

## TABLE OF CONTENTS

	<u>Page</u>
LECTURE 1.....	1.1
INTRODUCTION .....	1.1
Formulating a “Mathematical” Model versus a Physical Model .....	1.1
Sources of Error in a Mathematical Solution.....	1.3
Solutions to Governing Equations .....	1.4
Numerical Methods.....	1.5
How Numerical Methods Work.....	1.5
Why Study Numerical Methods.....	1.7
Typical Difficulties Encountered with Numerical Methods .....	1.8
Example - Geophysical Flows due to Tides and Winds in the Coastal Ocean .....	1.10
Taylor Series .....	1.12
<i>Example</i> .....	1.14
<i>Example</i> .....	1.15
<i>Example</i> .....	1.16
SUMMARY OF LECTURE 1 .....	1.17
 LECTURE 2.....	 2.1
DIRECT SOLUTIONS TO LINEAR SYSTEMS OF ALGEBRAIC EQUATIONS .....	 2.1
Cramer’s Rule - A Direct Procedure.....	2.3
<i>Example</i> .....	2.5
Gauss Elimination - A Direct Procedure .....	2.7
<i>Example application</i> .....	2.7
Gauss-Jordan Elimination - A Direct Procedure .....	2.11
Matrix Inversion by Gauss-Jordan Elimination .....	2.12
Gauss Elimination Type Solutions to Banded Matrices .....	2.15
<i>Banded matrices</i> .....	2.15
<i>Savings on storage for banded matrices</i> .....	2.16
<i>Savings on computations for banded matrices</i> .....	2.17
<i>Symmetrical banded matrices</i> .....	2.18
Alternative Compact Storage Modes for Direct Methods .....	2.19
Problems with Gauss Elimination Procedures.....	2.22
<i>Inaccuracies originating from the pivot elements</i> .....	2.22
<i>Partial pivoting</i> .....	2.22
<i>Complete pivoting</i> .....	2.23

	<u>Page</u>
LECTURE 3.....	3.1
DIRECT SOLUTIONS TO LINEAR ALGEBRAIC SYSTEMS -	
CONTINUED .....	3.1
Ill-conditioning of Matrices .....	3.1
<i>Effects of ill-conditioning</i> .....	3.1
<i>Detection of ill-conditioning in a matrix</i> .....	3.1
Factor Method (Cholesky Method).....	3.5
<i>Factorization step</i> .....	3.6
<i>Forward/backward substitution procedures to obtain a</i>	
<i>solution</i> .....	3.10
<i>Notes on Factorization Methods</i> .....	3.11
<i>Advantages of LU factorization over Gauss Elimination</i> .....	3.12
<i>Example comparing costs</i> .....	3.12
Other Factorization Methods for Symmetrical Matrices .....	3.14
<i>Cholesky Square Root Method</i> .....	3.14
<b>LDL<sup>T</sup> Method</b> .....	3.16
Computation of the determinant for Factorization Methods.....	3.18
 LECTURE 4.....	 4.1
ITERATIVE SOLUTIONS TO LINEAR ALGEBRAIC EQUATIONS.....	4.1
<i>Example</i> .....	4.2
(Point) Jacobi Method - An Iterative Method.....	4.4
<i>Example</i> .....	4.8
<i>Iterative convergence</i> .....	4.10
<i>Criteria for ascertaining convergence</i> .....	4.11
(Point) Gauss Seidel Method .....	4.12
Point Relaxation Methods (Successive/Systematic (Over)	
Relaxation - SOR).....	4.14
Application of Gauss-Seidel to Non-Linear Equations .....	4.16
Block Iterative Methods.....	4.17
Direct/Iterative Methods .....	4.17
 LECTURE 5.....	 5.1
INTRODUCTION TO INTERPOLATION .....	5.1
Linear Interpolation .....	5.3
<i>Example 1</i> .....	5.6
Error for Linear Interpolating Functions.....	5.7
Derivation of $e(x)$ .....	5.8
<i>Step 1</i> .....	5.8
<i>Step 2</i> .....	5.9
<i>Step 3</i> .....	5.10
<i>Example 2</i> .....	5.14

