implications to the African context. This can be done by concretising National, Regional and Continental Policy Frameworks, structures, resourced roadmaps and increased expenditure in Research, Science, Technology and Innovation and developing partnerships . The universities and other centers of knowledge creation and skills development must play a critical role. The Universities must be alive to this responsibility and aim to transform to be a research-intensive institutions – and is enhance their internal university innovation ecosystems including around data exploitation through innovations.

This talk will provide an update on the developments of around data in Botswana, this from the prism of policy and strategy development, research and Innovation, skills development and science communication for public and policy engagement – this to help address Botswana's socio-economic challenges and attainment of Vision 2036 – Prosperity for all and address 4IR preparedness. The talk will discuss developments around Botswana Open Data Open Science, Botswana Space Science and Technology Strategy Development, highlight example National Open Data projects and discuss the University Industry Government Co-creation Initiative that aims to foster innovation- including around exploitation of open data.

Supported Student:

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Discovery of selective Glucose transporter type 4 inhibitors as targets for anti-cancer therapy: A computer-based study

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Presently, many studies are focusing on exploring *in silico* approaches in the identification and development of alternative therapies for the treatment and management of cancer. Accordingly, solute carrier family-2-member-4-gene (Slc2a4) which encodes glucose transporter 4 protein (GLUT4), has been identified as a promising therapeutic target. Though Slc2a4 is known to play a major regulatory role in the pathophysiology of type 2 diabetes, emerging evidence suggests that successful pharmacological inhibition of this protein may lead to the development of a novel drug candidate for the treatment of cancer. In this study, Slc2a4 protein sequence was retrieved and analysed and we identified seven putative antimicrobial peptides (AMP1-AMP7) as possible targets for anti-cancer therapy using an *in silico* mathematical algorithm, Hidden Markov Models (HMMER). The structures of the protein and AMPs were modelled using the Iterative Threading ASSEmbly Refinement (I-TASSER) server, and the overall quality of the Slc2a4 model was validated using PROCHECK. Subsequently, the probable motifs and active site of the protein were computed. Lastly, the molecular interaction between the AMPs and Slc2a4 was ascertained using PatchDock. All seven AMPs successfully inhibited Slc2a4, with AMP1 having the highest binding affinity of 12,392 and binding energy of –39.13 kcal/mol. As Slc2a4 is usually responsible for the production of energy for cancer cells during angiogenesis, this suggests that inhibition of Slc2a4 could impair this process. Collectively, this study reveals that all seven AMPs could serve as targets for further development as anti-cancer drugs. This is the first report on AMPs as inhibitors of Slc2a4 for the treatment of cancer.

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SIG Poster / **32**

Does Size Really Matter? Structural Fragmentation and Efficacy in Lead Drug Design and Optimization – A Computational "Proof-of-Concept"

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Despite the potency embedded in natural products with regards to multiple disease treatment, the numerous challenges of toxicities and undesirable biological 'off-targeting" have limited its clinical transition. More recently, the synthetic reduction of complex natural products into simpler fragments has been identified as a viable strategy to develop next-generation leads with improved potencies and minimal toxic effects. Therefore, to validate the efficacy of this method, we employed combinatorial molecular modeling and cheminformatics techniques to describe the differential pharmacological and antagonistic activities of a selected fragment, SB640 and its parent compound, Anguinomycin D towards their target protein, Exportin Chromosome Region Maintenance 1 (CRM1), involved in pro-carcinogenic chemotherapeutic resistance. Our findings revealed that the fragment exhibited improved pharmacokinetics with minimal toxicities and off-target activities compared to the parent compound. Furthermore, truncation into a smaller fragment enabled optimal positioning and binding with crucial residues at the protein target site which in turn accounted for a more prominent CRM1 inactivation as compared to the parent compound that had minimal structural effects due to motion and dynamical constraints caused by its long polyketide tail. Our findings, therefore, indicate that the "size does not matter" and that reduction of complex bioderived compounds to fragments could be an essential strategy for improving potency and minimizing associable adverse drug reactions.

SIG Poster / 13

Dual targeting approach for Mycobacterium tuberculosis drug discovery: insights from DFT calculations and molecular dynamics simulations

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Abstract

Drug resistant Tuberculosis (TB) infections are on the rise and anti-tuberculosis drugs that inhibit Mycobacterium tuberculosis (M. tuberculosis) through a new novel mechanism could be an important component of evolving TB therapy. Pantothenate Kinase (PanK) and CTP synthetase (PyrG) are both essential for de novo pyrimidine biosynthesis. Given the extensive knowledge base on de novo pyrimidine biosynthesis inhibition of M. tuberculosis growth and survival, these enzymes present an interesting opportunity for anti-mycobacterial drug discovery. A recent experimental study shows that CDD-823953 and GSK-735826A act as dual PanK and PyrG inhibitors, respectively. However, the molecular mechanisms of their selective inhibition remain elusive. Herein, Density functional theory (DFT) calculation was applied to unveil the molecular and reactivity properties of two lead compounds targeting these enzymes in a shot. Molecular dynamics simulations were then employed to investigate the inhibitory mechanism as well as selectivity impact of these potential inhibitors for their enzymes. Computational modeling of the ligands and the enzyme—ligand systems reveal that CDD-823953 and GSK-735826A lead compounds, can potentially inhibit both PanK and PyrG thereby creating a pathway via the use of double target approach in tuberculosis treatment.

Keywords: Tuberculosis, PanK, PyrG, Dual Targeting, DFT, and Molecular dynamics simulation

DIRISA / 196

EOS storage system

Author: Sean Murray[1]

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EOS is the storage system of choice for CERN's data storage and is used by various WLCG Tier1 and Tier2 facilities, including at the CHPC. EOS is an elastic, adaptable, and scalable software based solution for central data recording, user analysis and data processing.

It has a multitude of supported protocols and authentication methods. We will present what EOS is, what is does, and how we use EOS in conjunction with our Tier 2 facility, and how EOS is used in a couple of other examples.

Supported Student:

16

ESTABLISHING MICROBES FOR PRODUCTION OF CELLULASE USING BANANA (Musa paradisiaca) PSEUDOSTEM DURING SOLID-STATE FERMENTATION

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ESTABLISHING MICROBES FOR PRODUCTION OF CELLULASE USING BANANA (Musa paradisiaca) PSEUDOSTEM DURING SOLID-STATE FERMENTATION

Mulaudzi, M. L.1, Ncube. I. 1
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Introduction: In nature, saccharification is done by a variety of microorganisms secreting a variety of cellulase in addition to other proteins. The aim of the study is to establish microbes for the production of highly active cellulase preparations. The objectives are to optimize production of cellulase co-cultures and monocultures of microorganisms producing high levels of cellulose and to use zymography in studying the variety of cellulase in secretions from monoculture and co-cultures.
Materials and Methods: Banana pseudostems were collected, cut, dried in an oven at 60 ℃ and ground to powder. Fungal isolates were cultured using Mendel salts with banana pseudostem as the carbon source for a maximum of 10 days at 30 ℃, during Solid-State Fermentation. Enzyme activity assays were performed to determine endoglucosidase and β-glucosidase. Zymography was performed to detect the active bands on a 12% sodium dodecyl sulphate-polyacrylamide gel electrophoresis (SDS-PAGE).
Results and Discussion: It was observed that 1B seemed to be the best producer of both cellulase activity; endoglucosidase (6.7 U/ml) and β-glucosidase (37 U/ml); hence, 2A as the least producer of endoglucosidase activity (2.5 U/ml) and β-glucosidase (28 U/ml). All these isolates seem to be cellulase producers, hence active bands observed on zymography.

Conclusion: The study concludes that single isolate 1B was best in producing high cellulase activity. It also shows that SSF which mimic the natural decomposition of lignocellulose was best condition to use in order to achieve a higher cellulase activity.

Supported Student:

Waive Fees Only

SIG Poster / 101

Effect of Ta, Hf and V on Structure and Stability of Ti50Pt50 shape memory alloys

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First principle density functional theory approach was employed to study the effect of Ta addition on the TiPt shape memory alloys (SMAs). SMAs have the ability to remember their shapes after deformation, and this is due to their shape memory effect and super elasticity properties. These alloys have the capability to operate as high temperature shape memory alloys considering that they possess a reversible martensitic transformation. All the calculations in this study are carried out at the Centre for High Performance Computing (CHPC), employing VASP code embedded in Material design MedeA platform. We employed the generalized gradient approximation parameterized by Perdew, Burke and Enzerhof using the supercell approach. The equilibrium lattice parameters, elastic properties and the phonon dispersions were calculated to investigate the stability of the Ti50Pt50-XMX. We have found that the calculated heats of formation predicted the 6.25 at.% V, Ta and Hf as the stable structures. Interestingly, the vanadium, tantalum and hafnium addition was found to stabilise the TiPt with all the Cij's being positive. The predicted phonon dispersion curves revealed that increasing the V, Ta and Hf content in the system stabilizes the structure.

HPC Technology / **172**

Evaluating the Compressibility of Elevation Data using Space-Filling Curves

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Two of the typical points of interest with elevation data, or Geographic Information Systems (GIS) data in general, are storage and query costs. The former is typically addressed by integrating standard compression schemes into already existing storage mechanisms, such as GZIP in HDF5. Space-Filling Curves (SFCs) have already been used to reduce access time for spatial operations on point and polygon data. In this research, we evaluate the effect of using SFCs as a pre-processing step for standard compression schemes on elevation data. We break up common compression tools into their base algorithms and identify canonical SFCs from the literature (for example, the Hilbert curve).

We use 1-arcsecond resolution elevation maps from the Shuttle Radio Topographic Mission (SRTM) as the comparative data-set upon which we apply all combinations of SFCs and compression schemes. The SFCs, in most cases, neither significantly improve nor worsen compression ratios when compared to non-preprocessed results. However, we show that certain pre-processing steps improve the compression performance of otherwise ineffective compression techniques. This research shows the potential for future work on compression schemes which allow for in-place search and modifications without the loss of compression performance. Another application is to apply these techniques to astronomical data from the Square-Kilometre Array, a major scientific and engineering project in South Africa, for which some preliminary results have been attained.

Supported Student:

DIRISA / **209**

Evolution of a South African eResearch support service

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INTRODUCTION

Given the complex relationship between eResearch stakeholders within universities and research organisations, a "one size fits all" solution to the development of a national eResearch support service is not practical. Services contributed by Libraries, IT and research administrations are at different stages of maturity, and the South African landscape is characterised by scarce skills in areas of software and systems support. To advance national eResearch capability, a considered approach requires both costly infrastructure investment and collaborative support services.

BACKGROUND

The emergence of a new paradigm, "sometimes called eResearch", gave rise to the examination of a national information service framework in 2005.( ) The need for joint action was identified to meet the challenges of eResearch cost-effectively in South Africa. A specialized agency was proposed to provide support services, with a governance model that should work well for all participants. Two reports commissioned by the Department of Science and Technology assisted in conceptualising strategic plans for the further development of South Africa's research infrastructure, including the cyberinfrastructure component. The recommendation to establish of a National Integrated Cyberinfastructure System (NICIS) was accepted and plans for follow-up activities approved in 2013. NICIS comprises several core components of the Tier 1 infrastructure: a national Center for High Performance Computing (CHPC), the South African Research Network (SANReN), and the more recently established Data Intensive Research Initiative for South Africa (DIRISA). Experience of the Research Data Management project component of the DIRISA Tier 2 ilifu infrastructure has provided valuable lessons the collaborative development of shared services that can now be evolved to the wider community.

FROM INFRASTRUCTURE DEVELOPMENT TO SERVICE ORIENTATION

As research becomes more multidisciplinary, more collaborative and more global, researchers seek to leverage the South African investment in specialist scientific equipment and domain-specific infrastructures, often generating massive data outputs for analysis in international collaboration. As the national research infrastructure moves from an experimental testbed to a user-oriented environment, a challenge faced by most eResearch infrastructures is the provisioning of sustainable services, and the monitoring of user experience (UX), to improve the interaction of researchers with the infrastructure. This critical component is seldom defined explicitly in the infrastructure development, and the research community have little interest in the expansion of cost-effective services beyond their own needs, and especially beyond the duration of their funded project. Responsibility at present, falls to the host entity to realise the full potential of the national cyberinfrastructure, and the collaboration enabled with global infrastructures. A limited science system suggests a federation of distributed support services, including multiple universities and institutional partners to meet the ever-increasing need to meet both current user support and ongoing data access.

A pilot project to support a South African eResearch support service will build on the eResearch Africa conference hosted bi-annually at the University of Cape Town since the initial event in 2013. An annual training workshop aimed at professional development and career enhancement opportunities recognizes the varied job roles associated with eResearch. Institutional eResearch capacity building will focus on selected teams of information professionals through sponsored participation in designated training programmes and national events.

CONCLUSIONS

The development of a national support service model is intended to improve distributed efficiency, rather than to centrally consolidate a limited pool of existing human resources. The effect of overextending the existing capacity poses serious threat to the realisation of the national cyberinfrastructure, with discussion of actual use cases in this presentation.

Due to the complex relationship between eResearch stakeholders within institutions, a "one size fits all" solution is impractical, and a phased approach is recommended, leveraging a brokerage model to access third party services and avoid scenarios where services are developed and implemented and then subsequently "orphaned" by lack of support and changing financial priorities.

The potential administrative overhead of service development projects, established by individual

service level agreements with multiple institutions, warrants further consultation on the project governance with university executives, senior researchers and infrastructure managers.

Capability approaches to advanced computing technologies must address more than the big shiny stuff. A considered approach requires both costly infrastructure investment and collaborative support services. The user experience of researchers, and their improved interaction with the national cyberinfrastructure should ultimately direct the project and its evaluation.

Supported Student:

24

Exploring the flap dynamics of the South African subtype C HIV-1 protease in presence of FDA-approved inhibitors: MD study

Author: Siyabonga Maphumulo[1]

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The abstract has been attached.
I was not able to add the names of the co-authors on the indicated section but they're as follows; Amit K. Halder,1 Thavendran Govender1, Sibusiso Maseko1 Glenn E. M. Maguire,1,2 Bahareh Honarparvar,1,* and Hendrik G. Kruger

Supported Student:

Travel & Accom.

DIRISA / 218

Federating the Ilifu Cloud

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Ilifu is an Infrastructure as a Service cloud that utilises OpenStack to provide its core services. It is run by a consortium of South African universities and provides data intensive computing resources to Astronomy and Bioinformatics users. This talk describes how we are utilising federated identity services enable the use of ilifu by users in a way that can be managed by individual project groups without needing to contact ilifu support to have them create or remove accounts. It will explain how this has been done using tools run by EGI, and using tools integrated locally.

Supported Student:

HPC Applications / 150

Field-induced exotic electronic phases in spin-filter tunnel junctions

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ABSTRACT:
The future of spintronics based on 2D-materials is dependent on the effectiveness of the injection of pure spin current into a tunnel barrier region. Here, first principles calculations are used to show that the efficiency of the spin-filtering across the semiconducting barriers of monolayer hBN is mainly limited by the dynamical response of tunneling electrons to the applied axial field. By projecting the effective electric field gradient densities and magnetic shielding constants across constitutive atomic layers in the scatter region of spin-filter tunnel junctions, an unusual site-dependent spin response is unraveled at the Fe/hBN and hBN/metal heterobilayer interfaces. Since the ground-state energy has no lower bound in extended electric fields, our analyses of the dependence of the Fermi surface topology on applied electric fields show the emergence of a frustrated electronic order. This exotic electronic phase is characterized by electric-field induced spin-flip relative to the ferromagnetic ground state, and observable as field-tunable perpendicular magnetic anisotropy.

HPC Content:
All the calculations were performed in parallel using version 6.4.1‘ of the Quantum ESPRESSO suite. Due to poor code scalability, all the computations were carried out on the ‘SMP que’ using 1 Node of 24 CPU cores. No net gain in computing speed was observed when more nodes were used on larger system sizes. In fact, the speed of the computations significantly reduced to > 6 CPU hours per scf-cycle when the same jobs were running on the ‘Normal que’ at 10 Nodes at double the system-size. The main computational challenge lies in solving the associated Poisson’s equation for atoms in the presence of the compensating potential due to externally-applied fields under gauge-corrections, in a more efficient manner. For fully-converged field-dependent computations, an average duration per task was timed at 2d 0h19m (CPU time) and 2d 0h40m (WALL time). This is still too ‘slow’ for scientific computing jobs executed on a supercomputer.

HPC Applications / 130

Finite volume modelling of dense granular flow in rotary kilns

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Granular materials are used in several industrial applications. One example of such an industrial application is rotary kilns, often used for drying, pre-heating and the reduction of a moving, high-temperature granular bed. The granular flow in these reactors have an important influence on capacity, product quality, and economic feasibility. Rotary kilns, in the pyrometallurgical industry, often have diameters up to 6m, with lengths in excess of 80m, and operating at temperatures of 1000 to 1400℃. Because of the size of these kilns, modelling the granular flow using the discrete element method (DEM) would result in excessively high computational costs. In this work, we therefore made use of a continuum approach to describe the granular flow.

We adopted the μ(I) dense granular flow model proposed by de Cruz et al. (2005) and later extended by Jop et al. (2006). This model is a rate-dependent, phenomenological description of dense granular materials and can be characterised as an elsto-viscoplastic material description with a frictional yield criteria. The flow model approximates an effective friction coefficient through a relationship between

plastic flow strain rates and a confinement time scale to account for the internal, inter-particulate motion.

We implemented the material model into OpenFOAM, an open source, finite volume (FV) based, partial differential equation toolkit. The volume of fluid (VoF) method was used to capture the discrete granular-fluid interface, enabling the simulation of large granular bed deformations. The numerical scheme was stabilised by using pressure and viscosity regularisation, along with a semi-implicit coupling between the internal pressure and velocity fields.

In our project we were faced with serious technical and computational challenges involving combustion, heat transfer, fluid flow, high-temperature chemistry, and the movement of a large granular bed. Our FV approach enabled us to make valuable computational modelling and simulation contributions to the development of a new high-temperature process technology.

SIG Poster / 100

First Principles Study on the Effect of Lithiation on the Spinel LixMn2O4 Structure using CASTEP and ONETEP Codes.

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Despite the poor performance demonstrated by layered and spinel cathode materials during cycling, their composite cathode material exhibits enhanced performance. Such distinction qualifies the composite electrode material as one of the promising cathode material to potentially accelerate the rate performance of lithium ion batteries and meet the high energy needs posed by the exponential growth in technology. A vast number of studies have focused on improving the specific capacity of these layered-spinel composites. However, the internal structural changes responsible for the noted enhanced performance of these materials during the discharge (lithiation) process are not yet fully understood. As such, we perform the spin polarised density functional theory DFT calculations using the CASTEP and the ONETEP (linear-scaling DFT) codes embedded in Material Studio to elucidate the effect of lithiation on the electronic structure of spinel LixMn2O4. The electronic structure of spinel LiMn2O4, the delithiated-Mn2O4 and the lithiated-Li2Mn2O4 spinel were investigated the generalized gradient approximation (GGA). The electronic structure analysis depicted semiconducting properties for delithiated-Mn2O4 with a band gap of ~0.65 eV whilst LiMn2O4 and lithiated-LiMn2O4 were found to be conductors. Furthermore, it was found that less amount of energy is required for electrons to occupy the eg orbitals of LiMn2O4 than of the eg orbitals of the delithiated-Mn2O4. This indicates that lithiation favours Mn3+ which is in line with what was observed experimentally. The LiMn2O4 DOS calculated with ONETEP clearly distinguish dx2-y2 and dz2 orbitals. The dx2-y2 orbital is filled and dz2 orbital is empty which is consistent with the dual-existence of Mn4+ and Mn3+. We also performed a scaling test with ONETEP on supercells of LiMn2O4 spinel structure and the best performance was achieved by ensuring that the product of MPI processes and OMPI_THREADS are equivalent to the requested number of cores in the Lengau cluster. Our current findings forms a basis for moving from traditional DFT to linear-scaling DFT which will enable the study of the electronic properties of Li-Mn-O layered-spinel nanoarchitectures at larger scales.

