# Chemical Engineering 541

*Final Review*

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## Final Review

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- Classes 31-41
- Homework 8-9
- Hyperbolic equations
- Numerical integration
- Sample PDF
- Interpolation
- Curve fitting
- Spectral methods
- Homotopy continuation

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# Overall

- Errors accuracy and roundoff
- Linear Algebra
- Linear Systems
  - Direct
  - Iterative
- Nonlinear Equations
  - 1-D
  - Multi-D
- Taylor Series
- ODEs:
  - IVP

- ODEs
  - BVP
  - BCs
  - Shooting
  - Relaxation
- PDEs
  - Parabolic
  - Elliptic
  - ADI
- Finite Difference
- Finite Volume

- PDEs
  - Convection
  - Diffusion
  - Hyperbolic
- Numerical Integration
  - Trapezoid, Simpsons
  - Adaptive quadrature
  - Gauss quadrature
  - Monte Carlo
- Interpolation
- Curve fitting
  - Polynomial
  - Least squares
- Spectral methods
- Homotopy continuation

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# Themes

- *Methods and implementation*
- PDEs to ODEs or algebraic equations
- ODEs to algebraic equations
- Linear, nonlinear, systems
- Taylor series
  - FD equations, consistency
  - PDE→FDE→MDE
- Stability analysis, Fourier analysis
- Eigenvalue decompositions
  - Separate equations, analysis, especially for systems

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# Homework Summary

- **HW 1**
  - Machine precision, roundoff error.
  - Floating point analysis, condition number
  - LU decomposition / Thomas Alg.
- **HW 2**
  - Iterative methods: Jacobi, GS, SOR, optimal omega
  - Nonlinear Root finding
- **HW 3**
  - Nonlinear systems,
  - FD derivatives.
- **HW 4**
  - IVP, EE, IE, MM, Euler stability
  - RK4 convergence
- **HW 5**
  - BVP: cylidrical heat conduction, Neumann BCs
  - Shooting, Relaxation methods
- **HW 6**
  - Parabolic PDE: flamelet equation
  - FTCS, BTCS, CN
- **HW 7**
  - Lid driven cavity (vorticity-streamfunction): F.D., F.V. equations
  - Nonlinear
  - ADI method
- **HW 8**
  - 1D linear wave equation
  - Upwind, 2nd order upwind, Lax Wendroff
- **HW 9**
  - Integration: Trapazoid, Simpson
  - Curve Fit
  - Spline

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# Hyperbolic Equations

- Methods:
  - FTCS
  - Lax
  - Lax Wendroff
  - MacCormack
  - Upwind
  - 2nd order upwind
  - BTCS
- Know:
  - Consistency
  - Order in time and space
  - Stability
  - Stencils
  - Characteristics
  - MDE
    - Lax Wentroff used this to fix the Lax method

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# Hyperbolic Equations

- Euler Equations
  - An example of a hyperbolic system
  - Inviscid fluid flow: solve mass, momentum, energy, for ideal gases.
  - Converted energy equation to pressure eqn.
  - Wrote as a matrix system
  - Decoupled using an eigenvalue decomposition to show form as 1-D wave equations
  - Eigenvalues were wave speeds.
- Flux Limiters
  - These are nonlinear methods to suppress oscillations and retain second order accuracy.
  - Write fluxes as the sum of two fluxes (nominally a low order that's good near sharp regions, and a high order thats good in smooth regions).
  - The flux limiter function switches between the two fluxes based on ratio of successive slopes (steepness of profile).
  - Many methods depending on the form of the flux limiter.





# Numerical Integration

- Direct fit polynomials
  - Fit a polynomial through data and integrate it
  - Limited to few points/low order else get poor results due to polynomial oscillation
- Trapazoid rule
  - Fit lines through adjacent points and sum the area of the resulting trapazoid.
  - Adjacent trapazoids double count points → build into the single summation equation.
  - Second order globally
- Simpson's rule
  - Fit parabola through groups of three points
  - Need odd number of points
  - How to fit the parabola?
  - Fourth order globally (error in notes: says its 3$^{rd}$ order).
- Boundary issues

# Integration

- Adaptive Quadrature
  - Recursive routine for trapazoid rule
  - Be familiar with this, it was not complicated to implement
  - Issues...
- Monte Carlo Integration
  - Introduction
  - Converges as $N^{1/2}$ (that is, error is proportional to $N^{1/2}$)
  - Integrate area in circle by ratio of points
  - Examples of why (weird domains, multi-dimensional, fiercly expensive).
  - Sample uniform random points on [a,b]?
  - Sample uniformly from a distribution (like a Gaussian)?
  - Sample uniformly under a curve?

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# Integration

- Monte Carlo Integration
- Sample from nonuniform distributions
  - Integrate and Invert
  - Rejection method
- Poisson Process example

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## Integration

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- Gauss Quadrature
  - Gauss Legendre
  - Scale the domain
  - Weighting function → Other quadratures
  - Exponential convergence rates
- Soot moments example

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## Interpolation

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- Direct polynomial fit to points
  - M points, M-1 degree polynomial
  - Limit to 5-6$^{th}$ degree
  - Don't extrapolate
  - Limitations?
  - Lagrange form
- Linear interpolation
- Cubic Splines
  - Allows smooth f, f', f" using low order polynomial (cubic).
  - Domain is coupled to solve though
  - Constraints to get number of equations and points.
  - Simpler version solves for f" at each point, then has the cubic in each interval in terms of f".

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# Curve Fitting

- Lagrange Polynomials
  - Formed to fit the points directly
- Least Squares approximation
  - Fit a function to data.
  - Minimize the sum of the square error.
  - Partial derivatives of the square error with respect to parameters=0
  - Try to transform to a linear system.
- Linear least squares
  - Matrix formulation

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# Spectral Methods

- Solution represented as sum of coefficients times basis functions.
  - Similarly used in finite element methods
- Periodic domains
  - Similar variations allow non-periodic domains (e.g., Chebychev polynomials)
- FFT, IFFT
- Spectral vs Pseudo-Spectral method
- Treats derivatives exactly
- Exponential convergence with # of points

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# Homotopy Continuation

- Challenging nonlinear problems
- Traverse a path from an easy problem with a known solution to the difficult problem.
- Common types
  - Newton
  - Fixed point
- Formulations
  - Step along path
  - ODE system to formalize the advancement along the path