Course	**Computational Modelling**
Code	**SCS 2209**
Lecturer	**S.M Nleya**
Year	**2023**
Office	**AG 15**
Email	**sindiso.nleya@nust.ac.zw**
Venue	**Part 2 Lab**
Lectures	**Wednesday: 1300-1500hrs** **Tuesday: 1300-1500Hrs**
Phone	**Ext 2208**

Course Objective (S)

Computational modelling is emerging as a "third pillar" of science and engineering alongside theory and experimentation. Computer simulations bridge between theory and experiment, generating hypotheses, forecasts and predictions about real-world systems. This reduces the number of experiments that need to be carried out in the real world and the number of design prototypes that have to be built, thereby reducing cost, encouraging innovation, optimising system design and enabling the study of systems for which experimental work is infeasible (for example due to prohibitive cost or risk of endangering lives, the environment, etc). As a consequence of this increasingly key role, computational modelling is now recognised as a priority

area by industry, government and academia. To this end, the course aims to introduce some principles of computational scientific modelling in the
wider scientific domain. A range of modelling approaches, numerical algorithms and the generic concepts of computer programming will be introduced. Students will also develop practical modelling skills through the study of a range of examples using the common computational framework such as MATLAB/PYTHON.

Synopsis

Introduction to computational modelling. Modelling methodologies. Modelling software tools. Data modelling, fitting curves and distribution to data. Pseudo code extraction. Stochastic and deterministic simulation. Algebraic application in modelling software tools.

Topics

1.Overview of Computational Science

2. Modeling Process

3.Software tools in Modelling

4.Data-Driven computational Modelling

5. Deterministic Modelling and simulation

6. Stochastic Modelling and simulation

7.Next Generation Computational modelling

Suggested Sources

- A FIRST COURSE IN DIFFERENTIAL EQUATIONS with Modeling Applications- (by Frank R. Gio
- **Introduction to Computational Science:Modeling and Simulation for the**

Sciences (Second Edition) Angela B. Shiflet and George W. Shiflet Wofford College © 2014 by Princeton University Press

- **Understanding Molecular Simulation(Second Edition):From Algorithms to Applications** *Author(s):**Daan Frenkel and Berend Smit***

Assessment

Students should expect assignments (theory and practicals) and tests that will monitor their progress in the course

Assessment	Dates	Points
Group and individual Assignments	TBA	40
Test1	TBA	30
Test 2	TBA	30
Total		100