SIG Poster / 48

First Principles study of Zn/Cu doped hematite surfaces for Photoelectrochemical water splitting.

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Co-authors: Refilwe Edwin Mapasha [2] ; Artur Braun [3]

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Abstract:

First principles studies of Zn/Cu doped {0001} and {012} surfaces of hematite for enhanced photoelectrochemical water splitting have been carried out. Doping was confined to planes in close proximity to the termination region, precisely from the top most layer to the third inner layer (plane P1, P2 and P3) of Fe atoms. The two surfaces and the three doped layers were found thermodynamically stable. The analysis of electronic properties reveals that even with mono doping of Zn on the top most layer (P1) of the {0001} α-Fe2O3 surface, the band gap can be decreased without impurity states in the band gap which normally acts as recombination centres. Cu doped surface systems do not only decrease in the band gap but also leads to the correct conduction band alignment for spontaneous water splitting. Furthermore, the conduction band minimum (CBM) of P2 and P3 of the {012} surface become wavier and delocalised suggesting improved electron mobility of hematite. Analysis of the charge density difference plots showed concentration of charge mainly at the top of the surface, which is the termination region, which suggests facile transfer of charges to the adsorbed water molecules due to the closeness of the charges to the adsorbate. It is envisaged that surface doping is more beneficial than bulk doping because it reduces the distance moved by the charge carriers and further reduce quick recombination resulting in efficient use of the charges. The concentration of the charges at the surface, the decreased band gap and the absence of recombination centres within the band gap suggest improved photocatalytic activity of the Zn/Cu doped α-Fe2O3 surface.

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Keywords: First principles study, hematite (α-Fe2O3); surfaces; Zinc (Zn), copper (Cu), Photoelectrochemical and band gap

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First principle density functional theory of M9S8 (M = Ru, Pd, Os, Ir, Rh, Pt), (Ru,Pd)9S8, (Os,Pt)9S8 and atomic simulations M9S8 (M = Rh, Ir) pentlandite-like structures

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Abstract: The platinum group elements (PGEs) exist in different structures which are known and studied to some extent. The existence of these PGEs in pentlandite-like structure is a promising host phase of these PGEs. In this study Viena ab-initio Simulation Package (VASP) density functional theory code at Lengau using 48 cores to investigate phase stability of the PGEs, M9S8 (M = Ru, Pd, Os, Pt, Ir,Rh), (Ru,Pd)9S8 and (Os,Pt)9S8 pentlandite-like structures. The phase stability was investigated by calculating heat of formation, elastic properties, density of states (DOS) and phonon dispersion curves. The heats of formation predicted that for M9S8, Rh9S8 and Ir9S8 were stable, and further showed that group 8 rich were more stable than the group 10 rich ternary Pn-like system The calculated heat of formations was plotted against average valence electron number per atom, the trends were comparable with the previous theoretical results. Furthermore, their density of states showed high stability in M9S8 (M = Rh, Ir)systems as their Fermi energy falls into the pseudo-gap, this is in agreement with previous work. Moreover, their phonon dispersion curves of M9S8 (M = Rh, Ir)

appeared to have no negative frequencies (soft modes), hence they are vibrational stable. Lastly, we performed atomistic simulations to the stable systems. In order to explore the structural behaviour of these stable systems (Ir9S8 and Rh9S8) under a certain temperature, molecular dynamics (MD) was employed. The former was achieved by firstly deriving empirical interatomic potentials of Ir9S8 and Rh9S8 which were fitted to DFT calculated data. MD results showed that Ir9S8 and Rh9S8 changes phase at 1800K.

Supported Student:

Travel & Accom.

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First principle study of E-centre defects in silicon.

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Silicon is the most widely used material in semiconductor industries, as such much attention has been given to the study of the electrical properties of silicon both experimentally and theoretically. With increasing miniaturization, the successful design of silicon-based devices requires complete knowledge of the physical parameters of defects, including the charge states in which they may occur. In order to gain deep understanding of the behaviour of semiconductors, it is important to be able to model their properties from a fundamental level.

Density functional theory (DFT) is often used to calculate the electronic properties of defects. The generalized gradient approximation (GGA), however, fails in predicting the band gap of semiconductors correctly, and therefore hybrid functionals, such as the functional by Heyd, Scuseria and Ernzerhof (HSE) is often used.

The E-centre defect is one of the prominent radiation induced defects in silicon and comprises a vacancy bound to a Group V (P, As, Sb) substitutional dopant atom. Experimentally, the various E-centres, also referred to as the V-P, V-As or V-Sb centres, are reported to have acceptor levels at Ec − 0.36 eV, Ec − 0.35 eV and Ec − 0.31 eV for P, As and Sb doping, respectively, while a donor level of Ev + 0.27 eV was found for the V-P defect.

In this study, the results of calculations using the HSE functional are compared to experimental results and the results of previous GGA calcuations. The HSE calculations, in common with the GGA calculations predicted acceptor levels for all the defect complexes, however the predictions by the HSE functional were closer to the experimental values.

The factors influencing the accuracy of these calcuations were studied in detail. These include finite size corrections according to the method of Freysoldt Neugebauer and Van de Walle, where 64 atom, 216 atom, 512 atom and 1000 atom supercells were compared. It was found that the larger the supercell size the closer the predicted defect levels were to the experimental results. We also observed that the 216-atom supercell using the GGA functional gave better results than the 64-atom super cell using the HSE functional with a major reduction in the computational cost.

Supported Student:

Accommodation Only

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First-Principle Stability Study of Solid Electrolytes in Magnesium-ion batteries

Authors: KHUMBULANI TIBANE[1] ; Mogahabo Morukuladi[2] ; Cliffton Masedi[2] ; Phuti Ngoepe[2]

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Magnesium-ion batteries are a promising energy storage technology due to their higher theoretical energy density and low cost of raw materials. Among the major challenges has been identification of cathode materials that demonstrate capacities and voltages similar to lithium-ion systems. A good introduction to the field of magnesium electrochemistry can be a short description of the more established and well understood world of lithium batteries. Lithium-ion batteries for high energy capacity, are coupled with problems such as safety, durability, uniformity and cost, which imposes limitations on the wide-rage applications of lithium-ion batteries. However, magnesium batteries appear a viable alternative to overcome the safety and energy limitations faced by current lithium-ion technology. Rechargeable magnesium-ion batteries are a promising candidate technology to address future electrical energy storage needs of large scale mobile and stationary devices, because of the high environmental abundance of magnesium metal and divalent character of magnesium-ion. However, low mobility of Mg2+ in solids limit the development of magnesium batteries. Therefore, in this study we investigate the stability of MgX2Z4 (where X = Sc, Y and In; Z = S and Se) structures by calculating their structural, mechanical, and electronic properties utilizing first-principle based calculations within generalized gradient approximation (GGA) was used. The heats of formation indicate that all structures are stable. Calculated elastic properties shows that structures are all mechanically stable in good agreement with the phonon dispersion curves. The total density of states (TDOS) indicate that all the structures are semi-conductors due to the direct bad gap. For all our calculations we used centre for high performance computing (CHPC) MedeA and material modelling centre (MMC) but CHPC was faster when calculating the properties of our systems and produced better results.

Supported Student:

Waive Fees Only

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From A to AI with Intel

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Note: Sunday workshop day

From A to AI with Intel

Join us for the one day workshop tailored for all the audience: from AI passionate to Data Scientist and System architects. Workshop will include hands-on sessions on Artificial Intelligence.

Experience a unique opportunity to learn about this incredible domain and test out the latest performance optimized frameworks and tools and best practices to get started implementing AI guided by experts from Intel® .

Target Audience:
Morning session: beginners, AI passionate
Afternoon session: Data Scientist, application developers and HPC bench markers targeting the deep learning and machine learning domain

Prerequisites:
Morning session: beginner to non-experts.
Afternoon: Basic skills of programming, ideally some Python and HPC knowledge

Type of tutorial:
Mix of lectures and hands-on tutorials

Special requirements:
Attendees should bring their laptop with an SSH- & VNC client
Attendees will get for hands on-labs also access to the CHPC cluster

Supported Student:

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From genomic variation to protein aberration: Mutational analysis of single nucleotide polymorphism present in ULBP6 gene and implication in immune response

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Genetic polymorphisms have been identified as one of the underlying factors in disease pathogenesis and drug resistance since they account for protein dysfunctionality, or in some cases, aberrancy. This explains the high degree of inactivity that characterize the polymorphic variants of ULBP6 binding protein, which in turn disrupts its primary interaction with human Natural Killer Hence, the possible identification of deleterious non-synonymous Single Nucleotide Polymorphisms (nsSNPs) present in the ULBP6 gene is essential for the development of novel gene therapies to prevent the translation of dysfunctional protein variants. Lengau cluster CHPC was used to perform the molecular dynamics (MD) simulations for this study. The openMPI 1.8.8 GNU compilers, the GCC 5.1.0, amber modules and the /apps/chpc/chem/amber/18 application code were integrated to access the Amber18 suite. In order to scale up and maximize computational space, we used Amber 18 on GPU module. For the first time, we employed SNP-informatics approach (SNPs retrieval, pathogenic/mutational analysis, phenotypic analysis and structural analysis) and molecular dynamics techniques to identify and characterize undesirable SNPs coupled with their impacts on ULBP6 structural activities relative to dysfunctionality. V52F was predictively pathogenic amongst SNPs studied. Conformational and dynamic studies revealed that in comparison to wildtype ULBP6 (ULBP6wt), pathogenic ULBP6V52F demonstrated considerable structural inactivity, which could in turn impede biological protein-protein interactions. Moreover, ULBP6V52F showed relatively limited motions in the conformational space as deduced from estimations of structural stability, fluctuations and principal components. Conclusion: This study provides a workable paradigm for investigating pathological nsSNPS using computational platforms which findings present ULBP6V52F as a novel and attractive immunotherapeutic target in combatting immune associated disorders. This study also provides an insight into future investigations of pathological nsSNPS using computational platforms.

Supported Student:

Travel & Accom.

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Fully sponsored test

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Fully sponsored test

Supported Student:

Travel & Accom.

141

Future Changes in crops suitability and planting season over West Africa

Author: Temitope Egbeyiyi[1]

Co-authors: Olivier Crespo ; Chris Lennard ; Phillip Mukwenha

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The changing climate is posing significant threats to agriculture, the most vulnerable sector, and the main source of livelihood in West Africa. This study assesses the impact of the climate-departure on the crop suitability and planting month over West Africa. We used 10 CMIP5 Global climate models bias-corrected simulations downscaled by the CORDEX regional climate model, RCA4 to drive the crop suitability model, Ecocrop over 150-year period for 12 different crops. Considering the number of simulations required (12crops x 10 regional model x monthly data of 3 rainfall, minimum and mean temperature over 150 years for 96 x 41 grids points in West Africa) for this study, high performance computing remains the only and most suitable platform. Hence, we requested one (1) node with about 24 cores from Centre High Performance Computing (CHPC) perform the crop suitability modelling experiment. We applied the concept of the crop-climate departure (CCD) to evaluate future changes in the crop suitability and planting month for five crop types, cereals, legumes, fruits, root and tuber and horticulture over the historical and future months. We utilized the assigned node (comprising of 24 cores) with several runs between 6-10days for our simulations, which assisted and contributed to our findings both in time and computing resources. Our result shows a reduction (negative linear correlation) and an expansion (positive linear correlation) in the suitable area and crop suitability index value in the Guinea-Savanna and Sahel (southern Sahel) zone, respectively. The horticulture crop was the most negatively affected with a decrease in the suitable area while cereals and legumes benefited from the expansion in suitable areas into the Sahel zone. In general, CCD would likely lead to a delay in the planting season by 2–4 months except for the orange and early planting dates by about 2–3 months for cassava. No projected changes in the planting month are observed for the plantain and pineapple which are annual crops. The study is relevant for a short and long-term adaptation option and planning for future changes in the crop suitability and planting month to improve food security in the region.

Keywords: crop-climate departure; Ecocrop; crop suitability; planting month; CORDEX; high performance computing, West Africa

Supported Student:

Travel & Accom.

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Generation of CHARMM force field parameters for zinc centres of the malarial enzyme: 6-pyruvoyl tetrahydropterin synthase

Authors: Afrah Khairallah[1] ; Ozlem Tastan Bishop[1] ; Vuyani Moses[1]

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In the pharmaceutical industry; drug discovery, development and finally commercialization can take a long period of time. In addition to that, the cost of drug development is increasing. Computer-aided drug discovery with the aid of High-Performance Computing (HPC) allows for speedy identification of candidate drugs. In this study, in silico approaches were used to develop accurate Force Field (FF) parameters for metal centers of the malaria parasite enzyme 6-pyruvoyl tetrahydropterin synthase. Quantum mechanics (QM) calculations were performed such as Potential Energy Surface (PES) scans to derive the FF parameters. Followed by validation of the generated parameters through all atom Molecular Dynamics (MD) simulations. The newly developed FF parameters will allow for accurate and reliable MD simulations, which can be of great use in the in-silico drug discovery attempts for malaria treatment. The resources available at the Centre for High-Performance Computing (CHPC) (Cape Town, South Africa) were utilized for the QM calculations and MD simulations via Gaussian software and the Chemistry at HARvard Molecular Mechanics (CHARMM) MD package. The use of HPC in this study was crucial as it accelerated the process of calculation by allowing the use of several nodes and parallel processing.

Supported Student:

Travel & Accom.

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HPC calculations to understand the reduction of 1,3-substituted-acetylacetone derivatives

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Poster abstract of MSc student N Mateyise.
I am submitting this poster on behalf of the presenting author N Mateyise. She wish to get a sponsorship from the CHPC to make it possible for her to attend the conference.

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HPC on OpenStack

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Presented by Boston Limited and vScaler

In this class users will be hands on and working in a Linux environment. It is expected that participants have a good understanding of Linux fundamentals and are comfortable at the CLI and performing basic administration tasks (such as networking, package management and file editing).

Supported Student:

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Halting ionic shuttle to disrupt the synthetic machinery – Structural and molecular insights into the inhibitory roles of Bedaquiline towards Mycobacterium tuberculosis ATP synthase in the treatment of tuberculosis.

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Therapeutic targeting of the ATP machinery of Mycobacterium tuberculosis (Mtb) has recently presented a potent and alternative measure to halt the pathogenesis of tuberculosis. This has been potentiated by the development of Bedaquiline (BDQ), a novel small molecule inhibitor that selectively inhibit mycobacterial F1Fo-ATP synthase by targeting its rotor c-ring, resulting in the disruption of ATP synthesis and a consequential cell death. Although, the structural resolution of the mycobacterial C9 ring in complex with BDQ provided a first-hand detail of BDQ interaction at the c-ring region of the ATP synthase, there still remains a need to obtain essential and dynamic insights into the mechanistic activity of this drug molecule towards a crucial survival machinery of Mtb. As such, for the first time, we report an atomistic model to describe the structural dynamics that explicate the experimentally reported antagonistic features of BDQ in halting ion shuttling by the mycobacterial c-ring, using molecular dynamic (MD) simulation and MM/PBSA methods. Results showed that BDQ exhibited a considerably high ΔG while it specifically maintained high-affinity interactions with Glu65B ¬and Asp32B, blocking their crucial roles in proton binding and shuttling which is required for ATP synthesis. Moreover, the bulky nature of BDQ induced a rigid and compact conformation of the rotor c-ring which impedes the essential rotatory motion that drives ion exchange and shuttling. In addition, the binding affinity of a BDQ molecule was considerably increased by the complementary binding of another BDQ molecule, which indicates that an increase in BDQ molecule enhances inhibitory potency against Mtb ATP synthase. Taken together, findings provides atomistic perspectives into the inhibitory mechanisms of BDQ coupled with insights that could enhance the structure-based design of novel ATP synthase inhibitors towards the treatment of tuberculosis.
HPC CONTENT
The lengau cluster CHPC was employed to perform the molecular dynamics (MD) simulations for this study. The openMPI 1.8.8 GNU compilers, the GCC 5.1.0, amber modules and the /apps/chpc/chem/amber/14 application code were integrated to access the Amber14 suite. For system parameterization, the ANTECHAMBER and LEAP modules were incorporated.In analyzing generated MD trajectories, the CPPTRAJ and PTRJ modules were used. Running on 2 nodes and 48 cores, the GPU accelerated PMEMD engine was used.

Supported Student:

Travel & Accom.

HPC Applications / 212

High Performance Computing for Medical Interventional Planning Applications

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Personalised solutions for healthcare are increasingly recognised as an important approach for treating a variety of conditions that have different outcomes, based on the patient. In the field of computational mechanics, different virtual pipelines have been developed in an effort to improve interventional planning and long-term patient outcomes. One of the major challenges to realising patient-specific treatment tailoring is a mismatch of timeframes. Clinical diagnoses and treatments need to be carried out in as short a timeframe as possible, while traditional CFD codes tend to run over longer time periods.

The use of high performance computing platforms has been beneficial in the development of interventional planning pipelines for cerebral aneurysm thrombosis and congenital heart disease. For aneurysms, it is important to determine what type of clot will form in the aneurysm sac, based on the treatment modality selected. In the case of congenital heart disease, treatments which are selected need to be optimised to ensure that solutions will remain suitable as the child grows to adulthood. This talk will explore the challenges encountered in developing these two pipelines for clinical use.

Supported Student:

HPC Technology / **12**

High Performance Data Access: the Hermes approach

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High-performance computing (HPC) applications generate massive amounts of data. However, the performance improvement of disk-based storage systems has been much slower than that of memory, creating a significant I/O performance gap. To reduce the performance gap, storage subsystems are under extensive changes, adopting new technologies and adding more layers into the memory/storage hierarchy. With a deeper memory hierarchy, the data movement complexity of memory systems is increased significantly, making it harder to utilize the potential of the deep memory-storage hierarchy (DMSH) architecture. In this talk, we present the development of Hermes, an intelligent, multi-tiered, dynamic, and distributed I/O caching system that utilizes DMSH to significantly accelerate I/O performance. Hermes is a US NSF supported large software development project. It extends HPC I/O stacks to integrated memory and parallel I/O systems, extends the widely used Hierarchical Data Format (HDF) and HDF5 library to achieve application-aware optimization in a DMSH environment, and enhances caching systems to support vertical and horizontal non-inclusive caching in a distributed parallel I/O environment. We will introduce the Hermes' design and implementation; discuss its uniqueness and challenges; and present some initial implementation results.

