22.15 Essential Numerical Methods

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6-unit Core Module

Bulletin Description

Introduces computational methods for solving physical problems especially in nuclear applications. Ordinary and partial differential equations for particle orbit, and fluid, field, and particle conservation problems. Their representation and solution by finite difference numerical approximations. Iterative matrix inversion methods. Stability, convergence, accuracy and statistics. Particle representations of Boltzmann's equation and methods of solution such as Monte-Carlo and particle-in-cell techniques.

Educational Objectives

Students who complete this module will

- Become familiar with computational engineering and its mathematical foundations, at an elementary level.
- Deepen their understanding of the basic equations governing the phenomena in Nuclear Science and Engineering.
- Understand the methods by which physical problems can be solved using computation.
- Develop experience, confidence, and good critical judgement in the application of numerical methods to the solution of physical problems.
- Strengthen their ability to use computation in theoretical analysis and experimental data interpretation.

Calendar

[Lecture schedule TR 9:30-11. Recitation TR 9am-9:30am. On line zoom.]

Sep	1	3	Fitting curves to data. ODE integration.
	8	10	2-point ODE problems. PDE intro.
	15	17	PDE diffusive relaxation. Iterative matrix inversion.
	22	24	Fluid flow. Boltzmann equation.
Oct	29	1	Neutron transport. Atomistic modelling.
	6	8	MC techniques. Uncertainty, Tracking and Tallying.
	-	15	?Finite Elements, Revision.
	20?		Final: 3 hours. 9am-noon. TBA.

Grade Basis

The grade basis will be

22% Homework (exercise) assignment evaluation.
3% Class (Zoom) attendance and interaction
75% Final examination. Closed book. No computational devices.

The homework evaluation will count only the best five assignment scores. However, it should be noted that some exercises build on earlier ones. Therefore students should recognize that it is not generally possible simply to omit early assignments. Moreover, the exercises are designed to develop understanding and skill with the material that will be valuable for the final exam.

Lecture Notes and Bibliography

The text is "A Student's guide to Numerical Methods" Ian H Hutchinson, (Cambridge University Press, 2015), and the lectures will follow this book closely because the book is based on the course. An outline is below. Students who lack specific mathematics or science background in the areas discussed may be advised to supplement the lectures with extra reading.

Reference Books

W H Press, B P Flannery, S A Teukolsky, and W T Vetterling *Numerical Recipes*, Cambridge University Press (1989)

> This is an outstanding, readable, and practical introduction to numerical methods in science and engineering. It covers more than this course, but is the number one book recommendation.

Stephen Jardin *Computational Methods in Plasma Physics* CRC Press (2010)

> Although focussed on plasma physics, this book gives excellent introductions to finite difference PDE equations and the methods for solving them, across the spectrum of equation types.

Shoichi Nakamura *Computational Methods in Engineering and Science with applications to Fluid Dynamics and Nuclear Systems* Robert E Kreiger Publishing (1986)

> This book covers numerical methods in the nuclear reactor context, and therefore has some useful specialist topics. However, its mathematics is not, in my opinion, clearly written, and it is hard to learn from because of it.

Alain Hébert *Applied Reactor Physics*, Presses Internationales Polytechniques (2009)

> This modern reactor physics text book has numerical methods liberally sprinkled in its development and a useful appendix addressing them directly. Naturally its reactor physics goes far beyond what we will cover.

G D Smith *Numerical solution of partial differential equations*, Clarendon Press, Oxford (1985)

George E Forsythe and Wolfgang R Wasow *Finite-Difference Methods for Partial Differential Equations*, Wiley (1960)

A R Mitchell and D F Griffiths *The Finite Difference Method in Partial Differential Equations*, Wiley (1980)

> These are three examples of the large selection of text books that address how to solve partial differential equations numerically.

R W Hockney and J W Eastwood *Computer Simulation Using Particles*, Taylor and Francis (1988)

> This is a classic on particle simulation, especially plasma PIC approaches, but has a lot of additional material on other topics of the course.

Recitations and Classroom Discussion

Informal open recitations will be held 9am - 9:30am before the lecture, Tuesdays and Thursdays. The main point of these recitations is for students to raise questions about points that were unclear or questions that have since arisen in doing the exercises. We may do some worked examples to help explain and develop deeper understanding, but we won't cover new material in the recitations.

Course sequence and content

The exercises include hands-on programming tasks. Essentially all of them can be done in Matlab, though that might not necessarily be the only or best way to do them. These exercises change from year to year so in the following are just examples of them.

1 Lecture Numerical Fitting of Data

1-D least squares fit of a line to a sequence of data. Its representation as a matrix pseudo-inversion problem to determine coefficients.

Exercise. Write a fitting program and fit a line to some data.

2 Lecture. Orbits and ODEs

Ordinary differential equation of order N in one dependent variable is equivalent to N simultaneous first-order ODEs, i.e. a first order vector ODE. The orbit of a field line or an electron in prescribed static EM fields.