	<u>Page</u>
LECTURE 6.....	6.1
LAGRANGE INTERPOLATION .....	6.1
Power Series Fitting to Define Lagrange Interpolation .....	6.3
Lagrange Interpolation Using Basis Functions.....	6.4
Lagrange Linear Interpolation Using Basis Functions .....	6.7
<i>Example</i> .....	6.8
Lagrange Quadratic Interpolation Using Basis Functions .....	6.10
<i>Example</i> .....	6.12
Lagrange Cubic Interpolation Using Basis Functions .....	6.14
<i>Example</i> .....	6.14
Errors Associated with Lagrange Interpolation .....	6.16
<i>Example</i> .....	6.19
SUMMARY OF LECTURES 5 AND 6 .....	6.21
 LECTURE 7.....	 7.1
NEWTON FORWARD INTERPOLATION OF EQUISPACED POINTS ...	7.1
Forward Difference Tables.....	7.2
<i>Example 1</i> .....	7.5
Deriving Newton Forward Interpolation on Equi-spaced Points .....	7.6
<i>Step 1</i> .....	7.7
<i>Step 2a</i> .....	7.7
<i>Step 2b</i> .....	7.9
<i>Step 2c</i> .....	7.11
<i>Step 3a</i> .....	7.13
<i>Step 3b</i> .....	7.14
<i>Step 3c</i> .....	7.15
<i>Example 2</i> .....	7.20
<i>(Part a)</i> .....	7.20
<i>(Part b)</i> .....	7.22
<i>(Part c)</i> .....	7.23
Newton Backward Interpolation .....	7.24
Newton Interpolation on Non-Uniformly Spaced Data Points .....	7.26
SUMMARY OF LECTURE 7 .....	7.27
 LECTURE 8.....	 8.1
INTERPOLATION USING CHEBYSHEV ROOTS .....	8.1
Chebyshev Polynomials.....	8.3
Properties of Chebyshev Polynomials .....	8.6
<i>Example</i> .....	8.8
Application of Chebyshev Roots as Interpolation Points .....	8.10
<i>Example</i> .....	8.12
Generalization of the Interpolation Interval.....	8.15

	<u>Page</u>
LECTURE 9.....	9.1
HERMITE INTERPOLATING POLYNOMIALS .....	9.1
Cubic Hermite Interpolation .....	9.4
General Hermite Interpolation Using Basis Functions .....	9.11
EXTRAPOLATION.....	9.15
SUMMARY OF LECTURES 8 AND 9 .....	9.16
LECTURE 10.....	10.1
SOLVING FOR ROOTS OF NONLINEAR EQUATIONS .....	10.1
<i>Example 1</i> .....	10.1
<i>Example 2</i> .....	10.2
<i>Example 3</i> .....	10.2
Bisection Method with One Root in a Specified Interval .....	10.4
<i>Example 4</i> .....	10.8
<i>Problems with the Bisection Method</i> .....	10.9
Newton-Raphson Method (a. k. a. Newton Method).....	10.11
<i>Derivation of the Newton-Raphson Method</i> .....	10.12
<i>Example 5</i> .....	10.14
<i>Notes on Newton's Method</i> .....	10.15
<i>Problems with Newton's Method</i> .....	10.15
<i>Secant Method</i> .....	10.17
SUMMARY OF LECTURE 10 .....	10.18
LECTURE 11.....	11.1
NUMERICAL DIFFERENTIATION.....	11.1
Taylor Series Expansion for $f(x)$ About a Typical Node $i$ .....	11.2
Approximating Derivatives by Linearly Combining Functional Values at Nodes.....	11.7
<i>Forward first order accurate approximation to the         first derivative</i> .....	11.7
<i>Backward first order accurate approximation to the         first derivative</i> .....	11.9
<i>Central second order accurate approximation to the         first derivative</i> .....	11.10
<i>Forward first order accurate approximation to the         second derivative</i> .....	11.13
TABLE OF DIFFERENCE APPROXIMATIONS .....	11.14

	<u>Page</u>
LECTURE 12.....	12.1
DERIVATION OF DIFFERENCE APPROXIMATIONS USING UNDETERMINED COEFFICIENTS .....	12.1
<i>Forward second order accurate approximation         to the first derivative</i> .....	12.2
<i>Forward first order accurate approximation         to the second derivative</i> .....	12.5
<i>Skewed fourth order accurate approximation         to the second derivative</i> .....	12.7
NUMERICAL DIFFERENTIATION USING DIFFERENCE OPERATORS.....	12.9
Difference Operators.....	12.9
<i>First order difference operators</i> .....	12.9
<i>Notes</i> .....	12.10
<i>Second order forward difference operator</i> .....	12.11
<i>Third order backward difference operator</i> .....	12.12
<i>Second order central difference operator</i> .....	12.13
<i>Second order mixed difference operator</i> .....	12.14
Approximation to Differentiation Using Difference Operators .....	12.15
<i>First order backward difference operator approximation             to the first derivative</i> .....	12.15
<i>First order central difference operator approximation             to the first derivative</i> .....	12.16
<i>Central difference approximation to the first derivative             as an average of first order forward and backward             difference approximations</i> .....	12.17
<i>General difference operator approximations             to derivatives</i> .....	12.18

