Applied Mathematics for Chemical Engineering, ChE 230A

Instructors: Prof. Baron Peters Rm. 3339, baronp@engineering.ucsb.edu
Office hours: 9:00-11:00 Wednesday

Reader: Joel Paustian Squires Laboratory

Course webpage: http://www.engineering.ucsb.edu/~baronp/ChE230A/

Homework (20%) is due each Tuesday. Homeworks will typically extend beyond the lecture content to introduce new geometries, boundary conditions, applications, etc.

Exams will be closed book. Necessary tables, formulas, and supporting material will be provided. This policy is intended to focus your studies the concepts and the situations in which they are applicable.

Midterm 1 (20%) October 25
Midterm 2 (20%) November 20
Final (40%) Tuesday, Dec. 11, 8:00-11:00pm

Objective: become skilled in analytic methods for typical ChE problems.

Topics
Multivariable calculus review
Ordinary differential equations review
Method of characteristics (1st order PDEs)
Linear algebra and the spectral theorem
Sturm-Liouville theory
Fourier series and generalized Fourier series
Separation of variables (homogeneous equations)
Eigenfunction expansion and Green's functions
Homogeneous boundary value problems
Non-homogeneous boundary value problems
Fourier transforms
Laplace transforms and Duhamel's principle
Calculus of variations

Texts (in order of importance)
Farlow, "Partial Differential Equations for Scientists and Engineers" Dover 1993
(Eigenfunctions, Poisson integral solutions, integral transforms, characteristics)
Mathews and Walker, "Mathematical Methods of Physics" Addison-Wesley 1970
(Sturm-Liouville, Hermitian matricies, and Green's functions)
Riley, Hobson, Bence, "Math Methods for Physics and Engineering" Cambridge 2006
(all-in-one: calculus, matrix/tensors, ODEs (very good), PDEs, statistics, etc.)

Boyce and DiPrima, “Elementary Differential Equations and Boundary Value Problems” Wiley 1992 (easy introduction to ODEs)

Other references

Rice and Do, “Applied Math and Modeling for Chemical Engineers” Wiley 1995
(geared to traditional chemical engineering problems)

Logan, “Applied Mathematics” Wiley 1996
(stability, asymptotics, calc. of variations, integral eqs, stochastic processes)

Zachmanoglou and Thoe, “Intro to PDEs with Applications” Dover 1986
(systems of ODEs and PDEs, method of characteristics)

Matthews and Walker, “Mathematical Methods of Physics” Addison-Wesley 1970
(Sturm-Liouville, Hermitian matricies, and Green’s functions)

Barenblatt, “Scaling, Self-similarity, and Intermediate Asymptotics” Cambridge 1996
(the reference on dimensional analysis and scaling)

Boyce and DiPrima, “Elementary Differential Equations and Boundary Value Problems” Wiley 1992 (easy introduction to ODEs)

Gradshteyn and Ryzhik, “Table of Integrals, Series, and Products” Academic 1994
(tables of everything imaginable)

Mathews and Walker:

this book evolved from the course by Feynman while he was at Cornell fresh from Los Alamos. Feynman later said that from the experience at Los Alamos he knew which mathematical methods worked and was useful, and he tried to teach those skills in his course.

Lectures

1) Linear algebra introduction
[RHB:]
a) vector spaces b) inner products c) change of basis
e) orthogonality f) linearity

S) Ordinary differential equations
[RHB: 13, 14]
a) classification b) special equations c) integrating factors
d) dimensional analysis and homogenous differentials
e) other solution techniques, a prep course for 230A!

2) Linear algebra continued
[RHB:]
a) determinants
b) linearly independent ODE solutions and the Wronskian
c) diagonalization, eigenvectors, eigenvalues
d) systems of ODEs

3) Linear algebra continued
[RHB:]
a) hermitian matricies, spectral theorem, completeness
b) quadratic forms and multidimensional Gaussian integrals
c) solving equations with matrix operators in terms of the diagonal basis

4) Sturm-Liouville theory
[RHB: 17]
a) adjoint operator as the “integrating factor” of a second order linear ODE
b) self-adjoint operators: a continuous generalization of the Hermitian matrix
c) boundary conditions, eigenvalues, eigenfunctions, and completeness

5) Fourier series and generalized Fourier series
[Farlow: 11, 10]
a) periodic functions, Fourier coefficients, and discrete frequency spectra
b) generalized eigenfunction expansions: Bessels, spherical harmonics, etc.

