Indian Institute of Technology Kanpur

Proposal for a New Course

Course Number: ChE6XX

Structure: *Two* Lectures per week each of 50mins duration and *One* lab per week of 3hrs duration. (2-0-1-9)

Duration of the Course: Full Semester

Proposing Department: Chemical Engineering

Other Departments/IDPs which may be interested in the proposed course: Chemistry, Sustainable Energy Engineering

Other Faculties Interested in Teaching this Course: Indranil S. Dalal (CHE), Harshwardhan H. Katkar (CHE), Himanshu Sharma (CHE), Dipin Pillai (CHE)

Proposer: Vishal Agarwal

Course Description:

Objectives: The course is targeted for graduate-level students employing numerical and computational techniques for their research. The aim is to equip students with the theoretical foundations and practical exposure to these methods for solving complex problems in (chemical) engineering. The course is designed to have a combination of lectures and hands-on sessions using programming environments such as python (or matlab) aiming to develop skills to model, analyze, and address problems that are difficult to solve analytically; preparing them for advanced research and industrial challenges.

Title: "*Computational Methods in Chemical Engineering*"

Course Contents and Lecture-wise Breakup*:

Introduction: Introduction to scientific computing, approximations and round-off errors. (1 lecture + 1 lab on programming)

Linear Algebraic Equations: Gauss-Seidel, Gauss-Jordan, LU decomposition and matrix inversion. (2 lectures + 1 lab)

Eigenvalues and Eigenvectors: Power iteration, inverse iteration, Rayleigh quotient iteration, QR iteration, Krylov subspace methods, Jacobi method. (4 lectures + 2 labs)

Non-Linear Equations: Bracketing methods, method of successive substitution, Wegstein method, Newton's method, Homotopy and DIIS, sensitivity and conditioning, convergence rates and stopping criteria. (4 lectures + 2 labs)

Unconstrained Optimization: Steepest descent, quasi-Newton methods, conjugate-gradient methods, MD-based methods. (5 lectures + 3 labs)

Probability and Curve Fitting: Probabilities, random and pseudo-random numbers, Gaussian distribution, maximum likelihood, Bayesian linear regression, Gaussian process regression (GPR). (6 lectures + 2 labs)

Monte Carlo Methods: Monte-Carlo integration, Metropolis algorithm, stochastic chemical kinetics. (5 lectures + 2 labs)

* Each lecture is assumed to be of 50 minutes duration.

Pre-requisites: ESO208 or equivalent, MTH102 or equivalent and ChE331 or equivalent.

Expected Enrolment: $\sim$ 20-30

- **Useful References**
  - "*Numerical Methods for Engineers*", Steven C. Chapra and Raymond P. Canale, McGraw Hill, 2021, Eight Edition, ISBN-13: 978-9354601361.
  - "*Numerical Methods for Chemical Engineering*", by Kenneth J. Beers, Cambridge University Press, 2007, ISBN-13:978-0-521-85971.
  - "*Pattern recognition and machine learning*", by Christopher M. Bishop, Springer, 2006, ISBN-13: 978-0387-31073-2.
  - "*Introduction to linear algebra*", by Edwin K. P. Chong and Stanislaw H. Zak, Wiley, 2013, Fourth Edition, ISBN-13: 978-8126567898.
  - "*An introduction to Optimization*", by Gilbert Strang, Wellesley-Cambridge Press, 2021, Fifth Edition, ISBN-13: 978-1733146654.

Dated: August 12, 2025 Proposer:

Dated: DPGC Convener:

The course is approved / not approved

Chairman, SUGC/SPGC

Dated:_____