	<u>Page</u>
LECTURE 13.....	13.1
NUMERICAL DIFFERENTIATION FORMULAE BY INTERPOLATING POLYNOMIALS .....	13.1
Relationship Between Polynomials and Finite Difference Derivative Approximations .....	13.1
Developing Finite Difference Formulae by Differentiating Interpolating Polynomials.....	13.2
<i>Concepts</i> .....	13.2
<i>Procedure</i> .....	13.2
Approximations to First and Second Derivatives Using Quadratic Interpolation .....	13.3
<i>Develop a quadratic interpolating polynomial</i> .....	13.4
<i>Evaluating <math>g^{(1)}(x_0)</math> to obtain a forward difference             approximation to the first derivative</i> .....	13.6
<i>Evaluating <math>g^{(1)}(x_1)</math> to obtain a central difference             approximation to the first derivative</i> .....	13.8
<i>Evaluating <math>g^{(1)}(x_2)</math> to obtain a backward difference             approximation to the first derivative</i> .....	13.10
<i>Evaluating <math>g^{(2)}(x_0)</math> to obtain a forward difference             approximation to the second derivative</i> .....	13.12
<i>Evaluating <math>g^{(2)}(x_1)</math> to obtain a central difference             approximation to the second derivative</i> .....	13.14
<i>Notes on developing differentiation formulae by             interpolating polynomials</i> .....	13.15
Approximations and Associated Error Estimates to First and Second Derivatives Using Quadratic Interpolation.....	13.16
<i>Developing a 3 node interpolating function using             Newton forward interpolation</i> .....	13.16
<i>Deriving a central approximation to the first derivative             and the associated error estimate</i> .....	13.18
<i>Deriving a forward approximation to the second             derivative and the associated error estimate</i> .....	13.23
SUMMARY OF LECTURE 11, 12 AND 13 .....	13.26

	<u>Page</u>
LECTURE 14.....	14.1
PRACTICAL ISSUES IN APPLYING FINITE DIFFERENCE	
APPROXIMATIONS .....	14.1
Derivatives of Variable Coefficients.....	14.1
Two Dimensional Finite Difference Approximations.....	14.4
<i>Example 1</i> .....	14.6
<i>Example 2</i> .....	14.7
 LECTURE 15.....	 15.1
APPLICATIONS OF FD APPROXIMATIONS FOR SOLVING ORDINARY	
DIFFERENTIAL EQUATIONS .....	15.1
Ordinary Differential Equations.....	15.1
<i>Initial Value Problems</i> .....	15.1
<i>Boundary Value Problems</i> .....	15.2
<i>General Initial Value Problems</i> .....	15.2
Solution to a 1st Order Single Equation IVP .....	15.4
<i>Euler Method</i> .....	15.4
<i>Example</i> .....	15.6
<i>General Observations for Solving IVP's</i> .....	15.11
Solutions to Boundary Value Problems .....	15.11
<i>Example</i> .....	15.12
<i>Example</i> .....	15.15
 LECTURE 16.....	 16.1
NUMERICAL SOLUTION OF THE TRANSIENT DIFFUSION	
EQUATION USING THE FINITE DIFFERENCE (FD) METHOD.....	16.1
Explicit Solution Procedure .....	16.2
<i>Example of heat conduction in a rod</i> .....	16.6
<i>General Notes on Instabilities</i> .....	16.9
Implicit Solution Procedure .....	16.9
Crank-Nicolson Implicit (C-N) Method .....	16.14
Weighted Average Approximation.....	16.18