SIG Poster / **74**

High performance computing of super heavy elements of the periodic table

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This talk in intended to International Year of the Periodic Table of Chemical Elements (IYPT 2019) by presenting a talk on small molecules that needs HPC calculations to optimize. However,the molecules are small enough that any person can understand their structure and follow the talk. If this talk is accepted in the main CHPC conference program, it will be presented in a public understandable language.

HPC Applications / **73**

High throughput in silico screening for tailored catalytic reactivity and selectivity

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First-principles simulation has become a reliable tool for the prediction of structures, chemical mechanisms, and reaction energetics for the fundamental steps in homogeneous and heterogeneous catalysis. Details of reaction coordinates for competing pathways can be elucidated to provide the fundamental understanding of observed catalytic activity, selectivity, and specificity. Such predictive capability raises the possibility for computational discovery and design of new catalysts with enhanced properties.

In the case of mesoporous materials like zeolites, the well-defined pore structures and adjustable reactivity centers in the pore walls allow for efficient control of the catalytic properties. In addition to the reactivity at the catalytic center, the mobility of the reaction components throughout the network structure is crucial to the design. In this contribution we will use GPU-accelerated molecular dynamics simulations to study the diffusion of small molecules through zeolite structures.

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High-Performance Computing in Processing of Scientific Big Data and Improvement of our Understanding of Mechanisms Driving the Air-Sea CO2 Fluxes in the Southern Ocean

Author: Laique Merlin Djeutchouang[1]

Co-author: Pedro Monteiro [2]

[1] *CSIR-SOCCO & Oceanography Dept., University of Cape Town*

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Even though it appears to be one of the most poorly sampled ocean regions on Earth, the Southern Ocean is the largest anthropogenic CO2 sink as it accounts roughly 40% of its global uptake since the beginning of the industrial era. With the aim to quantitatively assess the sensitivity of atmospheric and oceanic drivers of the sea surface pCO2 (partial pressure of CO2) in the Southern Ocean, we need to improve our understanding of the mechanisms driving the CO2 exchange at the atmosphere-ocean interface. For this oceanographic research in Ocean Systems and Climate, we use many computational and memory intensive applications for simulation such as NEMO/PIECES codes to produce scientific big data on high-resolution ocean. The processing and analysis of these scientific big data contribute to the production for all domains of enquiry and across domains, as well as providing essential information for decision-making in response to global challenges such as climate change, disaster risk reduction, sustainable development. In order to meet the many global challenges and to take advantage of the opportunities of the scientific big data revolution, it is imperative to develop skills and capacity in the science of scientific big data. However, producing these skills and performing them on the analysis and processing of those scientific big data (in order to extract useful information) are memory and computationally intensive. They demand huge CPU and memory capacity for each of the jobs and we need to perform multiple iterations of these jobs to arrive at the end results which could be useful for our oceanographic research. This could not be possible without the help of the High-Performance Computing (HPC) cluster hosted and managed at the Centre of High-Performance Computing (CHPC). Given that the Southern Ocean carbon sink is also modulated by the regional wind variability, we have managed to explore the sensitivity of the seasonal cycle on the variability of storm characteristics using high resolution data and HPC cluster.

Supported Student:

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SIG Poster / 3

Human Rhinovirus Inhibition through Capsid "Canyon" Perturbation: Structural Insights into the Role of a Novel Benzothiophene Derivative

Authors: Clement Agoni[1] ; Pritika Ramharack[2] ; Geraldene Munsamy[3] ; Mahmoud soliman [2]

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The challenge in targeting human rhinoviruses (HRV) over the years has been attributed to the wide variety in HRV serotypes. Nonetheless, the search for therapeutic agents against HRV continues unabated. These efforts have been augmented by the recent discovery of the novel benzothiophene derivative shown to inhibit HRV viral replication. Bound to subtype HRV-B14, the compound showed similar inhibitory activity as Pleconaril, a known capsid inhibitor. However, the molecular and structural basis of this inhibition remains unclear. In this in silico report, residue interaction network analysis revealed that the binding of the benzothiophene derivative into the "canyon" region of the active site of HRV-B14 distorts its initially extensively networked and compact residue profile. This was characterized by fewer inter-residue hydrogen bonds, reduced van der Waal interactions, and increased residue flexibility. Interestingly, however, the binding of this benzothiophene derivative decreased the flexibility of the north-south wall around the canyon region possibly impeding the "breathing motion" of HRV-B14, hence its inhibition. Atomistic insights also revealed the cruciality of Tyr152 towards inhibitor binding at HRV-B14. This was justified by the amino acid's high intermolecular interaction with both inhibitors. Findings provide important structural insights in the inhibitory activity the novel benzothiophene derivative, and reaffirm its promising

potential as an alternative capsid inhibitor towards common cold therapy upon further experimental validation.

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INM RAS-MSU land surface scheme development: physical and computational aspects

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Land surface models (LSM) are an inherent part of Numerical Weather Prediction (NWP) systems and Earth System Models (ESMs). They provide surface momentum, energy and mass fluxes at the land surface necessary for simulating evolution of atmosphere and climate system at all temporal scales.

This abstract presents LSM jointly developed by Institute of Numerical Mathematics (INM) RAS and Moscow State University (MSU) and used in the INMCM Earth System model (Volodin et al., 2017), participating in the CMIP (Coupled Model Intercomparison Project) series of climate simulations. The basis of INM RAS-MSU LSM is a soil model computing vertical distribution of temperature, liquid water, ice and water vapor content in each land grid cell of the ESM (Volodin and Lykosov, 1998). Heat and moisture transfer equations are discretized at 23 levels in soil, whereas for heat transport in snow, 4 levels are used. Each land grid cell is composed of 5 possible surface types: dry vegetation, vegetation covered by intercepted precipitation, bare soil, snow and inland waters. The snow fraction of bare soil surface depends on snow thickness. To get cell-averaged temperature and fluxes, tile approach or parameter aggregation method are used, depending on a variable. To obtain the averaged physical soil parameters in a cell, the global data on 8 soil types distribution are involved. Water area and depth are adapted from GLDBv2 dataset. Thermodynamic state of lakes is simulated by simplified version of 1D LAKE model (Bogomolov et al., 2016). The river module consists of diffusive wave equation model for dynamics and heat balance equation to compute river temperature. The model can be used in fully coupled mode in a framework of ESM or NWP, or in standalone regime. In the latter case, measured atmospheric forcing, reanalysis, or climate simulation data are used. The model is implemented in parallel mode using MPI protocol, with 2D longitude-latitude domain decomposition.

Traditional land surface models allow for straightforward parallelization and 2D longitude-latitude data decomposition, because vertical diffusion-type problems solved in each cell are independent. Inside each MPI-subdomain a set of vertical diffusion-type problems is again independent, allowing to use multi-thread (OpenMP or GPU) computations per every CPU. Given this high scalability, a small number of MPI-collective operations like summing array elements over large land regions may become a bottleneck. Concomitantly, while increasing a land surface model complexity, new algorithms appear imposing horizontal dependence of computations. In INM RAS-MSU LSM, it is a new comprehensive river routing scheme, which solves 1D equations for momentum and heat along each river. This leads to at least two challenges. First, problem solutions for different rivers in a given basin are not independent, and a maximally scalable algorithm should be found. And second, each river basins does not fit in single MPI-subdomain, so that collection of data from MPI-domains overlapping with the river basin should be optimized. This would involve novel approaches, not implemented in land surface models so far.

HPC Applications / 173

In search of novel energy materials

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The wide spread use of fossil fuels is complicit in the rapid climate change we have witnessed during the past few years. All possible resources to reduce the use of fossil fuels must be explored. At the centre of research in alternative energy technologies is the search for novel materials that can improve the efficiency of solar energy harvesting in solar cells, catalyse hydrogen production and convert waste heat into electricity. Accurate numerical simulations of the properties of compounds is a potential first step in this process. With access to constantly improving computational resources this simulation plays an essential role finding potential compounds. In this talk I'll give an overview of an ab initio numerical simulation approach that enables us to establish whether a compounds is stable, what its physical properties are and its potential as an energy harvester.

HPC Applications / 192

In search of novel energy materials

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The wide spread use of fossil fuels is complicit in the rapid climate change we have witnessed during the past few years. All possible resources to reduce the use of fossil fuels must be explored. At the centre of research in alternative energy technologies is the search for novel materials that can improve the efficiency of solar energy harvesting in solar cells, catalyse hydrogen production and convert waste heat into electricity. Accurate numerical simulations of the properties of compounds is a potential first step in this process. With access to constantly improving computational resources this simulation plays an essential role finding potential compounds. In this talk I'll give an overview of an ab initio numerical simulation approach that enables us to establish whether a compounds is stable, what its physical properties are and its potential as an energy harvester.

Supported Student:

HPC Applications / 86

In-silico investigations of metal coordinating enzymes: From Biofuel production to Antimicrobial drug resistance

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Enzymes which are directly bound to metal cofactors are referred to as Metalloenzymes. These enzymes play various biologically important roles from catalyzing electron transfer reactions to being important structural components of protein structures. Due to the abundance of metal containing enzymes and the role they play in important biological processes, it is important to study these enzymes. In-sillico approaches are readily used to study protein structure and Molecular Mechanics (MM) is an essential tool used for understanding protein dynamics. MM is used to describe protein behavior by applying a MM force field to describe bonded and nonbonded terms of a protein structure. The accuracy of the force field in describing a particular protein structure is highly dependent on the force field parameters. Unfortunately, for metalloenzymes there are no currently available force fields which can accurately describe the coordination environment of metals in metaloenzymes.

As a result, performing an accurate Molecular Dynamics (MD) for metalloenzymes is extremely challenging using available force fields. To overcome this limitation Quantum Mechanics (QM) may be applied to elucidate the parameters required for accurate description of metalloenzymes during MD simulations. This approach involves the use of potential energy surface (PES) scans to evaluate the angles, bonds and dihedral parameters that are important to describe the metal binding site. Experimentally derived energy profiles generated from PES scans are then fitted using least squares fitting to a theoretical force field to generate the force field parameters. This approach three cases of metal coordinating enzymes. The first are the Auxilliary Activity family 9 (AA9) enzymes which are Cu(II) containing enzymes that have been shown to increase the rate of cellulose degradation. Secondly, new parameters were also used in the identification of novel inhibitory compounds against the Mn(II) coordinating HIV-1 reverse transcriptase enzyme. Finally, this approach was applied to the Zn(II) Bi metallic active site center of Beta lactamase enzymes which are contributors to the development of bacterial antibiotic resistance. For all three cases force field parameters were successfully generated and validated using MD simulations

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Interaction between S. mansoni Universal stress G4LZI3 protein and selected polyphenols: a bioinformatics investigation.

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For decades, Praziquantel has been the undisputed drug of choice against schistosomiasis; a disease that affects more than 200 million people in over 78 countries and responsible for over 280 000 lives lost per annum, predominantly in sub-Saharan Africa. Rising concerns have been raised due to the unknown mechanism of action of the drug and unavoidable reports of the emergence of drug resistant strains. Moreover, current apprehension has been reinforced by the total dependence on a single drug for treatment. Therefore, the search for novel and effective anti-schistosomal drugs become imperative. This study made use of bioinformatics tools to determine the binding properties of a selective range of polyphenols docked onto the Universal stress G4LZI3 protein, a recently identified 'lead' molecule in the design of alternative treatment drug against schistosomiasis. Schistosomes have over several years, evolved mechanisms that include the presence of USPs, to counter biotic and abiotic stress. Up-regulation of the G4LZI3 protein throughout the multifaceted developmental cycle of the schistosome worm sparks interest in this protein, whose function is currently unknown. Ten polyphenols were docked onto the G4LZI3 protein; the best five complexes were selected for post-molecular dynamics analyses and binding free energy calculations. The strongest binding interactions were observed between the G4LZI3 protein with curcumin and catechin respectively. The major interacting residues conserved in all the complexes provides basis for further structure-based drug design of new compounds, with enhanced inhibitory potency and toxicity against G4LZI3. This study suggests an alternative approach for the development of anti-schistosomal drugs using natural compounds.

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Intermetallic study of Mechanical and Thermodynamic Properties of FeAl-N (N: Ag/Pd/Pt)

Authors: Hasani Chauke[1] ; Phuti Ngoepe[1] ; Chrestinah Mkhonto[1]

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Transition metal (TM)-aluminide intermetallic including TiAl, NiAl, FeAl and Fe3Al have unique properties and are of great significance because of their high melting points, enhanced oxidation resistance and relatively low density. They have attracted a lot of attention for their potential application in automotive parts and steel-IT coating. We employed the embedded-atomic method, based on density functional theory, as a means of calculating ground-state properties of realistic metal systems. The transformation temperature entirely depends on the concentrations and alloying element. This was evident for Ag, Pt (0.5 at %) and Pd (0.7 at %) doping was the most stable system with respect to Gibbs free energy. It was also deduced that the Ag, Pt (0.5 at %) and Pd (0.7 at %) dopant influence the elastic instability above 1200 K as well as the ductility of these systems. The X-ray diffraction method was used for studying the distribution of iron and aluminium atoms in the crystal lattice of B2 FeAl and FeAl-N phases. In this work we employed DFT to investigate the structural, electronic and mechanical properties of Ag, Pd and Pt doped on FeAl intermetallic. Molecular dynamics was used to investigate the influence of ternary addition and the effect of temperature by improving previous suggested concentrations.

HPC aspects: LAMMPS CODE, 432 atoms, 90 core, 6 priority, jobs queuing longer.

Supported Student:

Travel & Accom.

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Investigating the Interaction of Chitin in Organic Electrolyte Solutions using Molecular Dynamics Simulations

Author: Lenard Carroll[1]

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Abstract:

The dissolution, hydrolysis and fermentation of biopolymers afford biofuels, an alternative source of energy. Unfortunately, biopolymers have hydrogen bonding networks that are difficult to disrupt and dispersion forces to overcome, all of which make it insoluble in most common organic solvents and water under moderate conditions.

Much work has been devoted to improving the dissolution of biopolymers, via alternative solvents or by developing new ground-breaking processes. One alternative solvent that has become quite popular in biomass dissolution studies are ionic liquids (ILs). These are attractive solvents due to their broad range of uses and advantageous properties. ILs have been promising in its use in separation, extraction, catalysis, lubricants, fuel cells, batteries and liquid crystal research and have low vapour pressure, which implies low toxicity with respect to their clean-up. While many ILs are produced under environmentally unfriendly conditions, more studies are being done on finding ways to synthesise these species using the 12 design principles of Green Chemistry.[1]

While a plethora of studies has been done on the experimental dissolution of cellulose in ionic liquids, similar studies have been minimal for chitin. As such, a computational investigation on the dissolution of chitin in ionic liquids and organic electrolyte solutions (OESs) is presented here. OESs consists of an ionic liquid and an additional aprotic organic molecular solvent. These mixtures are important as ILs typically have high viscosities, which decreases its ability to effectively dissolve biopolymers; but, by adding co-solvents to the IL, the mixture's viscosity decreases, potentially improving on the solubility of the biopolymer.

In this work the separation of two 4-methyl-β-D-N-acetylglucosamine-(1$\rightarrow$4')-1'-methyl-β-D-N'-acetylglucosamine ((Glc(NAc)$_2$Me$_2$) monomers in various solvent systems are described using potential of mean force calculations. This models the dissolution of chitin. The ionic liquids of choice are 1-butyl-3-methylimidazolium acetate ([C_4C_1im][CH_3COO]) and 1-butyl-3-methylimidazolium methyl sulfate ([C_4C_1im][CH_3SO_4]), two ILs that have experimental physical properties available, a requirement for MD simulation validation. The co-solvents chosen were dimethyl carbonate, propylene carbonate and γ-valerolactone, three structurally similar bio-based solvents.

The solvation of a (GlcNAc)$_2$Me$_2$ monomer via radial distribution functions, interaction energies and hydrogen bond analyses is also presented, as to support the results produced from the separation study. Furthermore, the experimental swelling of chitin is investigated as to compare it to the interaction energy results, acting as further validation of the computational results.

[1] - 12 Design Principles of Green Chemistry https://www.acs.org/content/acs/en/greenchemistry/principles/12-principles-of-green-chfemistry.html (accessed Feb. 22, 2019)

HPC Content:

Potential of mean force calculations were performed with the AMBER PMEMD CPU code at the CHPC. This is one of the fastest MD codes available with a highly efficient MPI implementation and the option of an even more efficient GPU implementation. Simulations were limited to 64 processors across four nodes without high memory requirements. Array jobs, consisting of 13 independent windows of 50 ns, were used for each simulation. More than 10 array jobs were used in order to model all solvents systems, which equates to more than 130 batched jobs and 6.5 μs of simulation.

Supported Student:

Travel & Accom.

SIG Poster / 114

Investigating the Mechanical Properties of Lithiated Li1+XMn2O4, (0 ≤ x ≤ 1) Nanoporous Composites

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The demand for batteries with higher energy density and storage capacity has been increasing over the past three decades. As such spinel LiMn2O4 have been found to be one of the promising and paramount cathode materials due to its inexpensiveness, environmental friendliness and structural stability when compared to its counterparts, such as LiCoO2. However, this material suffers from high voltage fade due to the Jahn-Teller distortion. This is caused by volume expansion in bulk materials; resulting in a material that has reduced symmetry and energy, consequently causing fractures to the material. Nanoporous materials for rechargeable Li-ion batteries have been considered to be a solution for Li-ion batteries due to their large exposed surface areas within the pore. This rare features enhance ionic diffusion and consequently improves electrochemical performance and mechanical stability. Furthermore, they also have the ability to expand freely upon lithiation without compromising the structural integrity of the electrode material.
Herein, molecular dynamics simulations employing the DL_POLY code have been used in a quest to investigate the mechanical properties of lithiated Li-Mn-O nanoporous materials of different cell dimensions (75 Å, 69 Å and 67 Å) and lithium concentration (Li1+xMn2O4, 0 ≤ x ≤ 1). When the lithium concentration is increased, all the structures experience volume expansion and nanoporous 67 Å shows more resilience to fracture compared to nanoporous 69 and 75 Å, due to its high yield strength. However, at Li1.75Mn2O4 concentration, nanoporous 69 Å depicts a higher yield strength. This is also validated by cleaner XRDs at this concentration compared to the other nanoporous structures. This implies that the cavity to wall ratio of nanoporous 69 Å results in an electrode material that is more resilient and not prone to fracture.

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Investigating the Structural and Electronic Properties of LiMO2 (M: Mn, Ni, Co) as Potential Cathode Materials: A DFT Study

Author: Nkgaphe Tsebesebe[1]

Co-authors: Kenneth Kgatwane [1] ; Phuti Ngoepe [1] ; Raesibe Sylvia Ledwaba [1]

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Large scale power applications continue to drive research and development of advanced battery systems. In recent years, the need for portable power has accelerated due to the miniaturization of electronic appliances. However, one of the major difficulties for improving the performance of lithium-ion batteries required to meet the increasing demand for energy storage is the development of efficient and stable cathode materials. Hence, the co-doped layered lithium transition metal oxides, LiMO2 (M = Ni, Co, Mn) have been regarded as promising cathode materials for secondary Li-ion batteries, due to their unique properties including high energy density, good cycling stability, low cost, and low toxicity. In this work, we employ the spin polarized density functional theory calculations with on-site Coulomb interactions to probe the energy gap of the LiMO2 (M = Ni, Co, Mn) structures. The Mn3+, Co3+ and Ni3+ with low spin in LiMnO2, LiCoO2 and LiNiO2 structures produced direct band gaps of 1.64 eV, 2.45 eV and 0.4 eV respectively. The band gaps are less than 4 eV indicating the structures are semiconductors. The band structures depicts distance between the valence band of electrons and the conduction band. Our results are in considerably better agreement with experiments, and corrections methods are found to have a small effect. The results generated thus far validate the accuracy of DFT+U method and will enable accelerated discovery, synthesis and optimization of doped materials that will contribute to performance prediction of LMO doped cathodes.

