## Computational Techniques - Video course

### **COURSE OUTLINE**

## **Objectives:**

The development of fast, efficient and inexpensive computers has significantly increased the range of engineering problems that can be solved reliably.

Computational techniques use computers to solve problems by step-wise, repeated and iterative solution methods, which would otherwise be tedious or unsolvable by hand-calculations.

This course is designed to give an overview of computational techniques of interest to process engineer.

However, the focus being on the techniques themselves, rather than specific applications, the contents should be relevant to varied fields such as engineering, management, economics, etc.

### Software:

Since this is designed to introduce students to the art of scientific computation, it will rely on computer-based exercises to learn aspects of practical implementation. MATLAB is the official software used in this course.

Alternatively, if MATLAB is not available, SCILAB - an open-source scientific computation and visualisation package may also be used. SCILAB is available to download for free at <a href="https://www.scilab.org">www.scilab.org</a>

## **COURSE DETAIL**

S.No	Topics	No. of Hours
1	Introduction  Motivation and applications.	1
2	Computation and Error Analysis  Accuracy and precision; Truncation and round-off errors; Binary Number System; Error propagation.	2
3	Linear Systems and Equations  Matrix representation; Cramer's rule; Gauss Elimination; Matrix Inversion; LU Decomposition; Iterative Methods; Relaxation Methods; Eigen Values.	6
4	Algebraic Equations  Bracketing methods: Bisection, Reguli-Falsi; Open methods: Secant, Fixed point iteration, Newton-Raphson; Multivariate Newton's method.	5



# **NPTEL**

http://nptel.iitm.ac.in

# Chemical Engineering

### Hyperlinks:

Numerical Recipes in Fortran and C:

www.nr.com

### **Coordinators:**

**Dr. Niket S.Kaisare**Department of Chemical
EngineeringIIT Madras

5	Regression and Curve Fitting  Linear regression; Least squares; Total Least Squares; Interpolation; Newton's Difference Formulae; Cubic Splines.	5
6	Numerical Differentiation  Numerical differentiation; higher order formulae.	3
7	Integration and Integral Equations  Trapezoidal rules; Simpson's rules; Quadrature.	4
8	ODEs: Initial Value Problems  Euler's methods; Runge-Kutta methods; Predictor-corrector methods; Adaptive step size; Stiff ODEs.	8
9	ODEs: Boundary Value Problems  Shooting method; Finite differences; Over/Under Relaxation (SOR).	3
10	PDEs Introduction to Partial Differential Equations.	4
	Total	41

### References:

- 1. Gupta S.K. (1995) Numerical Methods for Engineers, New Age International.
- 2. Chapra S.C. and Canale R.P. (2006) Numerical Methods for Engineers, 5th Ed; McGraw Hill.

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