

# Theoretical & Computational Biophysics

**Facilitators:** *Mathebula Dephney (UNISA), Moila Mercy (UL), [Rendani Netshikweta](#) (UNIVEN)*

**Supervisor:** *Azwinndini Muronga (NMU)*

Theoretical and Computational biophysics is an emerging scientific field that applies the theories and computational and mathematical methods of physics to understand how biological systems such as the mechanics of how the molecules of life are made, how different parts of a cell move and function, and how complex systems in our bodies such as the brain, circulation, immune system, and others function.

In theoretical and computational biophysics, scientists from many fields including mathematics, chemistry, physics, statistics, computing sciences, engineering, pharmacology, and materials sciences, use their skills to explore and develop new tools for understanding how biology or all life works. Physical scientists use mathematics to explain what happens in nature. Life scientists want to understand how biological systems work. These systems include molecules, cells, organisms, and ecosystems that are very complex.

Biological research in the 21st century involves experiments that produce huge amounts of data. Analysing such big data will require mathematical and computational skills. Training in the quantitative sciences of physics, mathematics, and chemistry is necessary to tackle a wide range of topics, ranging from how nerve cells communicate, to how plant cells capture light and transform it into energy, to how changes in the DNA of healthy cells can trigger their transformation into cancer cells, to so many other biological problems.

In this field, you will be introduced to some of the following topics:

- (i) Mathematical and Computational modelling of infectious disease epidemiology (such as COVID-19), integrating deterministic and stochastic models and methods.
- (ii) Translation of biological assumptions into mathematics to construct useful and consistent models.
- (iii) Using biological interpretation and mathematical reasoning to analyse these models.
- (iv) Relating models to data through statistical inference, and how to gain important insights into infectious disease dynamics by translating mathematical results back to biology.
- (v) The use numerical algorithms to study the physical principles underlying biological phenomena and processes.
- (vi) Using Geant4 Monte Carlo radiation transport to simulate the interaction of biological systems with radiation. This has been used in high energy physics, nuclear physics, astrophysics, and medical physics research.
- (vii) Machine learning and artificial intelligence for solving biological/immunological problems. We will emphasize artificial neural network (ANN) based methods for artificial intelligence.
- (viii) Ecosystems and population dynamics
- (ix) Bioinformatics