Supported Student:

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10

Investigation of the interaction between some selected phytochemicals from Solanum xanthocarpum and GLUT4: Insights from molecular docking approaches

Authors: Tayo Alex Adekiya[1] ; Raphael Taiwo Aruleba[2] ; Babatunji Emmanuel Oyinloye[3] ; Pierre P D Kondiah[1] ; Yahya E Choonara[1] ; Viness Pillay[1] ; Pradeep Kumar[1]

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In recent years, there has been an exponential increase in the global burden of cancer which has been associated with several factors including environmental influence, aging, diet, infectious agents, hormonal imbalance and chronic inflammation, among others. Cancerous cells utilize more glucose for its proliferation and survival than normal cells. Thus, the regulation of glucose consumption of cancerous cells through the inhibition of glucose transporter-4-protein (GLUT4) encoded by solute carrier family-2-member-4-gene (Slc2a4) by selected phytochemicals from Solanum xanthocarpum may serve as a new therapeutic candidate for the treatment of cancer. The seven identified potential inhibitors of GLUT4 from *Solanum xanthocarpum* were retrieved from PubChem database. Examination of their drug-likeness, toxicity prediction and molecular docking studies of these compounds

with GLUT4 were carried out using online tools such as Molinspiration, PreADMET V.2.0 and Patchdock server. The findings revealed that, five out of the seven compounds fulfil oral drugability of Lipinski's rule of five (RO5) while two slightly meet the criteria of RO5. Conversely, five of the compounds are predicted to be mutagen while the remaining two are predicted to be safe for the body. Additionally, stigmasterol glucoside has higher binding-affinity (7590) with GLUT4 when compared to doxorubicin (6600) the control. These findings suggest that stigmasterol glucoside from *Solanum xanthocarpum* could be a promising therapeutic agent with better therapeutic efficacy than doxorubicin in the treatment of cancer via the inhibition of GLUT4.

KEYWORDS:
GLUT4; cancer; drugability; stigmasterol glucoside ; Solanum xanthocarpum

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SIG Poster / **34**

Jahn-Teller effect in high spin d4 and low spin d9 octahedral metal-complexes.

Authors: Jeanet Conradie[1] ; no coauthor[None]

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Abstract for Computational chemistry session, oral

KEYNOTE 2 / **201**

KEYNOTE 1: TBC

KEYNOTE 2 / **229**

KEYNOTE 1: Digital Transformation: Issues of the Public Service

Author: Mandla Ngcobo[None]

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Generally, a lot of awareness has been created around Digital Transformation/ the Fourth Industrial Revolution (4IR) with various stakeholders electing to focus on matters of interest to them. However, there are known challenges and requirements for the public service to be able to transform digitally. The presentation would talk about challenges/ issues (people/ process/ technology issues) that require interventions/ solutions to achieve a Digitally Transformed public service.

Supported Student:

KEYNOTE 2 / **203**

KEYNOTE 3 (SA NREN): TBC

Author: Josva Kleist[1]

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KEYNOTE 2 / 223

KEYNOTE 3 (SA NREN): eInfrastructures as enablers for global science and education

Author: Josva Kleist[1]

[1] *NORDUnet A/S*

Corresponding Author: kleist@nordu.net

Science and education are increasingly becoming global endeavors. Scientists collaborate internationally and questionnaires indicate that scientists today are more likely to collaborate with partners outside their home institutions than with local research fellows. Students no longer need to physically be on campus to take classes, as they follow courses remotely and can even take a degree at foreign university without leaving home. Furthermore, there is a growing number of international research infrastructures, some centralized and some highly distributed, in all areas of science. The construction of those infrastructures is partly driven by financial necessity, but also from a need to bring together the necessary competences. Furthermore, the paradigms of Open Science and Citizen Science foster foster an environment of sharing and inclusion. Collaboration is no longer just a matter of scientist visiting for weeks and months.

For these reasons, access to facilities, research infrastructures, and data must be global, universal, fine-grained, and instant. As an eInfrastructure provider, R&E Network organizations are one of the fundamental building blocks supporting today's global science, and just as scientific activities are becoming more and more global, we need to think global. With the network, we already see this happening, where leading NRENs, such as the South African NREN, participate in the Global Network Advancement Group, that works on the intercontinental aspects of the (GREN) Global R&E Network. Moreover, network services such as eduroam, eduGAIN, and eduVPN take a truly global approach. The infrastructure needed to support Open Science and Citizen Science drives us to break down silos between storage, compute, and network infrastructures. We need to think about it in its entirety. The same goes for some of the large international research infrastructures, where storage, compute, and the network become an integral part of the science instrument. In this talk, I will present my views on the role of R&E Networks as enablers for science and education, with an outset on what I see happening in the European Nordics, at a European level, and globally.

Supported Student:

KEYNOTE 2 / 207

KEYNOTE 4: Scientific Applications on Heterogeneous Architectures – Data Analytics and the Intersection of HPC and Edge Computing

Author: Michela Taufer[1]

[1] *University of Tennessee Knoxville*

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This talk discusses two emerging trends in computing (i.e., the convergence of data generation and analytics, and the emergence of edge computing) and how these trends can impact heterogeneous applications. Next-generation supercomputers, with their extremely heterogeneous resources and dramatically higher performance than current systems, will generate more data than we need or, even, can handle. At the same time, more and more data is generated at the "edge," requiring computing and storage to move closer and closer to data sources. The coordination of data generation and analysis across the spectrum of heterogeneous systems including supercomputers, cloud computing, and edge computing adds additional layers of heterogeneity to applications' workflows. More importantly, the coordination can neither rely on manual, centralized approaches as it is predominately done today in HPC nor exclusively be delegated to be just a problem for commercial Clouds. This talk presents case studies of heterogenous applications in precision medicine and precision farming that expand scientist workflows beyond the supercomputing center and shed our reliance on large-scale simulations exclusively, for the sake of scientific discovery.

Supported Student:

KEYNOTE 2 / **204**

KEYNOTE 4: TBC

Author: Michela Taufer[1]

[1] *University of Tennessee Knoxville*

KEYNOTE 2 / **194**

KEYNOTE 5 (DIRISA): DALI: A Data life cycle instrument for management and sharing of data: Towards the reproducibility and data reuse of scientific research

Author: Hakizumwami Birali Runesha[1]

[1] *University of Chicago*

Corresponding Author: runesha@uchicago.edu

Researchers today are generating volume of data from simulations, instruments and observations at accelerating rates, resulting in extreme challenges in data management and computation. In addition to publications, scientists now produce a vast array of research products such as data, code, algorithms and a diversity of software tools. However, scholarly publications today are still mostly disconnected from the underlying data and code used to produce the published results and findings, which need to be shared. This presentation will discuss a funded project to acquire and operate an extensible Data Lifecycle instrument (DaLI) for management and sharing of data from instruments and observations that will enable researchers to (i) acquire, transfer, process, and store data from experiments and observations in a unified workflow, (ii) manage data collections over their entire life cycle, and (iii) share and publish data. This presentation will also discuss our approach in generating and sharing data and artifacts associated with research publications, and therefore, providing access to a platform that makes data findable, accessible, interoperable, reusable and reproducible.

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KEYNOTE 2 / **161**

KEYNOTE 6: Eliminating Weapons of Math Destruction: Next-Generation Arithmetic

Author: John Gustafson[1]

[1] *National University of Singapore*

Corresponding Author: john.gustafson@nus.edu.sg

Users of floating-point arithmetic (floats) have long experienced the disconnect between mathematically correct answers and what a computer provides. Choices made in the 1986 IEEE 754 Standard for floats lead to irreproducible results that destroy the confidence we experience, say, when working with integers. After 33 years, language support for mandated internal flags (rounding, overflow, etc.) remains nil, so float hazards are almost invisible. The Standard does not require correct or consistent rounding of transcendental functions, so bitwise portability of float-based programs is nonexistent.

The emerging posit standard is a fresh approach to computing with real numbers that is fast, bitwise-reproducible, and capable of preserving mathematical properties like the associative and distributive laws of algebra without sacrificing performance. Complete hardware-software stacks supporting this new kind of arithmetic are beginning to appear, so we now have the hope of eliminating IEEE 754 "weapons of math destruction" with something much closer to the logical behavior we expect from computers.

KEYNOTE 2 / 205

KEYNOTE 7: TBC

Author: Thomas Sterling[1]

[1] *Indiana University*

KEYNOTE 2 / 221

KEYNOTE 7: The Future of Computing Will Be non-von Neumann

Author: Thomas Sterling[1]

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Seven decades of HPC has been empowered by the abstraction of "the von Neumann Architecture" and its many derivatives, driven to a significant degree by Moore's Law and the exponential growth of device density and concomitant clock rates yielding a performance gain over that period of more than ten trillion for floating point computation. But a perfect storm of recent technology trends has terminated this unprecedented expansion and challenges the future opportunities beyond exascale computing. But even as the end of conventional processing practices is flat-lining, a new world of non von Neumann execution models and architectures is emerging igniting a revolution for the next generations of computing systems orders of magnitude greater performance than is currently achieved. Even more important is that the reality of HPC users is that approximately 90% of the Top-500 machines measured with the HPL benchmark demonstrate only about 1% of the performance of the fastest machines. Thus we are much further away from exascale than is generally assumed and therefore much greater gains are required to truly bring the major base of HPC users into the exascale era. New non von Neumann architectures and models, such as Quantum Computing, Neomorphic

Computing, and Continuum Computing (this last presented at CHPC18) are offering important possibilities for the future. Earlier non von Neumann techniques previously explored in past decades, such as static and dynamic dataflow, cellular automata, systolic arrays, and special purpose designs may also serve as starting points for new classes of useful computing methods even as Moore's Law recedes. Finally, advanced technologies beyond conventional semiconductors such as cryogenic such as single flux quantum logic provides yet another dimension of potential post exascale strategies. This Keynote Address will convey a fast paced odyssey through the near future opportunities of HPC non von Neumann based computers. Questions will be encouraged by participants throughout the presentation as well as the Q&A session at its conclusion.

Supported Student:

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Leveraging Open Source Technologies to Rapidly Deploy Infrastructure with Minimum Human Capacity

Authors: Eugene De Beste[1] ; Peter van Heusden[2] ; Alan Christoffels[3]

[1] *SANBI - UWC*

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Limited access to skills and staffing required to configure High Performance Computer / High Throughput Computing (HPC/HTC) is a barrier to the growth of computing facilities in Africa. Automation of common systems administration tasks, an approach known as "infrastructure as code", can help overcome this barrier. We demonstrate the construction of an OpenStack computing cloud configured with Kubernetes and Jupyter Lab as a High Throughput Computing facility using entirely automated methods based on open source technologies. A key aspect is that this solution is for a single individual to be able to deploy the complete solution within a single day.

Supported Student:

No

HPC Technology / 152

ML approaches for HPC

Author: Peter Braam[1]

[1] *University of Oxford*

Machine Learning methodologies and tools have delivered new approaches to scientific computing ranging from new approximation methods to solve differential equations to leveraging advantages of ML hardware over traditional HPC hardware. It is not unlikely that such approaches will be helpful to computational problems that have seen little progress for decades. We will discuss a few examples, and discuss key themes in carrying this forward.

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Machine Learning Models for the Prediction of Isobaric Heat Capacities of Room Temperature Ionic Liquids

Authors: Tayla Wilson[None] ; Gerhard Venter[1]

[1] *University of Cape Town*

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Abstract attached below.

Supported Student:

Travel & Accom.

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Machine Learning and applications.

Author: Bruce Mellado[1]

[1] *University of the Witwatersrand and iThemba LABS*

Corresponding Author: bruce.mellado@wits.ac.za

Machine Learning and applications.

Joint proposal from the Wits Institute of Data Science (WIDS) and the Wits Institute for Collider Particle Physics (ICPP)

Big Data, Artificial Intelligence and applications.

The workshop will include few introductory lectures pertaining to Machine Learning and the handling of Artificial Intelligence with a large variety of data sets. The workshop will include a hands-on session using standard tools. This will include the use of python, TernsorFLow and others.

Anticipate two days for 20 to 30 people

SIG Poster / 84

Mechanical investigation of Ru as a third element on TiPt for high temperature shape memory applications

Author: Mordecai Mashamaite[1]

Co-authors: Phuti Ngoepe [1] ; Hasani Chauke [2]

[1] *University of Limpopo*

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Shape memory alloys (SMAs) combine great mechanical and practical properties identified with the thermoelastic martensitic transformation (MT) with astounding corrosion resistance, prompting the

probability of countless applications in various modern fields. In order to understand the mechanical properties of these alloy, first-principle method was utilized to substitute Pt with Ru on the equi-atomic B2 TiPt. The supercell approach in MedeA (VASP) was used to create large supercells (16-1024 atoms). The structures were evaluated on the CHPC cluster, using 48 cores to substitute Pt with Ru on TiPt structure to study the phase stability and mechanical properties. The calculated heats of formation predict that the Ti50Pt6.25Ru43.75 is the most thermodynamically stable structure with the lowest density of 9.08Mg/m3. The structure becomes mechanically stable with an increase in Ru content, the C' becomes higher which constitute to reduced martensitic transformation temperature, the bulk and shear moduli and Pugh's ratio are calculated. The structures become more ductile and more hardened with the increment of Ru content. In addition, the calculated phonon dispersion shows that Ti50Pt6.25Ru43.75 is vibrationally stable more the other structures. The Ru substitution is more promising as a B2 Phase stabilizer.

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Mechanistic insight on the inhibition of D, D-carboxypeptidase from Mycobacterium tuberculosis by β-lactam antibiotics: an ONIOM acylation study

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Abstract

Tuberculosis is an infectious disease caused by *Mycobacterium tuberculosis* that has challenged public health care. D, D-carboxypeptidase (DacB1) is an enzyme involved in the biocatalysis of the complex *M. tuberculosis* cell wall. DacB1 act on pentapeptide stems and cleave off the terminal D-alanine residue thus resulting in tetrapeptide precursors for transpeptidation and the mechanism under which it occurs is poorly understood in M. tuberculosis. Herein, we investigated the acylation mechanism of DacB1 by β-lactams, Faropenem (Faro), Imipenem (Imi), and Meropenem (Mero), using a 6-membered ring transition state model that involves a catalytic water molecule in the reaction pathway. A two-layered our Own N-layer integrated Molecular Mechanics (ONIOM) (B3LYP/6-311++G(2d,2p): AMBER) model was employed.

The computational resources (CPUs/GPUs) to carry out this project were provided by CHPC under project short name: HEAL0839 workspace (Lustre file system) on Lengau cluster. Two software programs (Gaussian09 and Amber18) were used to execute the jobs on 24 cores, 1 node and 96:00 hours wall time.

The obtained results revealed that the 6-membered ring transition state model is feasible and efficient for DacB1 inactivation via acylation by β-lactams in the presence of the catalytic water. Hence, the ΔG# suggests that the nucleophilic attack on the carbonyl carbon is the rate-limiting step of serine protease with 13.62, 19.60, and 30.29 kcal mol-1 for Imi—DacB1 Mero—DacB1, and Faro—DacB1, respectively. Furthermore, the thermochemical properties, ΔH and ΔS, indicated that the reaction mechanism is favorable. Additional analysis of electron density through the electrostatic potential (ESP) and electron delocalization via natural bond orbital (NBO) agree in concept with respect to atomic intuition in the reaction pathway.

Keywords: *Mycobacterium tuberculosis*(*M.tuberculosis*), D, D-carboxypeptidase (DacB1), A two-layered our Own N-layer integrated Molecular Mechanics (ONIOM), transition state, Electrostatic potential (ESP), Natural bond orbital (NBO).

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HPC Technology / 71

MeerKAT archive and data access

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The MeerKAT archive was made accessible from the internet earlier this year.
This allow researchers from across the world to pull data from the MeerKAT archive.
In this talk I'll describe the MeerKAT storage system that consists out of several petabytes of observations backed by a Ceph distributed storage system. The use of Ceph at SARAO and the infrastructure around the archive will be described. There after the data access methods from the internet and from partner institutes like the CHPC will be presented.

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Microbes, not humans: Exploring the molecular basis of Pseudouridimycin selectivity towards bacterial and not human RNA polymerase

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Objective Bacterial RNA polymerase (bRNAP) rep- resent a crucial target for curtailing microbial activity but its structural and sequence similarities with human RNA polymerase II (hRNAPII) makes it difficult to target. Recently, Pseudouridimycin (PUM), a novel nucleoside analogue was reported to selectively inhibit bRNAP and not hRNAP. Till date, underlying mechanisms of PUM selectivity remains unresolved, hence the aim of this study.
Results Using sequence alignment method, we observed that the b0 of bRNAP and the RPB1 subunits of hRNAPII were highly conserved while the b and RPB2 subunits of both proteins were also character- ized by high sequence variations. Furthermore, the impact of these variations on the differential binding of PUM was evaluated using MMPB/SA binding free energy and per-residue decomposition analysis. These revealed that PUM binds better to bRNAP than hRNAP with prominent bRNAP active site residues that contributed the most to PUM binding and stabilization lacking in hRNAPII active site due to positional substitution. Also, the binding of PUM to hRNAP was characterized by the formation of unfavorable interactions. In addition, PUM assumed favorable orientations that possibly enhanced its mo- bility towards the hydrophobic core region of bRNAP. On the contrary, unfavorable intramolecular interac- tions characterize PUM orientations at the binding site of hRNAPII, which could restrict its movement due to electrostatic repulsions.

Conclusion These findings would enhance the design of potent and selective drugs for broad- spectrum antimicrobial activity.

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SIG Poster / **41**

Molecular Finite Element Density Functional Calculations employing a Cusp Factor to enable convergence at the nuclei

Authors: Moritz Braun[1] ; Kingsley Obodo[1]

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FEM calculations have been performed in Cartesian coordinates in the finite element framework FEniCS1, using the density functional approach for a number of small molecules. In order to aid convergence of the orbitals and total energies a suitable cusp factor
F(**r**)=1+$\sum_{j=1}^{N_A} c_j \exp(-2Z_J r_j)$ with $r_j = |\mathbf{r}-\mathbf{R}_j|$.$wasemployed, suchthattheresultingeffectivepotentialisnon-singularatallnucleiandwherethecoefficients$c$_i$ are obtained by solving a linear system of equations. The finite element ansatz for the pseudo orbitals leads to a sparse generalized eigenvalue problem of dimension N up to 3.6 10^6, which was solved employing thethe Jacobi-Davidson method on a High Performance SMP Machine with 32 CPUs and 512 GB of memory.
The resulting total energies and densities were compared with those obtained using the Gaussian basis set package NWChem[2] and excellent agreement was found.

