PMM203: COMPUTATIONAL METHODS FOR MATERIALS USING C-PROGRAMMING

L	T	P	Cr
3	0	3	4.5

Course Objective: The aim of the course is to introduce the students to C programming and various models in materials engineering.

Introduction: Algorithms, Flow charts, Problem solving methods, Need for computer language, C-character set, Identifiers and keyword, Data types, Declarations, Expressions, statements and symbolic constants, Input-output statements, Preprocessor commands, Preparing and running a complete C-program.

Operators and Expressions: Arithmetic, Unary, Logical, Bit-wise, Assignment and conditional operators, Library functions.

Control Statements: While, Do-while, For statements, Nested loops. If else, Switch, Break, continue and goto statements, Comma operator.

Functions: Defining and accessing: Passing arguments function prototypes, Recursion, Use of library functions, Storage classes: Automatic, External and Static variables.

Arrays and Strings: Defining and processing, Passing to a function, Multi-dimensional arrays, Operations on strings.

Introduction of Modeling: Concept of model, Modeling in materials science, Simulation vs. modeling, Numerical solution of differential equations.

Monte Carlo Methods: Introduction, Metropolis Monte Carlo algorithm, Ising model, Resident time algorithm, Diffusion.

Molecular Dynamics: Introduction, Interatomic potentials, Equations of motion, Integration, Correlation functions, and their examples.

Phase-field Models: Introduction, Allen-Cahn model, Energy functional, Numerical solution methods, examples.

Laboratory Work:
Programs related to computational methods along with basic programs will be carried out in C language.

Course Learning Outcomes (CLO):
The student will be able to:

1. Understand concept of programming in C
2. Understand modelling and simulation
3. Appreciate monte-carlo, molecular dynamics and phase-field models.

Recommended Books:

1. *Kemighan, B. W. and Ritchie, D.M., The C Programming Language, PHI (1988).*
2. *Wolfson, M. M. and Pert, G. J., An Introduction to Computer Simulation, Oxford University Press (1999).*
3. *Raabe, D., Computational Materials Science, Wiley-VCH (1998).*
4. *Koonin, S. E. and Meredith, D. C., Computational Physics, Addison-Wesley (1990).*