Chemical Engineering 541

Numerical Methods

Exam 2 Review

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- Classes 17-29
- Homework 5-7
- ODEs
  - Boundary Value Problems—Shooting
  - Boundary Value Problems—Relaxation
- PDEs
  - Classification
  - Parabolic PDEs
  - Elliptic PDEs
  - Finite Volume Method
  - Advection/Diffusion

ODEs, BVP, Shooting

- BVP
  - Characteristics
  - Differences between IVP, BVP
  - Recognize linear vs nonlinear.
- BCs
  - Three types: identify each by name, by physics, example
- Two methods: shooting and relaxation
- Shooting method
  - Reduce 2nd order (or higher) ODE to system of 1st order ODEs
  - March from one end to the other
  - Don't know all BC's at one end → Guess.
  - Shoot to the end
  - Update guess at starting point based on BC values at end point.
  - Formulate as a nonlinear equation solve → Newton, secant, etc.

Relaxation Methods

- Shooting vs Relaxation
  - Advantages and disadvantages
- Relaxation
  - Discretize domain into a grid of points
  - Apply finite difference approximations to derivatives in ODE in terms of grid points
  - ODE is now a coupled system of algebraic equations
    - Solve this linear or nonlinear problem using any standard method
    - Direct solution of a linear system. Depends on number of points in the FDE. Tridiagonal can be convenient and fast.
    - Iterative solution.
    - Nonlinear → direct Newton's method, or linearize and iterate.
  - Formulation of the linear system including boundary conditions

BVP Relaxation Methods

- BCs
  - Dirichlet are straightforward, done before
  - Neumann and Robin conditions.
  - Discretize the boundary condition in all cases.
  - Ghost Cell method:
    - Include Boundary point in unknowns.
    - Apply BC to eliminate the Ghost Cell that arises.
  - Method 2:
    - Don't include the boundary point in unknowns, but boundary point arises in equation for point 1.
    - One-sided difference on boundary condition to eliminate the boundary point from equation for points next to boundary.
  - Advantages and disadvantages of each method
- Nonlinear Relaxation Methods
  - Iterate: factor nonlinear terms into a linear component, and a lagged component. Example: $(y^2)^{n+1} \rightarrow y^n y^{n+1}$. Can also linearize the term with a Taylor series.
  - Newton's method (fast convergence, but requires a linear system solve at each step).
- Nonuniform grids
  - Arbitrary grid
  - Analytic stretched grid.

PDEs

- Approach:
  - Nonlinear → linear with iteration
  - ODEs → algebraic systems (linear/nonlinear)
  - PDEs → ODEs and/or algebraic systems
- Examples of each
- Classification
  - Elliptic, Parabolic, Hyperbolic
    - Domains of dependence
    - Qualitative/physical sense for each type.
    - Characteristic Curves
  - Parabolic:
    - Conceptually: has an unsteady (d/dt) term and a diffusive (d^2/dx^2 second derivative) term. A first derivative (advective) term is optional.
  - Elliptic:
    - Conceptually: like parabolic above, but steady state (no d/dt term).
  - Hyperbolic:
    - Conceptually: has a d/dt term and a d/dx term, but no d^2/dx^2 diffusive term.

PDEs Parabolic

- FTCS
- BTCS
- Crank Nicholson
- Omega Method is a generalization (ω on the n+1 term)
- Advantages/disadvantages for FTCS, BTCS, CN
  - What is the order and stability of each.
- Method of Lines
  - How to get and setup. How it differs from others
- Coupling in space of the different methods and how this affects a numerical method

Stability

- Stability Analysis
  - Applied to FTCS, but works for others too.
  - What do we mean by stability?
    - How stability of ODE, relates to that of the FDE.
  - Von Neumann Analysis (basic ideas only)
- Limitation on $d = \alpha\Delta t/\Delta x^2$.
  - Physical interpretations of constraints:
    - d is a ratio of timescales. Don't step more than some factor of the intrinsic physical process timescale

Multi-D

- Solution of Multi-D parabolic equation
  - 2D grid in space
  - Discretize both directions
  - Stencil: depends on finite difference approx, but a 5 point stencil is common
- Explicit in time
  - Straightforward: solve each gridpoint in terms of itself and its (four) neighbors at the previous time.
- Implicit in time
  - Pentadiagonal matrix
  - How to set it up, BC issues, ordering of gridpoints

ADI

- ADI
  - Alternating Direction Implicit
  - Use with Thomas Algorithm (TDMA)
  - Works for Parabolic or Elliptic problems:
    - Elliptic are more obviously applicable as they are naturally "implicit"
  - Approach 1: matrix specific:
    - Order grid in one direction, move off-diags to RHS, then iterate, changing grid order each time.
    - Solves the whole grid: (nx*ny) x (nx*ny) system.
    - Hoffman's equation implies this method.
  - Approach 2: grid specific:
    - Sweep rows of grid, solving 1-D tridiagonal system for each row, then do the same for each column.
    - Solves an (nx) x (nx) system for each row, then an (ny) x (ny) system for each column, rather than whole grid of points as in Approach 1.
  - For unsteady problems, don't have to iterate to convergence.

Finite Volume Method

- Solve integral rather than differential equation on a grid of finite volumes rather than a grid of points.
- Three equivalent approaches
  - Apply standard: Accumulation = In – Out + Generation
  - Integrate the PDE over the CV
  - Start from scratch and apply the Reynolds Transport Theorem equation to each CV
- Properties are assumed constant in a CV, and along a surface (CS)
- Uses Gauss Divergence Theorem. $\int_V \nabla \cdot \vec{v} dV = \int_A \vec{v} \cdot \vec{n} dA$
- Face properties evaluated using averages (interpolation), or by using finite differences (for derivatives), or both.
- Usually flux-based, and conservative by construction. Often write directly in terms of fluxes, without doing full substitution.
- More naturally accommodates heterogeneous materials.
- Formulation can be similar to finite difference method for special cases.

Finite Volume Issues

- Interface conductivity (or viscosity, or diffusivity).
  - Harmonic mean not arithmetic mean.
  - Find the face conductivity by equating heat fluxes across cell ($q^+=q^-$ and $q^+=q$ gave two equations in k_{face} and T_{face}).
  - Linear interpolation is inferior.
- Grid decoupling for first derivatives
  - Pressure gradient in N.S. equations, or convective terms in general
  - Allows checkerboarding
  - Use a staggered grid for velocities
    - Eliminates checkerboarding, and is convenient for evaluating fluxes at cell faces (which is where the velocities are located).

Advection/Diffusion

- Two parameters: $c=u\Delta t/\Delta x$, $d=\Gamma\Delta t/\Delta x^2$. (Timescale ratios)
- FTCS
  - Conditionally stable, consistent, $O(\Delta t)$, $O(\Delta x^2)$
  - $d<1/2$, and $c^2 < 2d$
- BTCS
  - Unconditionally stable, consistent, $O(\Delta t)$, $O(\Delta x^2)$
- Central difference "bad" on advective terms
  - wrote in terms of Pe, unphysical increase without a source term
- Upwinding solves this, but lower order, and diffusive.

Advection/Diffusion

- Exponential scheme
  - Instead of central differences or upwinding, we incorporate the exact solution of the SS, 1-D problem with no source for the discretization
  - Use exact solution to evaluate the flux at a face in terms of its neighbors → coefficients of neighbors as before, but different form.
    - Simplify by approximating the exponentials using polynomials or piecewise linear functions.
    - Write in terms of Peclet number Pe (analogous to Re for scalars).