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SIG Poster / **126**

Molecular dynamics study of the influence of temperature on Ti7/LiCl structure

Authors: Andile Mazibuko[1] ; Hasani R. Chauke[1] ; Phuti E. Ngoepe[1]

Co-authors: Alexey A. Sokol [2] ; C. Richard A. Catlow [2]

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In this study, we employ computational modelling techniques to explore the structural behaviour of the Ti7 cluster in LiCl as a medium of interaction (problem size: 432 – 1024 atoms). We employed the molecular dynamics code (DL_POLY) using a core count of 48 and 24:00 wall time on a normal queue, to understand the Li-Cl, Ti-Cl, Li-Li, Li-Ti and Cl-Cl interactions of the system at a temperature range of 300 K – 1000 K. The LiCl structure was validated by comparing the lattice parameters of LiCl with experimental data and were found to be in good agreement. We observed that the interatomic Buckingham potentials used reproduced the structure to within 1% in agreement with experimental data. Furthermore, the radial distribution functions for the Ti7/LiCl system, show a phase transition from solid to liquid in the temperature range of 600 K - 800 K. The results of this study provide insight into understanding the growth of titanium in salt mediums, significant for maximizing titanium metal production.

BoF / **157**

Monitoring HPC Services with CheckMK

Authors: Kieran Leach[1] ; Philip Cass[1]

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Administrative monitoring of a range of HPC systems can be time consuming and inefficient with many HPC systems being provided with their own integrated monitoring solutions and an expectation that system managers will monitor each system separately. In order to save staff time, effort and in order to improve the potential for rapid and effective response to emerging problems where systems interact, a “single pane of glass” approach is considered optimal. HPC systems typically utilise relatively boutique technology however which is commonly not monitored by existing out-of-the-box monitoring solutions. In this presentation we detail the application of CheckMK, a general use monitoring system, to HPC systems using non-commodity hardware and software. We focus on the development and use of “check” scripts, which at EPCC have enabled the System Administrators team to simply and reliably monitor all relevant and service-critical aspects of a variety of HPC systems through a single “pane of glass” approac

DIRISA / **167**

More than meets the eye: Towards an Artificial Intelligence Observatory

Author: Matias Carrasco Kind[1]

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DIRISA / **166**

More than meets the eye: Towards an Artificial Intelligence Observatory

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HPC Technology / **158**

NEXTGenIO: exploring the potential of non-volatile memory in HPC

Author: David Homan[1]

[1] *EPCC*

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Memory and storage read and write costs can lead to a significant loss of time and energy in current HPC systems. Byte-addressable non-volatile memory (NVM) could provide considerable improvements in both time and energy requirements over conventional DRAM memory. Using Optane DCPMM, Intel's new byte-addressable and persistent memory, the NEXTGenIO project investigated the performance of NVRAM by designing, building and testing a bespoke prototype NVM system. The main goal of the project was to explore the potential of NVRAM in overcoming performance bottlenecks in I/O and main memory, which are considered significant barriers to Exascale computing.

In this talk we will give a brief overview of the NEXTGenIO system (192GB DRAM and 3TB of NVM per dual socket node), and the various NVRAM usage modes. The results from a number of investigative test cases run on the NEXTGenIO prototype system will be presented. In particular we will discuss I/O performance, run-time, and energy consumption for applications with large I/O demands, such as OpenFOAM and CASTEP. Comparison of the results from NVRAM and DRAM shows that NVRAM can indeed provide significant improvement in both performance and energy consumption.

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NEXTGenIO: exploring the potential of non-volatile memory in HPC

Author: David Homan[1]

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Storage read and write operations can represent a significant cost for many HPC applications. For I/O-bound applications these overheads can become prohibitively large. In this talk we will discuss a number of approaches for dealing with common HPC I/O demands. One prevalent solution is the use of parallel file systems. We will present the basic methodology of distributed memory and popular parallel file system solutions used in current HPC architectures, such as Lustre and GPFS, as well as general file system solutions. MPI I/O, NetCDF and HDF5 will also be discussed as possible strategies for improving performance by moving beyond the one-program-one-file structure and effectively exploiting parallel file systems.

An alternate approach for improving I/O performance is the use of non-volatile memory (NVM). In contrast to DRAM, NVM makes it feasible to greatly expand main memory usage, reducing typical

I/O requirements. We will give a brief overview of the NEXTGenIO project, which explored the use of NVM in HPC, and present energy usage and I/O optimisation performance results from a suite of benchmarks run using NVM.

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NVIDIA Deep Learning Institute (DLI) Deep Learning Fundamentals

Authors: Maz Lopez[1] ; Michael Li[1]

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This workshop teaches deep learning techniques for a range of computer vision tasks. After an introduction to deep learning, you'll advance to building and deploying deep learning applications for image classification and object detection, modifying your neural networks to improve their accuracy and performance, and implementing the techniques you've learned on a final project.

At the end of the workshop, you'll have access to additional resources to create new deep learning applications on your own.

On completion of this course, you will be able to start solving your own problems with deep learning,

Tools, libraries, and frameworks: Caffe, DIGITS

Earn an NVIDIA DLI certificate to demonstrate your subject matter competency and support career growth.

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Network Analysis reveals insights into cellular death regulation in the resurrection plant Xerophyta schlecteri

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The resurrection plant *Xerophyta schlechteri* is able to withstand extreme water loss: it dries down to equilibrium with the air, losing 95% of its water, and can remain in the desiccated state for months to years. When water becomes available, the plants astonishingly recover within hours to regain full photosynthetic and metabolic competence. The question of how these plants regulate cellular death processes during water deficit is of great interest to the generation of drought tolerance in crops. During drying, a small region of the leaves do indeed succumb to desiccation. The present study compared these senescent tissues to viable tissues from the same leaves over the course of a dehydration event and during recovery. Gene expression data was subjected to K-means clustering and correlation network analysis to reveal putative regulators of cellular death and its outcomes in the resurrection plant.

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HPC Applications / 93

Next Generation Sequencing: where big data and high-performance computing meet

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The advent and evolution of next generation sequencing (NGS) has considerably impacted genomic research, including precision medicine. High-throughput technology currently allows for the generation of billions of short DNA or RNA sequence reads within a matter of hours. This becomes extremely important in the case of genetic disorders where rapid and inexpensive access to a patient's individual genomic sequence is imperative and enables target variant identification. NGS technologies results in the generation of large data sets which require extensive bioinformatic and computational resources. Computational life sciences therefore relies on the implementation of well-structured data analysis pipelines as well as high-performance computing (HPC) for large-scale applications. Here, we report the sequencing of the first six whole human genomes in South Africa and the processing of the data in collaboration with the Centre for High Performance Computing (CHPC). Efficient parallel and distributed implementations of common time-consuming NGS algorithms on modern computational infrastructures are imperative. The latter becomes pivotal as NGS will continue to transcend from research labs to clinical applications in the near future.

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Numerical simulation of geophysical turbulent flows on HPC systems

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A review of the code developed at Lomonosov Moscow State University for numerical simulation of geophysical turbulent flows is presented. The code combines DNS (Direct Numerical Simulation), LES (Large-Eddy Simulation) and RANS (Reynolds-Averaged Navier-Stokes) approaches to turbulence modelling in a unified numerical framework and allows simulations with high spatial and temporal resolution on HPC systems by using MPI, OpenMP and CUDA. Some of the challenges in using GPU and Intel Xeon Phi architecture for hydrodynamic simulations are discussed.

Using DNS and LES simulations of stably stratified plane Couette flow we show that besides chaotic irregular turbulent motions the turbulent Couette flow exhibits large coherent structures in the whole range of stability: from neutral to extremely stable. The well known counter-rotating rolls found in neutral case become unstable even with small increase in stratification. But for moderate stability skewed layered structures may be identified. It is argued that this layers act as barriers for turbulent mixing of heat without blocking momentum turbulent transfer, which results in increase in turbulent Prandtl number. For very strong stratification the flow becomes intermittent but the turbulence may persist for very high bulk Richardson numbers. Intermittency in the plane Couette

flow corresponds to the formation of secondary large-scale structures elongated in the spanwise direction, which define spatially confined alternating regions of laminar and turbulent flow.

We discuss how the DNS and LES results may be used to improve RANS models and, in particular, boundary layer turbulence closures used in weather and climate forecast models.

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Workshops / **27**

OpenStack cloud installation

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The workshop will offer OpenStack software stack installation and configuration, focusing on delivering OpenStack solution to help develop the skill set that will enable the deployment of OpenStack clouds.

KEYNOTE 2 / **202**

Opening Session

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Overview of the University of Namibia High Performance Computer

Authors: Anton Limbo[1] ; J.N.S Shapopi[1] ; M Backes[1]

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High performance computing (HPC) refers to the practice of aggregating computing power of several computing nodes in a way that delivers much higher performance than one could be achieving by a typical desktop computer in order to solve large problems in business, science, or engineering. UNAM has so far received two HPC racks from the Centre of High Performance Computing (CHPC), South Africa. The delivery was facilitated by the National Commission on Research Science and Technology (NCRST). The racks are primarily for human capacity development and awareness in HPC and form part of Namibia's readiness in participating in the Square Kilometre Array (SKA) and African Very Long Baseline Interferometry Network (AVN) projects.
The two racks have a combined total of 88 computing nodes, with the currently operational rack having 48 nodes. Thus far, the operational rack has been used in various projects such as modelling the broadband emission of globular clusters and analyses of gamma-ray data of active galactic nuclei, recorded with the H.E.S.S. telescopes in the Physics department, Land Degradation Assessment Baseline report: Omusati Region" by the Department of Geography, History and Environmental Studies Geo-Information Science (GIS) unit in conjunction with GIZ and the Ministry of Agriculture, Water and Forestry, as well as various MSc and BSc projects in the School of Computing. Very recently, the UNAM HPC site was used to model weather case studies by in collaboration with the Namibia Meteorological Services.

This presentation will give an overview of the use-cases of the HPC cluster as well as of its performance.

Supported Student:

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HPC Technology / **62**

PETSc: High-Performance Software Library for Engineering and Science Simulation

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Portable, Extensible Toolkit for Scientific Computation (PETSc) is a suite of
data structures and routines for the scalable (parallel) solution of scientific applications. Due to its solid mathematical grounding, careful software design, and most importantly, evolution resulting from the usage of many users in various application areas, PETSc is enabling engineers and scientists to solve large scale problems, with previously unreachable resolution, in areas as diverse as groundwater contamination, cardiology, fusion, nuclear energy, astro-physics, and climate change.

As a PETSc developer, I will give an overview of the PETSc, and briefly introduce its basic use in algorithmic research, numerical production simulation and parallel performance evaluation. As an example, I will present our recent simulation of the U.S. river systems on extreme-scale computers.

HPC Technology / **79**

Parallel and Distributed Search Algorithms

Authors: Cornelia Inggs[1] ; Steve Kroon[1] ; Marc Christoph[1]

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We investigate the parallelisation and performance analyses of search and planning algorithms for artificial intelligence, machine learning, and software verification. These applications involve the exploration of large state spaces, which requires at its core a combinatorial search algorithm. Much of our work, therefore, focuses on evaluating and improving the scalability of algorithms used in all these tasks.

In recent work we have implemented various parallel and distributed MCTS algorithms with different enhancement strategies for artificial intelligence, tested them for scalability, and compared the performance of these approaches on the same domain and the same hardware infrastructure. We make use of the CHPC's large queue to determine scalability up to 128 12-core compute nodes with 32GB RAM each—values that are in line with previous publications and distributed search implementations. We wrote our application code in Java, using an actor model framework (Akka) to simplify concurrency and distributed computing. We make limited use of MPI—more specifically, just mpirun—in order to easily launch our application on the available nodes using the PBS nodefile.

This talk will provide an overview of our research and the problems we investigate, as well as a discussion of recent results.

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Poster sponsored for registration only

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Practical HPC Tutorial

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From Workflow to Job Script

Following on from the basic induction tutorial this short course covers advanced job scripting with the aim of helping users to convert their scientific workflow into an HPC job script.

HPC Applications / **108**

Predicting Thermodynamic Properties of Ionic Liquids—from Molecular Simulation to Machine Learning

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KEYNOTE 2 / **206**

Prize Giving Ceremony

SIG Poster / **20**

Probing Binding Landscapes and Molecular Recognition Mechanisms of Atypical Antipsychotic Drugs towards the Selective Targeting of D2 Dopamine Receptor

Author: Patrick Appiah-Kubi[1]

Co-authors: Fisayo Andrew Olotu [1] ; Mahmoud E. S. Soliman [1]

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Dopamine receptors constitute a unique class of G-protein coupled receptors that mediate the activities of dopamine, a neurotransmitter implicated in diverse neurological diseases when dysregulated. Over the years, antipsychotic drugs have been primarily directed towards D2 dopamine receptor (DRD2) while associable adverse effects have been centred on non-selective targeting. The recent crystal structure of DRD2 in complex with atypical antipsychotic could further aid the structure-based design of highly DRD2-selective antipsychotics. Therefore, in this study, we comprehensively investigate the molecular recognition and differential binding landscapes of class-I and II DRD2 atypical antipsychotics, using membrane-bilayer molecular dynamics simulation and binding free energy techniques. Findings revealed that selected class-I antipsychotics exhibited binding dynamics and poses dissimilar to the class-II types with different interactive mechanisms at the binding cavity of DRD2. More interestingly, the class-II drugs established a highly coordinated binding at the DRD2 active site with a pertinent and recurrent involvement of Asp114 via strong hydrogen interactions. Furthermore, while these compounds exert distinct effects on DRD2 structure, findings revealed that the class-II types favourably engaged the deep hydrophobic pocket of DRD2 compared to the class-I drugs. We speculate that these findings will be fundamental to the discovery of highly selective DRD2 antipsychotics.

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Probing protein-protein interactions and druggable site identification: Mechanistic binding events between Ubiquitin and Zinc finger with UFM1-specific peptidase domain protein (ZUFSP)

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Deubiquitinating enzymes (DUBs) protein family have been implicated in some deregulated pathways involved in carcinogenesis such as cell cycle, gene expression and DNA damage response (DDR). Zinc finger with UFM1-specific peptidase domain protein (ZUFSP) is one of the recently discovered member of the DUBs. In this study, we used computational approaches to explore the impact of ubiquitin binding on ZUFSP. Furthermore, we identified, cross-validated and characterized ZUFSP binding sites for potential drug targeting. Four binding pockets were predicted, characterized and cross-validated based on physiochemical features such as site score, druggability score, site volume and site size. Site 1 with a SiteScore 1.065, Size 102, D score 1.00 and size volume 261 was predicted to be the most druggable site. Structural studies revealed that upon ubiquitin binding, the motional movement of ZUFSP was reduced when compared to the unbound ZUFSP. Furthermore, It was also observed that the ZHA domain orient in such a way that it moves closer to the Ub, this orientation enable the formation a UBD which is very peculiar to ZUFSP. The characteristics of these predicted sites can facilitate the design of site-specific inhibitors that can be used in cancer therapy.
Keywords: Binding site, ZUFSP, Ubiquitin, Molecular Dynamic Simulation, Deubiquitinating enzymes

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Travel & Accom.

SIG Poster / 94

Reactivity of H2O and SOx (x = 0 – 3) on a Pt (111) surface – A DFT Study

Author: Marietjie Ungerer[1]

Co-authors: Cornie van Sittert [2] ; Nora de Leeuw [3]

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The current global energy demand is met by burning fossil fuels, which releases large amounts of carbon dioxide, contributing to climate change. Hydrogen is considered a sustainable energy carrier, when it is produced from renewable sources. An attractive technology currently receiving attention is the Hybrid Sulphur (HyS) cycle, which is a thermo-electrochemical process where sulphuric acid (H2SO4) is thermally decomposed (> 800℃) to produce sulphur dioxide (SO2), water (H2O) and oxygen (O2). In a second step SO2 reacts with H2O to form H2SO4 and H2. The net reaction of this cycle is the splitting of H2O into H2 and O2. The current catalyst of choice is platinum (Pt), a very expensive and rare noble metal. While various other metals have been investigated, Pt is still the best performing catalyst in terms of activity and stability.1

The SO2 oxidation mechanism on the Pt surfaces is shown in Figure 1, where the adsorption modes of SO2 and H2O was determined. The most stable adsorption mode for SO2 on the Pt (111) surface had a S,O-bonded geometry, where S-O were in the plane of the surface on the fcc binding site. For H2O, the most stable adsorption occurred when all the atoms were parallel to the surface2. The second part of this work will cover the effect of increasing the SO2 and H2O coverage on the surface, in terms of surface morphology and reactivity. This will be concluded with a discussion on the behaviour of the other SOx species on the Pt surface.

Figure 1. Wulff morphology of a Pt nanoparticle, showing the structures and adsorption sites on the Pt (111) surfaces along with the surface coverages of H2O and SO2.

In this paper, we have used density functional theory (DFT) calculations3 to predict the behaviour of SO2 and H2O on the Pt (111) surface. To that regard, we aim to develop a comprehensive understanding of the SOx chemistry, including the adsorption, desorption, oxidation, as well as side reactions

to determine the species that may occur on the major electro-catalytic surfaces of Pt. This work was made possible by the CHPC (Centre for High Performance Computing)4 and Supercomputing Wales5 were 16.6 years of CPU time was used.

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Reactivity of ethylene carbonate on the (0001) aluminium oxide (α-Al2O3) surfaces.

Authors: Brian Ramogayana[1] ; Khomotso Maenetja[2] ; Phuti Ngoepe[2] ; David Santos-Carballal[3] ; Nora de Leeuw[3]

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Aluminium oxide (α-Al2O3) attracted the most attention as a potential cathode coating material for lithium-ion batteries because of its electrical behaviour and catalytic activity. Surface coating with α-Al2O3 shows improved capacity retention and electrochemical performance compared to the uncoated cathode material. Its reactivity towards the electrolyte components yields an additional coating layer that further hinders the cathode-electrolyte interactions. In this study, density functional theory calculations were employed to investigate the reactivity of commonly used electrolyte component, ethylene carbonate (EC) towards the (0001) aluminium oxide coating layer. All the intensive calculations were calculated using the Centre for High-Performance Computing (CHPC) facility of South Africa using VASP code as embedded in MedeA software. The lowest surface energy of γr = 0.11 eV/Å2 was calculated for the Al-terminated slab, which was in agreement with the reported literature. Upon adsorption, the EC molecule preferred to interact when place parallel to the Al-terminated (0001) surface. Although a minor charge transfer of Δq = -0.09 e- was calculated for the parallel adsorption configuration, the electronic rearrangement within the EC molecule and the charge transfer accumulation on the neighbouring oxygen atoms on the surface was observed upon adsorption. This indicate that the contribution of ethylene carbonate to the degradation of α-Al2O3 coating material is minimal.

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HPC Applications / 174

Research highlights from the Molecular Bio-computations and Drug Design Research Group at UKZN

Author: Mahmoud soliman [1]

[1] *Molecular Bio-computation and Drug Design Laboratory, School of Health Sciences, University of KwaZulu-Natal, Westville Campus, Durban 4001, South Africa*

Prof Mahmoud Soliman (http://soliman.ukzn.ac.za/) will provide a presentation that highlights the various research scopes and outcomes of research that is being conducted in his research group at UKZN over the last 8 years with more emphasis on the applications of computational simulations and the contribution of CHPC in drug design and discovery as well as capacity development. A few selected research topics will be presented such as: the irony of chirality; covalent drug inhibition; does drug size matter; and other topics.

