

**Chemical Engineering Department
King Saud University**

CHE401: Computational methods for chemical engineers

Reference Book:

An Introduction to Numerical Methods for Chemical Engineers, Riggs

Contents:

- Introduction to FORTRAN programming
- Linear algebraic equations
 - (1) Matrix inversion/ Gauss Elimination
 - (2) LU decomposition
 - (3) LSARG subroutine
- Non-linear algebraic equations:
 - (4) Bisection method
 - (5) Newton method
 - (6) Secant method
 - (7) NEQNF subroutine
- Ordinary Differential equations (ODE):
 - (8) Euler method
 - (9) Runge Kutta method
 - (10) IVPAG subroutine
- Boundary value problem:
 - (11) Shooting method
 - (12) Finite difference method
 - (13) BVPDF subroutine
- Optimization:
 - (14) uni-dimensional problems
 - (15) multi-dimensional problems
 - (16) NCONF subroutine

Grading:

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|-----------------------------|-----------|
| • Hand-calculated homework: | 05 points |
| • Programming assignments: | 10 points |
| • Exam I | 20 points |
| • Term Project | 15 points |
| • Final exam | 50 points |