**Code** SCS 2209 **Course** Computational Modelling

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**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.

**Course Aim**

The aim of this course is to equip students with the skills needed to model and simulate complex systems, communicate results effectively, and contribute to advancements in computational science.

**Course Objectives**

Students should be able to:

1. To understand the fundamental principles and concepts of computational modelling.
2. To explore various modelling methodologies used in computational modelling.
3. To tackle and understand complex physical problems using mathematical models and simulations.
4. To work with both numerical and non-numerical algorithms to create mathematical representations of real-world systems and implement them on computers.
5. To develop technical communication skills by creating comprehensive reports and oral presentations, in which they incorporate accurate visual representations of models and their results.
6. To understand and explore the role and importance of modelling in science and engineering.
7. To verify and validate computational models.
8. To understand concepts of Data-Driven Modelling through integrating empirical data with mathematical models using techniques from machine learning and statistical analysis.
9. To explore both deterministic (precise rules) and stochastic (randomness and uncertainty) modelling approaches and their areas of application
10. To gain insights into innovations like quantum computing, improved algorithms, and handling massive datasets.
11. To explore the application of algebraic concepts within modelling software tools to solve modelling problems effectively.
12. To learn techniques for extracting pseudo code from mathematical models for implementation in computational simulations.
13. To develop skills in data modelling, including curve fitting and distribution fitting to empirical data.
14. Gain proficiency in using modelling software tools for creating and analysing models.

**COURSE CONTENT**

1. **Overview of Computational Science**

Definitions of a model, computational modelling, Computational modelling versus Mathematical modelling, Model Classifications (static model, continuous model, ), Where models are used, Why model (Purposes of Modelling - Prediction or forecasting, Explanation or exploration of future scenarios, Understanding theory or designs, Illustration or visualisation, Analogy). Noise, Challenges in Computational Modelling, Future of modelling

1. **Types of Models**

Non-deterministic models, Static models, Dynamic models, Discrete models, Continuous models, Individual-based models, Population models, Logic models, Automata and process algebraic models, Black-box models etc.

1. Modelling Process

Steps of the Modelling Process such as Analyse the problem, Formulate a model, Solve the model, Verify and interpret the model’s solution, Report on the model, Maintain the model.

* Model Validation and Model Verification, documentation, Quality assurance, Uncertainty, Communicating a model, Preserving a model, Ensemble modelling, the Role of data in modelling

1. Population models (Exponential growth and decay population models, population model with carrying capacity, Predator-Prey Models)
2. Modelling using Random Numbers (Monte Carlo Modelling)

Definition of Monte Carlo Method, Importance and Applications across Different Fields, Importance of randomness in simulations, Monte Carlo Simulation Process, Applications of Monte Carlo Modelling (Finance, Engineering, Science and Project Management), Advantages and Limitations

1. Software tools in Modelling

Categories of Computational Modelling Software, 3. Key Features of Computational Modelling Tools, Emerging Trends in Computational Modelling Software

1. Data-Driven computational Modelling

Definition of Data-Driven Modelling, Importance of Data in Modern Computational Modelling, outliers, noise, cross validation, Goodness-of-Fit Tests (Root Mean Square Error (RMSE)), Validation Metrics (accuracy, precision, recall, and F1 score)

1. Deterministic Modelling and simulation

Definition of Deterministic Models, Importance and Applications in Various Fields, Types of Deterministic Models (Algebraic equations, Differential equations, Linear and non-linear models), Applications of Deterministic Modelling and Simulation (Engineering, Operations Research, Environmental Science, and Economics:

1. Stochastic Modelling and simulation

Definition of Stochastic Models, Differences between Deterministic and Stochastic Models, Importance and Applications in Various Fields, Characteristics of Stochastic Models (Randomness, Probabilistic Outputs and Dynamic Nature), Types of Stochastic Models (Markov Processes and Random Walks), Applications of Stochastic Modelling and Simulation (Finance, Operations Research, Insurance and Healthcare), Advantages and Limitations

1. Solving optimisation problems using computational models

Definition of Optimisation. Importance of Optimisation, Linear Optimisation, Applications of Computational Modelling in Optimisation

1. Next Generation Computational modelling

Definition, Overview of the Evolution of Computational Modelling, Key Drivers of Next-Generation Computational Modelling (such as Advancements in Computational Power, Big Data and Data Analytics, Artificial Intelligence and Machine Learning and Interdisciplinary Approaches), Applications of Next-Generation Computational Modelling (Climate Modelling, Healthcare and Epidemiology, Engineering Design, Smart Cities and Urban Planning), Challenges and Considerations, Tools and Technologies for Next-Generation Computational Modelling

**7.0 ASSESSMENT**

Assessment comprises continuous assessment and examination, that is, one assignment, 1 group presentation and 1 group mini project and 3-hour end of semester examination. Continuous assessment to examination ratio will be 40:60%.

**Suggested Sources**

● A FIRST COURSE IN DIFFERENTIAL EQUATIONS with Modelling 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