	<u>Page</u>
LECTURE 17.....	17.1
NUMERICAL INTEGRATION.....	17.1
Trapezoidal Rule.....	17.2
Evaluation of Error for Trapezoidal Rule.....	17.5
<i>Evaluation of error by integrating <math>e(x)</math></i> .....	17.5
<i>Evaluation of the error for Trapezoidal Rule by</i>	
<i>Taylor Series expansion</i> .....	17.6
Extended Trapezoidal Rule.....	17.10
Romberg Integration.....	17.13
<i>Example</i> .....	17.18
Romberg Integration Using 3 Estimates of the Integral.....	17.21
SUMMARY OF LECTURE 17.....	17.23
 LECTURE 18.....	 18.1
NUMERICAL INTEGRATION CONTINUED.....	18.1
Simpson's 1/3 Rule.....	18.1
Evaluation of Error for Simpson's 1/3 Rule.....	18.4
Extended Simpson's 1/3 Rule.....	18.7
Newton Cotes Closed Formulae.....	18.11
Newton-Cotes Open Formulae.....	18.15
 LECTURE 19.....	 19.1
GAUSS QUADRATURE.....	19.1
Derivation of Gauss Quadrature by Integrating Exact	
Polynomials and Matching.....	19.4
<i>Derive 1 point Gauss-Quadrature</i> .....	19.4
<i>Derive a 2 point Gauss Quadrature Formula</i> .....	19.6
<i>Gauss Legendre Formulae</i> .....	19.9
Derivation of Gauss Quadrature by Integrating Hermite	
Interpolating Functions.....	19.11
<i>Hermite Interpolation Formulae</i> .....	19.11
<i>Example of defining a cubic Hermite interpolating</i>	
<i>function</i> .....	19.13
<i>Gauss-Legendre quadrature by integrating</i>	
<i>Hermite interpolating polynomials</i> .....	19.20
<i>Two point Gauss-Legendre integration</i> .....	19.27
<i>Step 1 - Establish interpolating points</i> .....	19.28
<i>Step 2 - Establish the coefficients of the derivative</i>	
<i>terms in the integration formula</i> .....	19.30
<i>Step 3 - Develop <math>A_0, A_1</math></i> .....	19.36

	<u>Page</u>
LECTURE 20.....	20.1
SOLUTION TO SINGLE 1ST ORDER INITIAL VALUE PROBLEMS (IVP's).....	20.1
<i>Runge-Kutta type formulas</i> → <i>Single Step Methods</i> .....	20.2
<i>Multi-step Methods</i> .....	20.3
Runge-Kutta type methods .....	20.4
Euler Method .....	20.5
<i>Derivation 1</i> .....	20.5
<i>Derivation 2</i> .....	20.7
<i>Detailed analysis of truncation error for the Euler Method..</i>	20.9
 LECTURE 21.....	 21.1
SOLUTIONS TO O.D.E.S Continued.....	21.1
2nd Order Runge-Kutta Methods.....	21.2
<i>Improved Euler Method (Modified Euler-Cauchy)</i> .....	21.6
<i>Modified Euler Method</i> .....	21.8
4th Order Runge-Kutta (often referred to as the “Runge-Kutta formula”).....	21.10
Summary of Runge-Kutta Methods .....	21.12
 LECTURE 22.....	 22.1
MULTI STEP METHODS.....	22.1
Open Formulae.....	22.3
<i>Derivation</i> .....	22.3
<i>1st Order Accurate Adams Open Formula</i> .....	22.3
<i>2nd Order Accurate Adams Open Formula</i> .....	22.4
<i>Example Application of 2nd Order Adams Open Formula</i> ....	22.6
<i>3rd Order Accurate Adams Open Formula</i> .....	22.9
<i>Summary of Adams Open Formulae</i> .....	22.11
Closed Formulae .....	22.12
<i>Derivation</i> .....	22.12
<i>First Order Accurate Adams Closed Formula</i> .....	22.13
<i>2nd Order Accurate Adams Closed Formulae</i> .....	22.15
<i>3rd Order Accurate Adams Closed Formula</i> .....	22.17
Predictor-Corrector Methods .....	22.19
<i>Example</i> .....	22.20
Implementation of Changes in Time Step.....	22.23
Comments Predictor-Corrector Methods .....	22.24

	<u>Page</u>
LECTURE 23.....	23.1
SETS OF SIMULTANEOUS FIRST ORDER O.D.E.'S.....	23.1
Boundary Value Problems.....	23.2
Matrix Methods.....	23.3
Shooting Methods.....	23.3