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Research highlights from the Molecular Bio-computations and Drug Design Research Group at UKZN

Author: Mahmoud Soliman[1]

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Prof Mahmoud Soliman (http://soliman.ukzn.ac.za/) will provide a presentation that highlights the various research scopes and outcomes of research that is being conducted in his research group at UKZN over the last 8 years with more emphasis on the applications of computational simulations and the contribution of CHPC in drug design and discovery as well as capacity development. A few selected research topics will be presented such as: the irony of chirality; covalent drug inhibition; does drug size matter; and other topics.

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SA NREN / **217**

SA NREN Talk 1

Author: Shadreck Chitauro[None]

SA NREN / **216**

SA NREN Talk 3

Author: Attlee Munyaradzi Gamundani[None]

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SAFIRE for Service Providers

Author: Guy Halse[1]

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This workshop looks at how the South African Identity Federation (SAFIRE) can assist with solving access management for research collaborations and other e-infrastructure service providers. It will introduce some of the basic concepts of federated identity and provide and provide a high-level overview of the AARC blueprint architecture.

SA NREN / 214

SANReN Data Transfer Pilot

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Moving masses of data is a challenge. It can be slow and frustrating to transfer vast quantities of data from the many places it can be stored or generated over general-purpose computer networks.

When scientists attempt to run data intensive applications over campus networks, it often results in slow transfers - in many cases poor enough that the science mission is significantly impacted. In the worst case, this means either not getting the data, getting it too late or resorting to alternative inefficient measures such as shipping disks around.

SANReN would like to provide an update on the Data Transfer Pilot service that is available for the South African Research and Education community, to assist them to move their data locally and internationally. This session will also provide Data Transfer updates within the National Integrated Cyber Infrastructure System (NICIS).

Supported Student:

HPC Applications / 190

SAVIME - Simulation Analysis and Visualization in-Memory

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The increasing computational power of HPC systems fosters the development of complex numerical simulations of phenomena in different domains, such as medicine 1, Oil & Gas [2] and many other fields [3,4,5]. In such applications, a huge amount of data in the form of multidimensional arrays is produced and need to be analyzed and visualized enabling researchers to gain insights about the phenomena being studied.

Scientists also generate huge multidimensional arrays through environmental observations, measurements of physical conditions and other types of sensors. For instance, satellite data for Earth's weather, oceans, atmosphere and land [6] are kept in the form of multidimensional arrays in scientific file formats. Data collected by sensors in physics

experiments, such as the ones conducted in the photon studies by SLAC National Accelerator Laboratory [7], are also represented and processed in the form of multidimensional arrays.

Machine learning is another context in which multidimensional arrays are present. They are the basic input format for the heavily optimized linear algebra algorithms implemented in deep learning frameworks, such as: TensorFlow, Keras and Torch. Deep Learning algorithms were able to achieve superhuman performance for image recognition problems in the past few years [8], and they are among the most promising alternative for tackling difficult problems in Natural Language Processing, Image and Video Recognition, Medical Image Analysis, Recommendation Systems and many others. Thus, managing these large arrays in the context of deep learning is a very important task.

The traditional approach for managing data in multidimensional arrays in scientific experiments is to store them using file formats, such as netCDF and HDF5. The use of file formats, and not a database management systems (DBMS), in storing scientific data has been the traditional choice due to the fact that DBMSs are considered inadequate for scientific data management. Even specialized scientific data management systems, such as SciDB [10], are not very well accepted for a myriad of reasons listed in

- the impedance mismatch problem [12,13], that makes the process of ingesting data into a DBMS very slow.
- the inability to directly access data from visualization tools like Paraview Catalyst [14] and indexing facilities like FastQuery [13].
- the Inability to directly access data from custom code, which is necessary for domain specific optimized data analysis.

However, by completely dismissing DBMSs, some nice features also become unavailable. Including the access for out-the-box parallel declarative data processing with the usage of query languages and query optimization, and management of dense and sparse matrices. In this talk, we will present SAVIME, a Database Management System for Simulation Analysis and Visualization in-Memory. SAVIME implements a multi-dimensional array data model and a functional query language. The system is extensible to support data analytics requirements of numerical simulation applications.

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Supported Student:

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SO2 adsorption on Pt: DFT study

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As a result of the increasing demand for energy, reliable and sustainable alternatives for fossil fuels are required. A viable option is the hybrid sulphur cycle (HyS) in which SO2 and H2O are converted into H2SO4, which is subsequently split to give H2 as a fuel source. Platinum (Pt) is currently the most preferred catalyst for the HyS cycle due to its selectivity and durability 1. Despite the high durability of Pt, SO2 poisoning is still a matter of concern due to its inhibition of catalyst activity 2. Lowering of Pt d-bands by SO2 adsorption poses a further problem towards electron availability. Since experimental investigations regarding the HyS-cycle are often time-consuming and significantly environmentally dependent, it is hereby proposed to utilise molecular modelling, in Vienna-Ab-Initio-Simulation-Programming (VASP) with the Centre for High Performance Computing (CHPC) Lengau supercomputer, to investigate the fundamental processes and properties involved in the HyS Cycle 2,3.

Thus far, modelling results have indicated that SO2 is preferentially adsorbed in the fcc Sb,Oa configuration as displayed in Figure 1 2,4. This will be used in further calculations in order to evaluate

different proposed SO2 adsorption mechanisms and reactivity as well as identifying possible intermediates and transition states. VASP will be utilised further to investigate the interaction between SO2 and co-adsorbed compounds on the Pt surface. Electronic properties such as adsorption energy, bond length and bond angle will be investigated by employing VASP in order to identify all species involved in SO2 adsorption process. The influence of other gaseous and adsorbed molecules, such as pre-adsorbed O2, on the SO2 adsorption process, will be compared.

Overall, the study would have not been possible without the use of the CHPC since it would have taken 136 years to complete all the calculations performed for the aforementioned study.

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Supported Student:

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Schrödinger Materials Science Suite

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Computational approaches to establish the relation between chemical composition, material morphology, and macroscopic properties can help in the rational design of more robust, better manufacturable and environmentally friendly materials. Rapid advancements in computer science and computational power have brought about tremendous developments in recent years. Yet the impact of modeling in industrial R&D is somewhat hindered by an unclear connection between calculated and experimental parameters, the complexity of the calculations, and tedious analysis. Towards the resolution of these problems we discuss how a combination of combinatorial chemistry, machine learning, quantum chemistry, classical molecular dynamics and automated calculation workflows provide the basis for rational materials design.

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Security by Design and flaws in IoT Architectures

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Security by Design and flaws in IoT Architectures

The Internet of Things (IoT) has enormous potential, but connecting everything increases vulnerabilities. Ransomware remains one of the most damaging cyber threats facing organizations today, unlike other threats, Ransomware's most goal is to maximize the business and operational pain to the victim enterprise, by freezing its data and ability to function. This makes any organization or industry a potential target of Ransomware. The actual damage and loss of a Ransomware attack are almost always much higher than the cost of the Ransom itself.

Defending against such attacks is a top priority for security teams, This typically includes addressing weaknesses and vulnerabilities that Ransomware use, adding detection and response tools, and establishing data backup and recovery plans. However, the only way to truly prevent Ransomware damage is to stop the attack before assets are affected and damage is done, Vulnerability management plays a critical role in this area. However, vulnerability management has become one of the most challenging task for Cyber Security and IT Teams, who typically have far more vulnerabilities than they could ever hope to patch.

Security by design is becoming crucial in the developing IoT environment, One of the major challenges of IoT security is the fact that security has not traditionally been considered in production design for networking appliances and objects that have not traditionally been networked.
The Workshop will focus on Security Architectures and best practices to reduce Cyber Threats, the workshop will serve also as a great meeting place among Cyber defence experts in HPC seeking solutions to protect critical HPC infrastructures.

The Objective of the Workshop is for attendees to:

- Learn about the potential risks and vulnerabilities associated with IoT systems and connected devices
- Gain an understanding of IoT security best practices and guidelines
- Hear from leading experts and organisations providing guidance and best practices
- Meet companies offering security products, solutions and services

Guest Speakers

- Dr David Johnson
- Dr Kiru Pillay
- Dr Jabu Mtswene
- Mr Simphiwe Mayisela
- Mr Richard Hlalele
- Mr Paul Beyleveld
- Mr Sikhumbuzo Mthombeni
- Mr Len Lotz
- Mr Mvikeli Maninjwa
- Mr Bigani Sehurutshi

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Simplifying Research Data Management with Gobus

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Globus is a non-profit research data management service developed and operated by the University of Chicago and used by research computing centers at hundreds of universities, government agencies, and commercial R&D organizations around the world. In this workshop we will describe and demonstrate Globus capabilities that support data management throughout the research lifecycle. System administrators will learn about installing and configuring Globus endpoints at their institutions, while developers will learn how the Globus APIs provide intuitive access to authentication, authorization, sharing, transfer, and synchronization capabilities. We will use web applications, command line tools, Jupyter notebooks and virtual machines to demonstrate and allow participants to experiment with the service in various forms. We will also provide numerous examples and open source code that you can adapt to realize your own research data portals, science gateways, and other web applications for supporting research data workflows.

We target researchers new to Globus, and system administrators who are responsible for delivering data management services. Some sections are intended primarily for those who develop and maintain research applications and services but will also appeal to those familiar with Globus that wish to develop a deeper understanding.

We assume no prior knowledge of Globus. We provide sufficient background for researchers to use Globus in their daily work, and for system administrators to manage service delivery. Some sections will be of most value to those with an understanding of web application programming and REST APIs, but can still provide a perspective on where Globus can add values for those with little or no software development knowledge.

The workshop comprises presentation and hands-on exercises for new users, and experimentation with deploying Globus on campus systems. We will also review code and allow participants to follow along with Jupyter notebooks.

While it is not required, attendees may benefit from having a laptop with a recent version of a modern web browser (Firefox, Safari, Chrome, Vivaldi). Those attendees that wish to experiment with the Globus API, a working Python environment is required.

Supported Student:

HPC Applications / 37

Smoke and ventilation simulation using the CHPC

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Greenplan Consultants undertook a combined smoke, ventilation and wind study for a basement/underground parking area of approximately 27 000 m^2. This presentation gives an overview of the project and the experience of running it at the CHPC. In order to reduce the size of the transient model, the full domain (about 0.25 km^3) was modelled under steady-state conditions using OpenFoam. The wind flow patterns around the basement were then imposed as boundaries on the transient model of the basement. Even with this approach, the transient model was too large to simulate on a small office network, so high performance computing (HPC) was essential.

Fire Dynamics Simulator (FDS) 6.7.0. was used for the transient simulations. It is purpose-written for simulating fire and smoke, and uses the computationally intensive Large Eddy Simulation (LES) method. The FDS model CHPC requirements were as follows - RAM: ≈ 100 GB; Nodes used: 10-15; Cores used: 240-360; Simulated time per case: ≈ 1-2 min; Wall time per case: ≈ 20-60 hours; Total cells: max. 70-80 million; Cell size: 100 mm; Data output per simulation: 200-250 GB.

FDS can make use of OpenMP (Multi-Processing) and MPI (Message Passing Interface). Tests on the CHPC with OpenMP enabled showed little-to-no improvement, so OpenMP was set to 1 (disabled). An experiment was made whereby all cores per node were booked on PBS but only half were used to run MPI process. This did not give better performance – possibly because of ghost processes running on one or two of the cores. Subsequently, all models were run with 1 MPI process per core, with 24 MPI processes per node. This seemed to be the best option for cost-effective performance.

FDS makes use of manually-specified rectilinear meshes. Unfortunately, where parallel simulation is desired, each MPI process requires at least one mesh, which means the mesh domain must be manually split up into sub-meshes. Any mismatch in mesh size leads to uneven loading on the cores, which means that the less heavily loaded cores have to wait. Due to the rectilinear grid, there are also "wasted" cells in walls/floors/roofs which have no function but contribute to the computational load. Thus, although the initial CSIR scaling tests on the CHPC (6 million cells) were promising for cell counts as low as 30 000 cells per core, scaling tended to be less efficient than expected.

On a number of occasions the simulations progressed at different speeds despite having the same configuration, flow speeds, and boundary conditions. It is possible that this might have been caused by ghost processes on individual cores and the CHPC architecture effect – in particular, the blocking ratio between racks. As an experiment on our final model geometry, we reduced the number of nodes in use from 15 (360 cores) to 10 (240 cores). The cell count per core was a factor of 2.5 higher, the area modelled was larger, and there were more jet fans and extraction fans than in the previous model. Despite this, the CHPC wall time required per unit simulated time increased by a factor of only 2. Rigorous testing is necessary before any conclusions are drawn, as a rough test like this does not provide sufficient data and there might be factors not taken into account. While the above meant that simulations did not run as fast as desired, they ran far faster than they would have on a small office network (it would have taken years, if they ran at all). Greenplan had a good experience with the CHPC and are keen to use it for future projects of this nature.

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Solvation Energies of the Proton in Ammonia

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The absolute solvation energies (free energy and enthalpy) of the proton in solution are of great importance in biological and chemical processes in that solution. The absolute solvation free energy of the proton is used to compute the pKa of organic compounds. Furthermore, these absolute solvation energies are used in the development of continuum solvation models and force fields. They are also used to determine the absolute solvation energies of other ions from experimental data. Despite their importance, the absolute solvation energies of the proton cannot be determined experimentally. In the last century, several methodological approaches have been proposed to determine the absolute solvation energies of the proton in solution [1, 2, 3]. Most of these approaches are based on computational chemistry. Despite these efforts, there is no consensus estimate of the absolute solvation free energy of the proton in the literature. In this work, we calculated the solvation energies of the proton in ammonia using two different approaches. In the first approach, we used hybrid solvation model, where some ammonia molecules (less than 10 explicit molecules) around the proton are treated quantum mechanically and the remaining molecules are considered as dielectric medium. In the second approach, we treated up to 50 explicit ammonia molecules quantum mechanically, and we calculated the solvation energies directly without considering dielectric continuum medium. Considering recent progress in computational resources, 50 ammonia molecules can be treated quantum mechanically. However, this is only possible using HPC facilities. For each isomer, more than 90 hours have been used only for frequecies calculation on an Intel® Xeon® 24 cores, 2.6 GHz and 128 GB memory at CHPC. As a result, the solvation free energy of the proton in ammonia is calculated to be -1205 kcal/mol and -1192 kcal/mol at room temperature using the first and the second approach,

respectively [4, 5]. These values are in good agreement with the solely available estimate of Tutle and coworkers [6].

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SIG Poster / 81

Solving the Schrodinger equation in one and two Dimensions using Sinc functions and employing Python and Numpy.

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The Schrodinger equation in one and two dimensions is solved using Sinc functions, applying the variational principle and employing Python and Numpy. Our goal is to examine how the Sinc function method [1,2] employing the set of functions
$s_i(x) = \frac{1}{\sqrt{h}} \frac{\sin(\pi(\frac{x}{h} - i))}{\pi(\frac{x}{h} - i)}$,
performs with respect to its convergence rate. The Python codes are tested with the quantum harmonic oscillator potential and Morse potential, for which analytical solutions are available. It is found that the method converges quite quickly.
We also demonstrate the speed up achieved by optimizing the Python code via
the unrolling of loops. In addition we also consider the problem of
H_2^+ and what changes to the algorithm are needed and present initial results for this system.

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HPC Applications / 59

Speech data harvesting and factorized deep neural network development for the low-resource indigenous languages of South Africa

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Speech-enabled human-machine interfaces are becoming increasingly prevalent. There is, however, a disparity between the languages these systems are available in and the languages spoken in South Africa. This is because a tremendous effort is required to collect and refine large speech corpora. For the majority of South Africa's languages, very little speech data is available. This creates a challenge

due to the "data hungriness" of automatic speech analysis techniques, specifically those which yield the best performance such as deep learning. Once sufficient initial resources exist, automatic data harvesting strategies can be used to further increase the amount of available data in under-resourced languages. The aim of the work we report on is to improve existing ASR systems for the 11 official languages of the country. These systems are currently based on the recordings of the NCHLT (National Centre for Human Language Technology) corpus, which consists of an estimated 55 hours of speech obtained from 200 speakers for each language. During the NCHLT project additional speech data was collected but not released. To determine whether this additional data is useful, acoustic evaluation of the audio is required to detect both low signal-to-noise ratios (SNRs) and transcription errors. The decoding process with state-of-the-art Deep Neural Network-based models is more than an order of magnitude slower than real time on CHPC's Lengau Dell cluster's processors. It requires more than 10 CPU hours to process one hour of audio data. We therefore used CHPC to run the jobs required for processing one language in parallel. This allowed for approximately 200 hours of auxiliary data to be processed and used less than 50 GB of memory. The harvested data from this process was subsequently used to train factorized time-delay neural networks (TDNN-F). This model architecture was recently shown to yield good results in resource constrained scenarios (less than 100 hours of speech). These models significantly reduced phone error rates for the 11 languages. Each TDNN-F model trained in about 8-12 hours on CHPC's Lengau GPU cluster.

HPC Technology / 159

Stitch It Up: Using Progressive Data Storage to Scale Science

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Generally, scientific simulations load the entire simulation domain into memory because most, if not all, of the data changes with each timestep. This has driven application structures that have, in turn, affected the design of popular IO libraries, such as HDF-5, ADIOS, and NetCDF. All of these libraries assume that each output written will be a complete simulation domain. While a time dimension may be an "unlimited" dimension in NetCDF, the size of an array variable is fixed for the entire file. While for many cases, this assumption makes sense, there is a significant collection of simulations where this approach results in vast swaths of unchanged data written each timestep.

Some prior work has looked at compressing the output by only storing a difference. This reduces data size, but does not reduce the compute requirement. This paper explores a two-pronged approach to addressing the computation and the data sizes. First, an out-of-core-like computational framework is developed enabling simulation across a large domain by only computing over the part that is affected by the simulation. Second, and the primary focus of this paper, is a new IO approach that is capable of stitching together a coherent global view of the total simulation space at any given time. This benefit is achieved with no performance penalty compared to running with the full data set in memory, at a radically smaller process requirement, and a radical data reduction with no loss in fidelity. Additionally, the structures employed offer significant additional capabilities for simulation monitoring and easy data analytics.

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Structural Evolution of LiMn2O4 Nanoporous Cathode Material upon Lithiation

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Voltage and capacity fade of electrode materials encountered during the charge and discharge process of lithium-ion batteries is one of the setbacks in battery development. These in return affects the battery performance and shorten their lifespan. In order to enhance and optimise the battery performance, understanding of the structural changes that occur within the battery during lithiation is crucial. In this study, molecular dynamics simulations using the DL_POLY code were used to investigate the lithiated nanoporous structures with various cell dimensions (75Å, 69 Å and 67 Å) and lithium concentrations (Li1+xMn2O4, $0 \leq x \leq 1$). This was done at atomistic level in a quest to investigate their structural and cell dimension effect during the discharge process. The simulated structures showed efficiently recrystallised materials, which evolved into single and multiple crystals due to lithiation. The captured structural and microstructural snapshots depicted emergence of spinel and layered co-existing in the materials. Furthermore, the microstructures capture crystallographic defects which reduce with increased lithiation. Analysis of X-ray Diffraction patterns further confirms the structural composites nature of the nanoporous structures and further depicted shifting and splitting of peaks, which could be ascribed to phase transitions or change of symmetries. The volume plots depict expansion of the materials as the lithium content increased; however, nanoporous 69 Å at Li1.75Mn2O4 shows a minimal increase, compared to the other structures of 75 and 67 Å. And finally, again the stress-strain curves show more resilience to fracture for nanoporous 69 Å at Li1.75Mn2O4.