Finite difference expressions for derivative. Accuracy and Stability. Implicit and explicit advancing schemes. Runge-Kutta techniques.

Simple Leapfrog scheme as an example of centered time differences.

Exercises. Reduction to first order. Accuracy. Build and run a simple orbit integrator, or compare implicit and explicit integration.

3 Lecture. Two-point Boundary Conditions

Second order ODES. Two point boundary conditions.

Example(s) of two-point problems: slab charge, cylindrical volumetrically-heated conduction.

Shooting method. Bisection.

Second order differences. Linear ODE: expression of 2-point problem as a matrix equation. Finite difference boundary condition implementation in matrix. Non-uniform derivatives.

Exercise. Solution of 2-point problem by brute force matrix inversion

4 Lecture. Partial Differential Equations

Examples of partial differential equations of engineering physics.

Fluid flow and derivation of the continuity equation. Diffusion. Waves. Electromagnetism. Poisson's equation.

Classification of PDEs. Elliptic, Parabolic, Hyperbolic. Consequences for boundary conditions. Finite difference representation of partial derivatives. Structured (and unstructured) meshes. Difference stencil.

Exercise. Construct a difference stencil and demonstrate its conservation properties

5 Lecture. Diffusion. Parabolic PDEs.

The diffusion equation and boundaries in space and time.

Explicit FTCS scheme for time evolution of multidimensional PDEs first order in time (parabolic). Stability requirement.

Implicit BTCS scheme for time evolution: unconditionally stable. Crank-Nicholson and θ-implicit schemes.

Expression of the time advance as a matrix equation. Requirement for inversion in implicit schemes. Multidimensional cases leading to non-tridiagonal sparse matrices. The matrix size difficulty for multiple dimensions.

Example of time-dependent diffusive relaxation to a steady state.

Exercise. Build and run code for time-stepping a matrix diffusion equation to steady state.

6 Lecture. Elliptic Problems and Iterative Matrix Solution

Elliptic equation as steady state of a parabolic equation. Need for matrix inversion. Iteration's equivalence to diffusive relaxation. Solving matrix problem without explicit inversion.

Jacobi, Gauss-Seidel and SOR methods. Convergence.

Nonlinear equations, linearization and iteration.

Exercise. Improve your time-stepping code to make it a matrix solver.

7 Lecture. Fluid Dynamics and Hyperbolic Equations.

The fluid momentum conservation equation derived. Fluid closure.

The Navier-Stokes equation in conservation form. Hyperbolic equations in advection form. Eigenvalue of the Jacobian and Characteristics.

Finite differences and stability: FTCS unstable. Lax-Friedrichs and CFL condition. Lax Wendroff, second order accuracy.

Exercise. Verify stability of Lax Freidrichs scheme. Find eignvalues (analytically) for a compressible fluid.

8 Lecture. Boltzmann's Equation and its solution

The distribution function, and flux-density, energy-density.

Boltzmann's equation derivationas an expression of particle conservation in the presence of collisions and sources.

Integration along orbits/characteristics. Vlasov equation distribution behavior.

The collision term. Simple collision process examples.

Exercise. Demonstrate phase-space divergence. Solve simple collision problem.

9 Lecture. Neutron Transport

The Boltzmann equation in terms of flux. Neutron total loss, scattering and fission source terms. Reduction of Boltzmann equation to a (speed-resolved) diffusion equation.

Groups. Multigroup equations and their numerical representation. Leakage. Diffusive timestep stability.

Eigenvalue nature of the steady problem. Power iteration method to solve for dominant eigenvalue.

Exercise. Formulate the 1-group steady diffusion for a uniform 1-D slab reactor with non-reflective boundaries as a matrix eigenvalue equation. Optionally solve it!

10 Lecture. Atomistic and Particle in Cell Methods

Atomistic simulation. Time and space scales. Generic approach. Interparticle force examples: Lennard-Jones, Morse. Computational requirements. Neighbor lists and blocks.

The computational problem of long-range forces. Particle in Cell solution for plasmas. Pseudo-particle representation. Phase space. Direct Simulation Monte Carlo (DSMC) treatment of tenuous gas. Boundary conditions and their implementation.

Exercise. Build a three-body simulator in 2-D with specified interparticle force law.

11 Lecture. Monte-Carlo techniques for computational modelling

Collisions. Random numbers and statistical distributions. Basic introduction to probability (random variables, pdf, cumulative probability) and statistics (mean, variance, standard error). Random sampling from basic distributions used in Monte Carlo simulations (uniform, exponential, ...) and rejection sampling technique. Flux weighted injection.

Exercise. Construct a statistical distribution function using a random number generator.

or

Exercise. Sample distributions using direct and rejection sampling. Implement binary search algorithm?

12 Lecture. Monte Carlo Radiation Transport

Transport and collisions. Random walk step length; Poisson statistics. Collision-type choice. New particle generation.

Tracking and tallying of collisions. Statistical uncertainty, and tallying methods to reduce it. Importance sampling.