22.15 Essential Numerical Methods
I H Hutchinson

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 9am-9:30am Tuesday. All room 24-121.]

<table>
<thead>
<tr>
<th>Sep</th>
<th>5</th>
<th>Fitting curves to data.</th>
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<tbody>
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<td></td>
<td>10</td>
<td>ODE integration. 2-point ODE problems.</td>
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<td>17</td>
<td>PDE intro. PDE diffusive relaxation.</td>
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<td>24</td>
<td>Iterative matrix inversion. Fluid flow.</td>
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<td>Oct</td>
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<td>Boltzmann equation. Neutron transport.</td>
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<td>8</td>
<td>Atomistic modelling. MC techniques.</td>
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<td>17</td>
<td>Uncertainty, Tracking and Tallying. Finite Elements, Revision.</td>
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<td>24</td>
<td>Final: 3 hours. 9am-noon. NW14-1112.</td>
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Grade Basis

The grade basis will be

- 20% Homework (exercise) assignment evaluation.
- 5% Class interaction

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


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.


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.


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.


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.


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


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 on Mondays 9am - 9:30am before the lecture. If there is a demonstrated interest or need, they will also be offered on Wednesday at the same time. 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 are intended to be hands-on programming tasks that the students undertake. Essentially all of them can be done in Matlab, though that might not necessarily be the only or best way to do them. Probably not all exercises can be included in any one term, so some can be considered alternative options.

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.


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.

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

4 Lecture. Partial Differential Equations

Examples of partial differential equations of engineering physics.

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.
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


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

7 Lecture. Fluid Dynamics and Hyperbolic Equations.


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

8 Lecture. Boltzmann’s Equation and its solution

The distribution function, and flux-density, energy-density. Boltzmann’s equation derivation as 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.


9 Lecture. Neutron Transport

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


Exercise. Build a three-body simulator in 2-D with specified inter-particle 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


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