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Structural Variation of Nano-Li2MnO3 Cathode Material during Li and O Extraction

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The degradation of Li2MnO3 during cycling has been found to be the limiting factor for its practical use as a high capacity lithium ion battery cathode. Previous studies have insinuated that this degradation was due to complex phenomena within the electrode material, such as the oxygen release, phase transformation and Li+ /H+ exchange reaction encountered during cycling. However, detailed mechanisms governing these degradation behaviors have not yet been fully understood to enable complete diagnosis of the drawback. In the current study, the DL-POLY code is employed in carrying out the simulated synthesis of the charging process by simultaneous removal of lithium and oxygen from Li2-xMnO3-y (x = y = 0.25, 0.50, 0.75 and 1.0) nanoporous structures. This is carried out in a quest to explore the different internal structural transitions that occur within the intermediate phases and their impact on the cycling capabilities of Li2MnO3 cathodes. The concurrent removal of both lithium and oxygen from Li2MnO3 resulted in highly disordered structures which crystallised into multi-grained crystals. Simulated XRD patterns reveal extensive peak broadening at lower angles, emergence of peak at around $2\Theta \sim 29^0$ and strong cubic spinel LiMn2O4 at $2\Theta \sim 38^0$. Microstructural analysis reveal migration of Mn ions into Li layers resulting in the formation of layered (LiMnO2) and cubic spinel-type structures at lower Li/O concentrations. These findings shed light towards mechanisms that take place during the cycling of nanostructured high capacity oxide electrodes during lithium and oxygen extraction that will help guide the optimization of new Li-rich materials for rechargeable lithium batteries.

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Travel & Accom.

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Structural stability of some graphene oxide formations

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The classical molecular dynamics was used to study various forms of graphene oxide possible formations focusing mainly on the structural stability. The structures were modelled at 300 K through the NVT ensemble. Variations of the total energy against the a-axis was explored in which the equilibrium properties were computed. Pair distribution functions as well as structure factors were plotted. In the plots nearest neighbour distances and their neighbouring number of atoms were obtained. To probe the mobility of oxygen in the systems, the mean square displacements as well as the velocity auto-correlations were plotted.

Supported Student:

Travel & Accom.

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Structural stability of the two dimensional white graphene

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The two dimensional white graphene structural and stabilities properties are being investigated using the classical molecular dynamics approach. The formulation uses the NVT Evans ensemble and Tersoff potentials to obtain reliable structural properties. The Verlet leapfrog algorithm is adopted throughout the calculations to integrate the equations of motion. The radial distribution functions and structure factors are used to predict the most probable structural form. Mean square displacement are utilised to study the mobility/motion of boron (B) and nitrogen (N) atoms in the system. Results obtained are compared with the bulk hexagonal boron nitride.

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Studying Tantalum Arsenide (TaAs) bulk properties using Density Functional Theory (DFT)

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Tantalum arsenide is the first Weyl semimetal discovered. It is a nonmagnetic material which has a crystal structure without inversion symmetry and shows linear dispersion around nodes (Weyl points) in its electronic band-structure. The behaviour of Weyl fermions makes TaAs a metal-like compound that shares desirable features with graphene and topological insulators. We have calculated the band-structures of bulk TaAs with and without spin-orbit coupling (SOC), and we showed that when taking into account the SOC, a gap is opening along the path $\Sigma - N - \Sigma_1$ around Fermi level. Through the density of state (DOS) and projected density of state (PDOS) we have also calculated, we showed that Without SOC, orbitals As($2p$) and Ta($4d$) contribute the most in the valance band and the conducting band of the DOS while with SOC orbitals As($2p_{j0.5}$), As($3p_{j1.5}$) and Ta($5d_{j1.5}$), Ta($6d_{j2.5}$) are those contributing the most. The states around the Fermi level are pure states of orbitals d.

Supported Student:

Travel & Accom.

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TBC

HPC Applications / **199**

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Author: Malebogo Ngoepe[None]

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Tapping on the Crucial Role of Asp1116 in Selective Drug Targeting of CREB (cAMP- responsive element binding protein) Implicated in Prostate Cancer

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The selective targeting of CREB-cAMP-responsive element-binding protein (CBP) has recently evolved as a vital therapeutic approach for curtailing its aberrant upregulation associated with the development of prostate cancer. Inhibition of CBP has therefore been discovered to be an important therapeutic option in androgen receptor signalling pathway mediated prostate cancer. Y08197, a novel selective inhibitor of CBP has shown promising therapeutic outcome in prostate carcinogenesis over non-selective analogues, CPI-637. Herein, we used molecular dynamics simulation to gain insights into the mechanistic and selective targeting of Y08197 at the bromodomain active site. Molecular Mechanics/ Poisson-Boltzmann Surface Area (MM/PBSA) analysis revealed similar inhibitory effect between Y08197 and CPI-637. Furthermore, in exploring the selective affinity of Y08197 towards CBP in relative to Bromodomain and PHD finger-containing protein 1(BRPF1), our findings highlighted Asp1116 as the 'culprit' residue responsible for this selective targeting. Upon binding, Asp1116 assumed a conformation that altered the architecture of the bromodomain active site, thereby orienting the helices around the active site in a more compacted position. Interestingly, in addition to some specific structural perturbations mediated by Asp1116 on the dynamics of CBP, our study revealed that the strong hydrogen bond interaction (N-H···O) elicited in CBP-Y08197 sequestered Y08197 tightly into the CBP bromodomain active site. Conclusively, the inhibition and selective pattern of Y08197 can be replicated in future structure-based CBP inhibitors and other bromodomain implicated in carcinogenesis.

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Target-bound/ Tailored Pharmacophore- Virtual Screening (TP-VS) approach in drug discovery: A case study in the treatment of HIV/breast cancer co-infection

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HIV/breast cancer co-infection is a global threat and demands for the discovery and identification of potent inhibitors. The role of Cathepsin D, a prognostic marker in the treatment of breast cancer, has also been identified in HIV infection. Pharmacophore-based virtual screening techniques have proved to be an efficient approach in drug discovery. In this study, we present an approach to further enhance the potency of the conventional pharmacophore-based virtual screening method by incorporating a tailored pharmacophoric approach and per-residue energy contribution footprint from molecular dynamics simulation. Results presented herein confirm that pharmacophore models based on wild and mutant enzymes (bound and unbound drug conformations) significantly change the outcome of the virtual screening. The generated pharmacophore library is based majorly on highly contributing amino acid residues, instead of arbitrary pharmacophores. To the best of our knowledge, this is the first attempt in the literature using such an approach. Thus, we present a model for a per-residue energy decomposition coupled with the tailored-pharmacophoric approach in generating a more trustworthy pharmacophore model, which can be applied in current drug discovery and development machinery. Results presented herein could serve as a beneficial tool to enhance native virtual screening as well as novel drug discovery.

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Ternary alloying additions on Zr78Nb22-xMx (M: Sn, Co and Fe) systems for high temperature cladding purposes.

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Zr based alloys are promising materials for the atomic industry and power engineering ever and are considered of exceptional practical importance. Moreover, Zr alloys are structural material with a wide range of technological applications basically in the nuclear and chemical industries. Recently, advanced Zr-based alloys are aimed for service in more severe operating conditions such as higher burn-up, increased operation temperature, and high-pH operation. Most of these Zr alloys contain Niobium as the major alloying element, which is recommended for developing new fuel cladding materials since it is an effective strengthening element. With the renewed interest in nuclear energy, developing new materials that can respond to the stringent requirements of the next generation fission and future fusion reactors has become a priority. In the quest for developing new alloys, we investigated the effect of ternary additions on Zr78Nb22-xMx (M: Sn, Co, and Fe) systems at high temperatures. The influence of partial substitution of Nb with metal (M) was thus investigated using ab initio DFT calculations on the Zr78Nb22-xMx system, within the plane-wave pseudopotential method as implemented in the CASTEP code. It is seen that the Zr78Nb22-xMx system accommodates at. % M to within 1-2 percentage range. The individual additions of Co, Sn, and Fe appear to be stiff, ductile and isotropic which is favorable for applications at higher temperatures, particularly in nuclear.

DIRISA / **98**

The Capture, Storage and Consumption of the MeerKAT Radio Telescope's Sensor Data

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The Control and Monitoring (CAM) Team at the South African Radio Astronomy Observatory (SARAO) is responsible for implementing software solutions for the collection of sensor data from all of the components, user-supplied equipment and ancillary devices that make up the 64-dish MeerKAT Radio Telescope. Recently, the CAM Team developed and deployed a new solution called KatStore64 which provides services to the MeerKAT Telescope Operators, Astronomers and academia to access the telescope's sensor data.
In order to capture, store and consume all of this data, the CAM Team makes use of the services offered by the Centre for High Performance Computing (CHPC) for long term storage of the data and employs APIs to extract and present the stored data to users.

My poster/talk will illustrate how the CAM Team has built and implemented the KatStore64 service for the storage and retrieval of sensor data for the MeerKAT Radio Telescope.

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The Challenges and Opportunities of the using HPC at the University of Fort Hare

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HPC is a technology that is changing the academic and research landscape of universities. The technology is known to enhance the capacity of universities to do large and complex research, especially that involve complex computation. The University of Fort Hare is one of the first recipients of the first set of Ranger servers from CHPC. The HPC infrastructure, as much as it brings opportunities, there are also challenges in using and managing them. Fort Hare also experienced challenge. From the beginning, setting up the server room was a big challenge because the opportunity of getting the equipment came through personal contacts and there was no plan for its use and management. On the other hand, as complex as the system is, there was only a one week training opportunity offered to the university where one of the Masters student was sent to attend. Unfortunately, the student left the university when he finished his studies and the initiative became inactive. As a result, there was no activity in using the device for some time. However, because of requests from CHPC for reports on the status of the project, a move was made to revive the project. In a bid to involve itself much into using the HPC technology, in 2018 the Computer Science Department, which is the custodian of the server room, introduced an Honours course that is related to HPC. A big publicity campaign was also done by the Department through presentations about the infrastructure and currently the resource is getting much attention from other academic communities of the University. This poster presents the opportunities that HPC equipment presents to the University and the challenges surrounding the use and management of these devices. Other aspects, such as lessons learnt and future directions are also discussed.

Supported Student:

No

SIG Poster / **2**

The Perplexity of Synergistic Duality: Inter-Molecular Mechanisms of Communication in BCR–ABL1

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Background: Aberrant and proliferative expression of the oncogene BCR-ABL in bone marrow cells is one of the prime causes of chronic myeloid leukemia (CML). It has been established that the tyrosine kinase domain of the BCR-ABL protein is a potential therapeutic target for the treatment of CML. Although first and second line inhibitors against the enzyme are available, recent studies have indicated that monotherapeutic resistance has become an aggrieved challenge.
Objective/Methods: In recent studies, the dual inhibition of BCR-ABL by Nilotinib and Asciminib was shown to overcome drug resistance. This prompted us to investigate, with the use of computational tools, the molecular dynamics behind this novel drug combination.
Results: Conformational ensemble analysis presented a sustained inactive protein, as the activation loop, inclusive of the characteristic Tyr257, remained in an open position due to the unassailable binding of Asciminib at the allosteric site. Nilotinib also indicated more propitious binding at the catalytic site in the presence of Asciminib, thus exposing new avenues in treating Nilotinib-resistance. This was in countenance with intermolecular hydrogen bond interactions with key binding site residues GLU399, Asn259 and Thr252.
Conclusion: The investigations carried out in this study give rise to new possibilities in the treatment of resistance in CML, as well as assisting in the design of novel and selective inhibitors as dual anti-cancer drugs.

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The adoption of Deep Learning in Weather Forecast

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Technological development and the internet of things (IoT) increased the data assimilation sources in meteorology through satellites, sensors, weather stations, solar panels, cell phones, traffic lights, to name a few whose number grows daily. This begins to build an ideal scenario for Artificial Intelligence where the demand for data is high. This combined information generates spatio-temporal maps of temperature, rainfall, air movement, etc., with high precision in regions with larger data sources. Applying AI techniques in conjunction with a physical understanding of the environment can substantially improve prediction skill for multiple types of high-impact weather events.

In 2017, the American Meteorological Society (AMS) published a paper 1 with a broad summary indicating how modern AI techniques are helping to improve insights and make decisions in weather prediction. Among the most used techniques are Support Vector Machines (SVM), regression trees, k-means for radar image segmentation and traditional neural networks (ANN). These techniques lack temporal and spatio-temporal analysis, typical of meteorological phenomena. Today, most of the temporal analysis done on meteorological data is through statistical algorithms, such as autoregressive methods. However, the AMS recognizes that the novel Deep Learning techniques could soon be the cause of new improvements and says, “In the future, convolutional neural networks operating in a deep learning framework may reduce the need for feature engineering even further” .

Complementarily, recurrent neural networks, designed for analysis of natural language processing, are known by their results in numerical problems like temperature prediction, among others. In order to improve the temporary forecasts of spatio-temporal phenomena, such as rain and temperature, hybrid architectures have emerged that build the temporary forecast coding the spatial pattern of the neighborhood.

In [7], Shi et al. formulate precipitation nowcasting as a spatio-temporal sequence forecasting problem in which both the input and the prediction target are spatio-temporal sequences. They extend the fully connected LSTM (FC-LSTM) to have convolutional structures in both the input-to-state and state-to-state transitions, they propose the convolutional LSTM (ConvLSTM) and use it to build an end-to-end trainable model for the precipitation nowcasting problem. Experiments show that the ConvLSTM network captures spatio-temporal correlations better and consistently outperforms FC-LSTM and the state-of-the-art operational ROVER algorithm for precipitation nowcasting.

In [8], Souto et al. use a ConvLSTM architecture as a spatio-temporal ensemble approach. The channels in the convolution operator are used to input different physical weather models. In this way the ConvLSTM encodes the spatial information which are subsequently learned by the recurrent structures of the network. The results show that ConvLSTM achieves superior improvements when compared to traditionally used ensemble techniq ues such as BMA [9].

As a matter of fact, there are a plethora of opportunities to be investigated extending the initial results we have achieved in adopting Deep Neural networks to weather prediction. Linear and causal convolution operators (the latter also known as temporal convolution), for instance, have resulted in deep networks architectures that use convolutions to encode and decode time and space with greater precision. Raissi and colleagues [10] investigate the integration of physical laws described as a set of partial differential equations to the training process. By means of such integration, the training process is bound to obey the physical laws, an approach that has been dubbed as model teaching . Another area of interest is multimodal machine learning (MML) [11]. In MML, data from different representations are complementarily used in building models, including: images; textual data; quantitative dataetc... This can be extremely interesting in weather forecast as more data is captured from satellite images and sensors data to weather bulletins and predictive physical models.

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The driving force for the acylation of β-lactam antibiotics by L,D-transpeptidase from Mycobacterium tuberculosis: Molecular Dynamics and Quantum Mechanics/molecular mechanics (QM/MM) study

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The driving force for the acylation of β-lactam antibiotics by L,D-transpeptidase from Mycobacterium tuberculosis: Molecular dynamics and Quantum mechanics/molecular mechanics (QM/MM) study

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Abstract
β-lactam antibiotics, which are used to treat infectious diseases (tuberculosis), are currently the most effective class of antibiotics. This study focused on the chemical reactivity of five- and six-membered ring systems attached to the β-lactam ring. A partially constrained Molecular dynamics for 20 ns was performed on the precomplex system. The last snapshots from the final 5 ns were used as starting structures for the unconstrained ONIOM TS calculations. The ring strain energy (RSE), force constant (FC) of amide (C—N), acylation transition states and second-order perturbation stabilization energies of 13 basic structural units of β-lactam derivatives were computed using the M06-2X and G3/B3LYP multistep method. In the ring strain calculations, an isodesmic reaction scheme was used to obtain the total energies. RSE is relatively greater in the five-(1a-2c) compared to the six-membered ring systems except for 4b, which gives a RSE that is comparable to five-membered ring lactams. These variations were also observed in the calculated inter-atomic amide bond distances (C—N), which is why the six-membered ring lactams C—N bond are more rigid than those with five-membered ring lactams. The calculated ΔG# values from the acylation reaction of the lactams (involving the S—H group of the cysteine active residue from L,D transpeptidase 2) revealed a faster rate of C—N cleavage in the five-membered ring lactams especially in the 1-2 derivative (17.58 kcal mol-1). This observation is also reflected in the calculated amide bond force constant (1.26 mDyn/A) indicating a weaker bond strength, suggesting that electronic factors (delocalization) play more role on reactivity β-lactam ring, than ring strain.
The Centre for high Performance computing (CHPC, www.chpc.ac.za) provided the computational resources (CPUs) for this work. Drawing allocation from CHEM0808 workspace (Lustre file system) on Lengau Cluster. The Gaussian09 (D01) program was used to execute the jobs. 24 cores, 1node and 48:00 hours wall time were used. Also, AMBER 14 was used for the MD studies with mpirun -np 72 -machinefile, walltime=48:00hours and ncpus=24

Keywords: β-lactam antibiotics; Transition state (TS); Ring strain energy (RSE); Force constant (FC), Activation energy.

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The identification of new plasmodium falciparum phosphatidylinositol 4-kinase (PfPI4K) inhibitors using Computer-aided drug design approaches.

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The impact of the solvent media and substituents on the energy band-gap and redox potential of hydroxybenzophenone (HBP) using both experimental and computational methods

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The interest of this research is to study the electrochemical properties, energy band-gap and stability of five derivatives of hydroxybenzophenone (HBP). Hydroxybenzophenone derivatives are important compounds that are being used as chromophore in sunshades to protect the human skin from sunburn and are known to be photostable with little to no formation of a photoreactive radical that can penetrate the body to cause DNA damage. HBP are also organic pi–conjugated molecules that can demonstrate a good charge transport and/or electroluminescent properties in their application as organic semiconductors (OSCs).
The aim is to gain insights into the energy band-gap, current peaks and the redox potential of the five derivatives of HBP in different solvent media using both experimental and computational methods. The five derivatives was selected to span the range of those with strong electron withdrawing substituents to those with strongly electron donating substituents. This study will give more insight into their light absorption, photocarrier properties and will also help in their rational design approaches to improve their efficiency as OSCs.
The band gap energy of organic pi-conjugated materials is very important for their application in organic and hybrid electronic devices such as organic light emitting diodes (OLEDs), organic photovoltaic cells (OPVs) and organic field-effect transistors (OFETs). Besides corroborative information that will be gathered from computational approach, it will also helps to gain insight into the preferred type of isomeric form that the derivatives are prone to assume in different solvent media as shown in Scheme 1.

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The research benefits of improving equity, diversity and inclusion

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Equity, diversity and inclusion seem to be the magic words of the 21st Century. We've all been told they are important, but for many, it is nice-to-have but difficult-to-implement. As there is an increasing shortage of highly skilled technology specialists and an increasingly large array of applications, it has never been more important to implement workable equity, diversity and inclusion practices to ensure that we can attract and retain talent

This session will discuss the benefits of diversity and what we all need to be doing to ensure our community benefits. Discussions will include the work being carried out by Women in High Performance Computing to diversify the international supercomputing community and what the African HPC community can learn from this.

