Chemical Engineering 541

Computer Aided Design Methods

Material Review, Exam 1

Exam Review, by Classes

- Overview
- **Errors, accuracy, roundoff, floating point**
- Linear Algebra
- **Numerical Linear Algebra**
- **Nonlinear Root Finding**
- **Finite Differences**
- **ODEs: IVPs**

Class 1—Overview

- What are numerical methods, what differentiates them from other methods.
- Examples of methods from research, chemical engineering
- Different types of methods, specifically.
- Issues/Aspects:
  - Computers, algorithms, errors, stability, order, convergence, etc.

Class 2—Errors, accuracy, roundoff

- Binary numbers: conversions, fractions
- Number representation: parts of floating point numbers on a machine
- Integers versus floats
- F.P. summation vs. multiplication and how this relates to roundoff error.
- Floating point analysis
  - How it works, why we use it.
- Pitfalls and solutions (e.g. what kinds of problems can arise (e.g. divide by zero.)

Class 3 – L.A. Review

- Matrix multiplication, different interpretations, A*B, A*x, rows vs. cols
- Definitions: rank, transpose, symmetric, inner/outer prod, singular
- Types of “solutions” or systems
- An alternate interpretation of inverse
- Decomposition/basis change: Inverse, EV
- Norms– vector, induced matrix, types, props.
- Condition number. What it is , why it matters, how it affects numerics.
- Most of this is review

Class 4— L.A. Direct Methods

- Gauss Elimination, LU decomposition, Thomas Algorithm
- Differences between iterative and direct methods, when they are applicable
- Gauss Elimination
  - How it works, what are the major steps involved, and how are they implemented. What is the cost?
- L.U. Decomposition versus Gauss Elimnation
  - When to use, differences in the algorithm
- Thomas algorithm
  - Where it comes from, types of systems it applies to, cost.

Class 5—L.A. Iterative methods

- Jacobi, Gauss Seidel, SOR, Convergence
- Many convergence issues, what does convergence mean, what does it depend on.
- Role of R.O. error with respect to iteration
- Know about the J., G.S., SOR formulas and how they differ.
- Convergence criteria: relative versus absolute error, forms for multiple eqns.

Class 6—Nonlinear Equations, Closed

- Types of Methods: open, closed
  - Advantages, disadvantages, when to use.
- 1D versus multi-D
- Problems that may arise.
- Closed methods: know the methods.
  - Bisection
    - How to test for root bracket
  - Regula Falsi
    - Equation for a line

Class 7—Nonlinear Root Finding, Open

- Two types of convergence criteria here:
  - f(x) versus x
- Fixed point method
  - Why it looks good, but may not perform
  - Convergence criteria: how did we get it
  - Convergence rate.
- Secant method: know how it works (this will allow you to get the equation)
- Newton's method: how to derive it, how it converges

Class 8—Nonlinear Root Finding

- Multi-D Newtons method
  - How to derive, know the formula.
  - Can under-relax it and the 1D version
- Fixed point is also easily multi-D and the convergence can be similarly derived.
- Examples
- Step size for numerical derivatives for Newton's method.
- Approach for numerical Jacobian

Class 9—Taylor Series, Finite Differences

- Taylor Series
  - You should be able to write a T.S. any time
- Procedure to derive finite difference approximations.
  - T.S. at a point, about a base point.
  - Use multiple eval points and combine to eliminate high order terms, retaining the derivative of interest.
- Taylor Table
  - What's the idea (don't worry about the details)

Class 10—Intro to ODEs

- IVP vs BVP
  - Corresponding physical problems
  - Order, linearity
  - Method of solution: start at initial condition, step along the slope
- Euler methods: Explicit vs. Implict
  - Advantages, disadvantages.
  - Derive, know order, know basic stability, qualitative properties
- Local vs. global truncation error.

Class 11—Higher Order Methods

- Modified Midpoint
- Implicit Trapazoid
- Modified Euler
- You should know the formulas for these or be able to write them from a basic understanding of what they are.
- 2nd Order R.K.
  - Procedure (not details) for how to derive:
    - Recall general form $y_{n+1}=y_n+c_1\Delta y_1+c_2\Delta y_2$, etc.
    - Plugged in steps for $\Delta y_{1,}$ Δy_2
    - Did a T.S. for RHS to write about the initial point.
    - Did a T.S. for y_{n+1} (generic)
    - Equated terms to solve for constants.
- 4th Order R.K.
  - Know the idea, combo of slopes at intermediate points
  - (which points, how did you get there).

Class 12—Higher Order ODEs

- Higher order of derivative: y’ vs y” vs y”’
- Systems of coupled equations
  - Implicit
  - Explicit
  - Nonlinear
- Decoupled equations
- Adaptive timesteps
  - given the error, how to pick a new step; how to get the error.

Class 13—Stability, Stiffness, Coupled Eqns.

- Stability
  - EE versus IE.
  - Linear homogeneous form (or get that form by linearization).
  - Stability does not mean "no wiggles," it means "does not blow up"
  - The ODE has to be stable, not just the FDE
- Stiffness
  - What causes it.
  - Cures for stiffness
- Consistency and the MDE