MS4671 – Introduction to Materials Simulation

Course Code	MS4671					
Course Title	Introduction to Materials Simulation					
Pre-requisites	MS1008	Introduction to Computational Thinking				
	MS0003	Introduction to Data Science and Artificial Intelligence				
Pre-requisite for	NIL					
No of AUs	3					
Contact Hours	Lectures	26	Tutorials	13		

Course Aims

The aim of this course is to introduce to year-4 students some of the most important computational modelling techniques for materials simulation, such as continuum methods, atomistic and molecular simulation methods, quantum mechanics methods, and machine learning techniques that includes artificial neural networks.

Students will gain insights into fundamental, theoretical, and numerical aspects of materials simulation through examples and exercises, appreciate the utility of computational modelling as an essential aid to uncover the underlying physics of experimental studies.

Intended Learning Outcomes (ILO)

By the end of this course, you (as a student) would be able to:

1. Identify the utility of computational modelling as an essential aid to uncover the underlying physics of experimental studies.
2. Explain various techniques of computational modelling of materials.
3. Differentiate between the usage of the continuum Finite Element Method, the atomistic Molecular Dynamics simulation method, and the ab-Initio Density Functional Theory method.
4. Explain the fundamentals of quantum physics and their applications to nanoscale materials.
5. Explain different machine learning techniques and their applications to materials datasets.
6. Identify the utility of Design of Experiments and demonstrate the advantages of using machine learning based optimization to accelerated process development and achieve targets.

Reading and References

There is no single textbook for the course. The following books and resources will be used as references and if necessary, notes will be provided.

The Practice of Computing Using Python: W. Punch and R. Enbody (3rd edition, Pearson).

Principles of Quantum Mechanics: R. Shankar (2nd Edition, Plenum Press).

Applied Finite Element Analysis: L. J. Segerlind (2nd Edition, Wiley).

Electronic Structure: Basic Theory & Practical Methods: R. M. Martin (Cambridge Univ Press).

An Introduction to Machine Learning: E. Alpyadin (3rd edition, Cambridge MS, MIT press).

Artificial Intelligence: A Modern Approach: S. Russell and P. Norvig (3rd edition, Pearson).

Course Policies and Student Responsibilities

As a student of the course, you are required to abide by both the University Code of Conduct and the Student Code of Conduct. The Codes provide information on the responsibilities of all NTU students, as well as examples of misconduct and details about how students can report suspected misconduct. The University also has the Student Mental Health Policy. The Policy states the University's commitment to providing a supportive environment for the holistic development of students, including the improvement of mental health and wellbeing. These policies and codes concerning students can be found in the following link.
https://www.ntu.edu.sg/life-at-ntu/student-life/student-conduct

Academic Integrity

Good academic work depends on honesty and ethical behavior. Quality of your work as a student relies on adhering to the principles of academic integrity and to the NTU Honor Code, a set of values shared by the whole university community. Truth, Trust and Justice are at the core of NTU's shared values.

As a student of NTU, it is important that you recognize your responsibilities in understanding and applying the principles of academic integrity in all the work you do at the University. Not knowing what is involved in maintaining academic integrity does not excuse academic dishonesty. You need to actively equip yourself with strategies to avoid all forms of academic dishonesty, including plagiarism, academic fraud, and collusion and cheating. If you are uncertain of the definitions of any of these terms, you should go to the academic integrity website for more information. Consult your instructor(s) if you need any clarification about the requirements of academic integrity in the course.