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The thermodynamic phase transitions in Ti17 metal nanocluster: A molecular dynamics study

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Titanium clusters are one of the central theme in cluster science to investigate the evolution of the electronic, structural and magnetic properties of the metal clusters as a function of cluster size. Nanoclusters provide a nice prototype to investigate and understand the thermodynamics of finite systems. Small nanoclusters exhibit physical and chemical properties that are often different from the bulk phase. In particular, the titanium metal clusters have been shown to strongly dependent on their internal clusters energy which dictates the geometrical arrangement and growth patterns. In this study, classical molecular dynamics simulation software (DL_POLY), on normal queue, using 8 notes and 24:00 walltime was used to investigate the temperature effects on pure Ti17 metal nanocluster. The dynamical properties were interrogated by subjecting the nanoclusters to various temperatures in the range of 300 – 2400 K. The radial distribution functions, density profiles and potential energies were examined to study the structural changes as a function of temperature. It was found that the vacuum structures undergo several transitions as a function of temperature. The phase transition from solid to liquid has been identified by a simple jump in the total potential energy curve. Furthermore, the RDF's peaks decrease as the temperature is increased and the potential energy smoothly increases with temperature. These observations are important in the production of titanium metal and development of titanium metal components for industrial and aerospace applications

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Theoretical Model for HIV-1 PR That Accounts for Substrate Recognition and Preferential Cleavage of Natural Substrates

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The Human Immunodeficiency Virus type 1 (HIV-1) protease is a crucial target for HIV/AIDS treatment and understanding its catalytic mechanism is the basis on which HIV-1 enzyme inhibitors are developed. Several experimental studies have indicated that HIV-1 protease facilitates the cleavage of the Gag and Gag-Pol polyproteins and it is highly selective with regards to the cleaved amino acid precursors and physical parameters. However, the main theoretical principles of substrate specificity and recognition remain poorly understood theoretically. By means of a one-step concerted transition state modeling, the recognition of natural substrates by HIV-1 PR subtypes (B and C-SA) was studied. This was carried out to compare the activation free energies at varying peptide bond regions (scissile and non-scissile) within the polypeptide sequence using ONIOM calculations.
The computational resources (CPUs/GPUs) used in this research were provided by CHPC under project name: HEAL0839 workspace (lustre file system) on lengau cluster. The Gaussian 09 and Amber 18 were the two software programs utilized on the cluster to execute the project, using 24 cores, 1 node and 48 hours wall time.

We studied both P3-P3' and P5-P5' natural substrate systems. For P3-P3' substrates, excellent recognition was observed for the MA-CA family but not for the RH-IN substrates. Satisfactory recognition for the latter was only observed for the longer sequence (P5-P5') after the substrate was subjected to an MD run to maximise the interaction between the enzyme and the substrate. These results indicate that both sequence and structure are important for correct scissile bond recognition of these natural substrates.

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Theoretical infrared Spectrum of the Ethanol Hexamer

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Experimental infrared spectrum of a sample is used to characterize different compounds that are present in the sample. Two different compounds will always have different infrared spectra. For a compound with several isomers, the experimental spectrum will be a combination of the spectra of different possible isomers. It is not possible to determine these possible isomers experimentally. Using computational chemistry, one can locate these isomers and compute their theoretical infrared spectra. Combining the theoretical and the experimental spectra, one can then be able to identify different isomers that can contribute to the experimental sample. In this work, we applied this procedure to determine the structures of the ethanol hexamer that could contribute to the population of the cluster. We started by sampling different isomers which have been optimized at the APFD/6-31++G(d,p) level of theory. 139 different isomers have been located 1. From the 139 APFD optimized isomers, we selected 98 for further optimization at the MP2/aug-cc-pVDZ level of theory for the accuracy of the results. Frequencies calculation for all the isomers is performed at the MP2/aug-cc-pVDZ level of theory. For one isomer, about 70 hours have been used on an Intel® Xeon® 24 cores, 2.6 GHz and 128 GB memory at CHPC to compute the frequencies and their intensities. The computed frequencies, as well as their intensities, are used to produce the theoretical spectra of the isomers. Then we used the infrared spectra of these possible isomers weighted by their canonical probability to produce a unique theoretic infrared spectrum of the ethanol hexamer using Voigt profiles [2]. The computed theoretical spectrum is in qualitative agreement with the experimental spectrum of the ethanol hexamer [3].

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Tuning and optimisation of parallel programs on the CHPC's Lengau cluster

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This session will cover various aspects of analysing and optimising parallel programs to achieve optimum performance on the supercomputer. Tuning and Analysis Utilities (TAU) callgraph visualization system will be used to demonstrate the performance of different objects (e.g. modules, routines and functions) within parallel applications. Moreover, scaling of parallel programs running on the CHPC's Lengau cluster will be examined and presented accordingly.

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Tuning the electronic properties and interfacial interactions of WS2/ZrO2(001) heterostructures by an external electric field, interlayer coupling and monolayer to few–layer of WS2 sheets

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Understanding the connection between interfacial interactions and electronic properties are vital for the fabrication of ZrO2–based optoelectronic and nanoelectronics materials with desirable properties. In this study, the interfacial interactions, optical and electronic properties of WS2/ZrO2 heterostructures in the presence of an external electric field, interlayer coupling and monolayer to few–layer WS2 sheets are investigated for the first time using a first–principle calculations. All calculations were performed using the Cambridge Serial Total Energy Package (CASTEP) code 1 implemented in Materials Studio 2016 [2] with the plane-wave ultrasoft pseudopotentials method [3] and Perdew-Burke-Ernzerhof (PBE) functional for the exchange and correlation contribution [4]. All the simulations were done using the resources provided by the Centre for High Performance Computing (CHPC), Rosebank, Cape Town [5]. The charge density distribution and Mulliken population charge analysis reveal that the charge carriers can effectively separate in the layered WS2/ZrO2 interface. The optical absorption spectra and band shape of these hybrid heterostructures are similar, with their bandgap decreases, as well as their charge transfer and redshift of the absorption edge increase upon increasing the number of WS2 sheets. Moreover, by varying the interlayer coupling or by applying a suitable external electric field with different strengths, the cohesion energy, work function and bandgap energy of WS2/ZrO2 heterostructure can be effectively tuned. These theoretical results are expected to offer useful insights into the design of future optoelectronic and nanoelectronic devices based on two–dimensional van der Waals heterostructures.

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Tuning the electronic, optical and structural properties of two-dimensional C2N/GaS van der Waals heterostructure in a photovoltaic cell: First-Principle Calculations

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The two-dimensional materials have drawn a lot of attention due to their wide applications in the photovoltaic cell and photocatalysis. In this computational study, carbon-nitrogen (C2N) sheet with gallium sulphide (GaS) monolayer is studied as C2N/GaS heterostructure for photovoltaic performance. The calculations of this study are performed by means of plane-wave density functional theory (DFT) method as implemented in the Cambridge Serial Total Energy Package (CASTEP) code of Material Studio 2016 with the pseudopotentials method and Perdew-Burke-Ernzerhof (PBE) functional encountering for the exchange and correlation of the heterostructure. In this study, the GaS monolayer is coupled on top of C2N sheet for improvement of absorption of C2N sheet.

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Updating the Outdated Storage Paradigm to Handle Complex Computational Workloads

Accelerating discovery in computational science and high performance computing environments requires compute, network and storage to keep pace with technological innovations. Within a single organization, interdepartmental and multi-site sharing of assets has become more and more crucial to success. Furthermore, as the growth of data is constantly expanding, storage workflows are exceeding the capabilities of the traditional filesystem. For most organizations, facing the challenge of managing terabytes, petabytes and even exabytes of archive data for the first time can force the redesign of their entire storage strategy and infrastructure. Increasing scale, level of collaboration and diversity of workflows are driving users toward a new model for data storage.

In the past, data storage usage was defined by the technology leveraged to protect data using a pyramid structure, with the top of the pyramid designated for SSD to store 'hot' data,' SATA HDDs used to store 'warm' data and tape used for the bottom of the pyramid to archive 'cold' data. Today, modern data centers have moved to a new two-tier storage architecture that replaces the aging pyramid model. The new two-tier paradigm focuses on the actual usage of data, rather than the technology on which it resides. The new two-tier paradigm combines a project tier that is file-based and a second or perpetual tier which is object based. The object based perpetual tier includes multiple storage media types, multi-site replication (sharing), cloud, and data management workflows. Data moves seamlessly between the two tiers as data is manipulated, analyzed, shared and protected – essentially creating yin and yang between the two storage tiers. Solutions designed to natively use the Perpetual Tier empower organizations to fully leverage their primary storage investments by reducing the overall strain on the Primary Tier, while at the same time, enabling data centers to realize numerous benefits of the Perpetual Tier that only increase as the amount of storage to manage increases.

The next logical question is how to manage data between the two tiers while maintaining user access and lowering overall administration burdens. Join us for a deeper look into the nuances of the two-tier system and data management between them. We will cover storage management software options; cloud vs. on-premise decisions; and using object storage to expand data access and create a highly effective storage architecture to break through data lifecycle management barriers

Supported Student:

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Use of high-throughput sequencing to uncover resistance mechanisms in sugarcane

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The sugarcane industry is an important agricultural activity in South Africa generating an annual estimated average direct income of R14 billion. Economic loss due to Eldana saccharina (eldana), a lepidopteran stem-borer, is estimated to be R1 billion per annum. Commercial sugarcane cultivars (Saccharum spp. hybrids), have different susceptibility ratings to eldana, varying from low to high risk of sustaining economically damaging infestations. The South African Sugarcane Research Institute has utilised the resources of the Centre for High Performance Computing in an approach involving high-throughput RNA sequencing (RNA-seq) to identify early and late response genes that are differentially expressed in two sugarcane cultivars possessing contrasting resistance phenotypes when challenged with eldana herbivory. The results will be used to identify molecular mechanisms

involved in the successful defence response and identify candidate genes which are most likely to be useful in breeding for resistance to eldana.

HPC content:
Annotation and assembly is a computationally intensive process that requires considerable CPU time and effort. Various bioinformatic tools were used for the de novo transcriptome assembly and the differential expression analyses required in this project.

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Using PBSPro on Lengau

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The primary task of the PBS scheduler is to allocate computing resources to a computational task (job). We have noticed that our new users and some of the old users are struggling to use this important tool properly.

This workshop is intended to help users to understand PBS and to promote better usage of Lengau. The following will be discussed:-

- PBS Policies that are implemented on the system.
- Mistakes done by users PBS.
- Options and variables available.
- Challanges we are experiencing with some of the jobs.
- Explain the role of PIs on allocation manager.
- We will also allow users to ask questions.

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Using Site Occupation Disorder and Surface Energies to Determine Pt3Pd2 and Pt2Pd3 Electrocatalyst Models

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A potential means of energy production is the hybrid sulphur (HyS) cycle 1. The HyS cycle is a two-step water-splitting process, which is used to produce hydrogen, with no harmful by-products that are typically produced from hydrocarbon fuels. The HyS cycle oxidises aqueous SO2 to produce

hydrogen and H2SO4, with the H2SO4, then thermally decomposed back to SO2. The oxidation can be promoted by use of an electrocatalyst, typically a platinum catalyst.[2] Research are conducted at North-West University [3] to improve these electrocatalysts, by developing multi-metal thin film catalysts. The best preforming catalysts were Pt3Pd2 and Pt2Pd3, which had the same performance as the standard platinum catalyst, but had increased stability, chemical resistance. Thus in order to understand the surface properties of these catalysts, computational models of these catalysts were constructed using Sutton-Chen interatomic potentials. The program, Site-Occupation Disorder (SOD),[4] was used to prepare all possible bulk combinations of Pt3Pd2 and Pt2Pd3 catalysts, and the configurations were optimised using General Utility Lattice Program (GULP).[5] Each catalyst had 101 possible combinations, however at a thermal annealing temperature of 800℃ [6] all combinations were possible and had to be taken into account. Thus to find optimum configurations, surface energies were calculated, using the two-region method, for 101 configurations of both catalysts. The bulks were cut to expose the (111) surfaces using the program METADISE [7] (minimum energy techniques applied to dislocation interface and surface energies). Figure 1 shows the calculated surface energies for both Pt3Pd2 and Pt2Pd3 catalysts. The surface energies of Pt3Pd2 catalyst indicated that one configuration, namely configuration 3, had a notably lower surface energy (0.817 J.m-2) than the rest. The Pt2Pd3 system had three configurations with lower than average energy, namely configurations 17, 81 and 8 with energies calculated at 0.887 J.m-2, 0.888 J.m- 2 and 0.889 J.m-2 respectively. These configurations will be used in future studies as the representative surfaces of these catalysts. This study was made possible thanks to the computational resources obtained from the Centre for High Performance Computing (CHPC), which provided both hardware and software used in this study.

a)
b)
Figure 1: Surface energies for the 101 configurations of the (a) Pt3Pd2 and (b) Pt2Pd3 catalysts

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Vinyl and phenyl halide's dissociation on Pd(111)

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Carbon-coupling reactions, such as the Suzuki and Stille reactions, play a vital role in pharmaceutical synthesis (1). Usually, these synthesis reactions make use of homogeneous Pd catalysts, which often end up in the product mixture. This is undesirable given the stringent regulatory limits on the

concentration of Pd in pharmaceuticals (2). Although there are means to separate homogeneous catalysts from product mixtures, such as nano-filtration, they are expensive and often destroy the catalysts. This has been prompting research into the development of heterogeneous Pd catalysts, such as nanoparticles, for carbon-coupling reactions.

During the last three decades, uncertainty has risen on whether Pd nanoparticle surfaces are active catalytic sites for carbon-coupling reactions (3). Some argue that molecular Pd species are leached from the Pd surfaces, and act as the active catalysts instead. This uncertainty regarding the true mechanistic nature of these catalysts has hampered this area of research. Our work focuses on modelling heterogeneous mechanism of common Pd catalysed carbon-coupling reactions using density functional theory. By modelling the mechanisms for heterogeneous Pd catalysts, and comparing our results to the known mechanism of homogeneous Pd-containing catalysts, we hope to shed light on the mechanistic nature of some of these proposed Pd catalysts.

We would like to present work at the CHPC National meeting 2019 which illustrates that vinyl and phenyl halides adsorb and then readily dissociation on Pd(111) form stable adsorbed species. Although these results pertain only to carbon-halide cleavage (i.e. the first stage in a carbon-coupling reaction), they illustrate that Pd nanoparticle surfaces have a role to play in the heterogeneous catalysis of the Suzuki and Stille reactions. Using the Vienna ab initio simulation package (VASP) (4-6), we found that chemisorption of vinyl and phenyl halides cause weakening of the carbon-halide bonds. According to our modelling of the dissociation reactions, using the nudged-elastic band method, the dissociation of vinyl and phenyl iodides has the lowest activation energy, followed by vinyl and phenyl bromide, then vinyl and phenyl chlorides.
We did some of these calculations using the CHPC's Lengau cluster, typically using two to three nodes for geometry optimization and single-point energy calculations, while using six to ten nodes for the nudged elastic band calculations. We also made use of the Supercomputing Facilities at Cardiff University (Advanced Research Computing @ Cardiff, ARCCA) in Wales.

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Supported Student:

Accommodation Only

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Weather and Climate Modelling

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In this SIG seminar a number of presentations focusing on weather and climate modelling will be made. Areas of discussion include modelling from first principles, machine learning and the use of HPC hybrid architectures, especially GPUs. The seminar will showcase work done in Brazil, Russia, and South Africa. The SIG seminar also supports the Climate Research for Development (CR4D) fellowship aimed at improving weather and climate early warning systems over southern Africa through the improvement of numerical weather and climate models. Work done by meteorological services in six SADC countries will be discussed; this work supports the implementation of the SADC Cyber-Infrastructure Framework.

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Women in High Performance Computing in South Africa

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Women in HPC BoF proposal is attached.

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Workshop: Receptor based virtual screening, molecular docking and molecular dynamics to explore promising molecules

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Virtual screen of small molecular databases is a pivotal computational drug discovery approach. This tutorial aim for the reduction of chemical space of large number of molecules available in public and private databases through freely available molecular docking tools. Finally, there will also be exploration of dynamic behaviour of protein-ligand complexes through molecular dynamics simulation using Gromacs.

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iRODS

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Description:
iRODS core competencies, capabilities, patterns and use cases. iRODs demonstration using metalnx, webdav and nfsrods

The iRODS workshop details are as follows:

- **Introduction to iRODS**
- Core Competencies
- Capabilities
- Deployment Patterns
- Use Cases
- **Resource Composition**
- **Automated Ingest**
- **Storage Tiering**
- **Interface demonstration**
- Metalnx web interface
- WebDAV
- NFS

Lecturer:
Jason Coposky, Renaisasnce Computing Institute.

Target Audience:
Technical and non technical.The workshop will not include hands on practicals, instead it will showcase the capabilities of iRODS.

Supported Student:

SIG Poster / 146

ng Against Tuberculosis Drug Resistance: Dual target Extirpation through a "Double-Edged" Antifolate Derivative

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Despite the availability of clinically approved drugs and the incessant flurry of innovative research techniques, tuberculosis has escalated to the leading cause of death in its category, worldwide. The increasing prevalence of multidrug and extensively drug-resistant tuberculosis strains, due to target-specific inhibitors, have created an imperative need for new antibiotics that can overcome bacterial resistance and still maintain efficiency. In recent years, multi-target modulation or, "polypharmacology", has been a focal point in drug discovery. Polypharmacology is broadly defined as the affinity of a variety of biological targets toward a single "master-key" molecule. One of the key beneficial outcomes of multi-facetted inhibitors against bacteria, such as Mycobacterium tuberculosis, is its ability to overcome resistance by inhibiting an alternate target within the network of metabolic pathways. A recent study elucidated on one such antifolate derivative, which demonstrated inhibitory characteristics against DHFR and RV2671 within the folate pathway. However, a clear understanding of UCP1172's structural mechanism of action and molecular characteristics allowing for inhibition of the enzymatic dyad was not established. In this study, we conducted predictive pharmacokinetic

profiling of UCP1172, as well as demonstrated a comparative structural mechanism of inhibition against the above-mentioned enzymes. It was evident from the pharmacokinetic analysis that the molecular characteristics of UCP1172, including its increased lipophilicity permitted increased GIT absorption. Predictive analysis also exposed UCP1172 as an antagonist against drug-metabolizing enzymes CYP3A4 and P-gp, thus extrapolating an enhanced biological half-life of the compound. Subsequent to molecular dynamic simulations, free-energy analysis and molecular interaction plots of the enzyme complexes revealed distinct similarity in the energy contribution of UCP1172 to both enzymes, with increased enzymatic contribution from RV2671. Catalytic residues (Serine, Threonine and Aspartate), common to both enzymes, also participated in key molecular interactions with UCP1172. This indicated a common molecular mechanism of inhibition of enzymatic dyad. By elucidating on the structural and molecular mechanism of UCP1172's inhibitory characteristics, inhibiting folate production and combating drug resistance can be sustained in tuberculosis therapy. This study could also act as a model in the design of effective polypharmacological inhibitors against drug-resistant diseases.