6) Partial differential equations introduction
[Farlow: 1, 4, 8, 31, 23, 41, 22]

a) formulation and interpretation b) common equations
c) transforming hard equations to the usual suspects
d) classification, canonical forms, and characteristics of solutions
e) overview of solution techniques

7) Similarity solution – dimensional analysis
[notes from Barenblatt]
a) pi theorem and intuition
b) reduced variable that makes PDE an ODE *and* makes ICs and BCs redundant

8) Spectral solution by separation of variables – finding the eigenfunctions
[Farlow: 3, 5, 6, 7, 26]
a) homogeneous boundary conditions (BCs)
b) separate variables, solve Sturm-Liouville, superimpose spectrum of solutions
c) how to get homogeneous BCs from time varying BCs
d) solving harder problems by separation of variables

9) Nonhomogenous partial differential equations
[notes from Logan + Farlow: 9]
a) eigenfunction expansions
b) the impulse response function – aka the Green's function
c) the Green's function by eigenfunction expansion

10) Boundary value problems (steady-states, potentials, etc)
[Farlow: 32, 33, 34]
a) Laplace's equation (eigenfunctions again)
b) Poisson's integral formula
c) example: Soap films

11) Boundary value problems continued – nonhomogeneous problems
[Farlow: 36]
a) nonhomogeneous equations – (Green's functions again)
b) nonhomogeneous boundary conditions – (Poisson integral formula)
c) nonhomogeneous BCs and nonhomogeneous PDE – (superposition)

12) Conformal mapping: boundary value problems on complicated domains
[Farlow: 47]
a) invariance of Laplace's equation to conformal change of variables
b) the complex plane and functions of a complex variable
c) example: steady-state temperature distribution of a wedgie

13) Integral transform methods
[Farlow: 10, 25, 12]
a) the basic idea of integral transforms
b) Finite Fourier transforms …better to expand in eigenfunctions if known
c) the Fourier transform and its characteristics
d) linear equations with constant coefficients and homogeneous BCs at infinity
e) Fourier transform inversion

14) The Laplace transform (constant boundary conditions)
[Farlow: 13]
a) why another transform? existence of the Laplace transform
b) characteristics of the Laplace transform
c) linear equations with constant coefficients

d) “An inconvenient truth”: inversion by tables, residues, and worse

15) Duhamel’s principle (time-varying boundary conditions)
    [Farlow: 14]
    a) derivation of Duhamel’s equation
    b) interpretation as weighted superposition of the homogeneous solutions
    c) example: heat equation with heat sources and time varying BCs

16) Calculus of variations
    [notes from Fredrickson + notes from Logan]
    a) functionals, variational principles, and functional derivatives
    b) Euler-Lagrange equations
    c) Rayleigh-Ritz method
    d) intro to the inverse problem: variational principle from differential equation

17) First order partial differential equations
    [Farlow: 27, 28]
    a) method of characteristics
    b) conservation equations (nonlinear first order equations)

18) Systems of PDEs – linear algebra revisited
    [notes from Logan + Farlow: 29]
    a) writing higher order equations and systems as first order systems
    b) decoupling first order systems
    c) stability of PDE solutions, pattern formation, and lengthscales

19) (time permitting) PDEs for the evolution of distributions
    [notes from van Oudenaarden and O’Shaugnessy]
    a) transition probabilities, master equations, and Fokker-Planck equations
    b) cursory notes on integral equations
    c) example: chain length distribution in polymerization

Syllabus

I. Introduction
- A. review of ordinary differential equations: methods of solution, nullclines, bifurcations, … <2e>
- B. review of linear algebra: vector/function spaces, basis, inner product, orthogonalization, symmetric/adjoint, spectral thm <2e>
- C. eigenfunctions and sturm-liouville eqns <1>

II. Formulation of PDEs, boundary/initial conditions, canonical forms, the Laplacian <1>
- A. classification and physical characteristics
- B. dimensional analysis, scaling
- C. similarity transforms

III. overview of solution strategies: <1>
- A. Characteristics (for first order PDEs)
- B. ODEs from a PDE (restricted to certain BC/IC) sep. of variables, integral transforms, similarity transforms
- C. Expansion/superposition (eigenfunctions and Greens functions)
- D. Variational approaches: (PDE => functional minimization)
- E. Perturbation theory: (hard problem => series of easy problems)

IV. Fluid flow, shock waves <1>
- A. method of characteristics
- B. front propagation rate

V. Electrostatics, steady-state temperature and concentration <6>
- A. Green's function approach for Laplace's equation
- B. eigenfunction expansions of the Green's function
- C. the Poisson-Boltzmann equation
- D. complex boundaries
  - perturbation theory
  - conformal mapping

VI. Transient diffusion and heat conduction <6>
- A. separation of variables
- B. Laplace transform, Duhamel's principle and time varying BCs
- C. Fourier series, Parceval's thm and quantum mechanics
- D. infinite domains: Fourier transform, continuous frequency spectrum, and the similarity solution as the Green's function
- E. Reaction-diffusion equations
  - stability and pattern formation

VII. Waves <2>
- A. separation of variables
- B. Fourier transform
- C. modes, nodes, frequencies

VIII. Time-independent Schrodinger equation <4>
- A. WKB approximations

B. Calculus of variations and variational principles

- Euler-Lagrange equations
- functional minimization: H_2^+

IX. Stochastic processes and the Fokker-Planck equation <2>

A. noise in gene expression (van Oudenaarden)

B. living polymerization (O'Shaughnessy)

<28+2e>