	<u>Page</u>
REVIEW NO. 1 .....	R1.1
TAYLOR SERIES.....	R1.1
NUMERICAL SOLUTION TO LINEAR SYSTEMS OF ALGEBRAIC	
EQUATIONS .....	R1.5
Direct Methods.....	R1.5
<i>Gauss elimination</i> .....	R1.5
<i>LU decomposition - Cholesky decomposition (a factor</i>	
<i>method)</i> .....	R1.6
<i>Matrix conditioning</i> .....	R1.7
<i>Matrix storage</i> .....	R1.7
Iterative Methods .....	R1.8
INTERPOLATION .....	R1.9
Lagrange Interpolation.....	R1.9
<i>Method 1 to derive g(x): Power series</i> .....	R1.10
<i>Method 2 to derive g(x): Lagrange basis functions</i> .....	R1.10
<i>Method 3 to derive g(x): Newton forward interpolation</i> .....	R1.13
<i>Interpolation using Chebyshev roots</i> .....	R1.15
Extrapolation.....	R1.16
Hermite Interpolation.....	R1.16
ROOT FINDING ALGORITHMS .....	R1.17
Bisection Method for Finding Roots .....	R1.17
Newton-Raphson Method .....	R1.17

## REVIEW NO. 2

NUMERICAL DIFFERENTIATION	
Generic Method to Derive a Difference Formula .....	R2.2
Numerical Differentiation Formulae Using Interpolating	
Polynomials .....	R2.2
Errors for Numerical Differentiation .....	R2.3
INTRODUCTION TO O.D.E.'s AND P.D.E.'S.....	R2.5
Partial Differentiation .....	R2.5
Solving Single Equation O.D.E. I.V.P.'s .....	R2.5
Solving O.D.E. Boundary Value Problems.....	R2.6
Solutions to P.D.E.'s.....	R2.7
NUMERICAL INTEGRATION .....	R2.9
Basic Development of Integration Formulae .....	
<i>Newton Cotes Closed Formulae</i> .....	R2.10
<i>Newton Cotes Open Formulae</i> .....	R2.10
<i>Gauss Legendre Integration Formulae</i> .....	R2.11
Methods for Evaluating the Accuracy of Integration Methods	
For a Sub-interval.....	R2.13
<i>Method 1: Develop Taylor Series expansions for <math>f(x)</math> and</i> <i>the functional values at the nodes</i> .....	R2.13
<i>Method 2: Use error terms from the interpolating function</i> ..	R2.14
Accuracy of Extended Integration Methods .....	R2.15
Rombert Integration .....	R2.18

	<u>Page</u>
REVIEW NO. 3 .....	R3.1
O.D.E. CLASSIFICATION .....	R3.1
I.V.P. SOLUTIONS - 1ST ORDER EQUATIONS - SINGLE STEP	
METHODS .....	R3.2
Runge-Kutta Formula .....	R3.2
Procedure for Deriving R.K. Methods .....	R3.3
Step 1 .....	R3.3
Step 2 .....	R3.4
Step 3 .....	R3.4
Step 4 .....	R3.5
Step 5 .....	R3.5
Advantages of R.K. methods .....	R3.6
Disadvantages of R.K. Methods .....	R3.6
SOLUTIONS TO I.V.P.'S - MULTI-STEP METHODS.....	R3.7
Open Formulae.....	R3.8
How to Derive Open Formulae .....	R3.8
Step 1 .....	R3.8
Step 2 .....	R3.9
Advantages of Open formulae .....	R3.10
Disadvantages of Open formulae.....	R3.10
Closed Formulae .....	R3.11
How to Derive Closed Formulae.....	R3.11
Step 1 .....	R3.11
Step 2 .....	R3.12
Advantages of Closed Formulae .....	R3.12
Disadvantages of Closed Formulae.....	R3.12
Predictor-Corrector Methods .....	R3.13
Predictor $\rightarrow$ Open Formula .....	R3.13
Corrector $\rightarrow$ Closed Formula .....	R3.13
Starter .....	R3.13
Modifier.....	R3.13
Advantages of Predictor-Corrector Methods .....	R3.14
SIMULTANEOUS FIRST ORDER I.V.P.'S .....	R3.15
B.V.P. SOLUTIONS .....	R3.15
COURSE SUMMARY .....	R3.16
Survey of Many Numerical Methods.....	R3.16
Numerical Interpolation.....	R3.16
Numerical Differentiation .....	R3.16
Numerical Integration.....	R3.17
O.D.E./I.V.P.'s $\rightarrow$ Time Dependent Problems.....	R3.17
O.D.E./B.V.P.'s $\rightarrow$ Spatially Dependent Problems .....	R3.17
P.D.E. Solutions .....	R3.18
Solutions of Simultaneous Linear Algebraic Equations .....	R3.18
Course Concepts .....	R3.19