

Contents

1	Introduction.....	1
1.1	Introduction to Maple	1
1.1.1	Getting Started with Maple.....	1
1.1.2	Plotting with Maple	3
1.1.3	Solving Linear and Nonlinear Equations	5
1.1.4	Matrix Operations	6
1.1.5	Differential Equations.....	11
1.1.6	Laplace Transformations	16
1.1.7	Do Loop.....	18
1.1.8	While Loop.....	19
1.1.9	Write Data Out Example.....	19
1.1.10	Reading in Data from a Text File.....	23
1.1.11	Summary.....	24
1.1.12	Problems	24
	References	27
2	Initial Value Problems.....	29
2.1	Linear Ordinary Differential Equations	29
2.1.1	Introduction.....	29
2.1.2	Homogeneous Linear ODEs.....	29
2.1.3	First Order Irreversible Series Reactions.....	31
	Example 2.1. Irreversible Series Reactions (see equations (2.8)).....	32
2.1.4	First Order Reversible Series Reactions	37
	Example 2.2. Reversible Series Reactions (see equations (2.10)).....	38
2.1.5	Nonhomogeneous Linear ODEs	47
	Example 2.3. Heating of Fluid in a Series of Tanks	49
	Example 2.4. Time Varying Input to a CSTR with a Series Reaction	56
2.1.6	Higher Order Linear Ordinary Differential Equations	63

Example 2.5 A Second Order ODE	65
2.1.7 Solving Systems of ODEs Using the Laplace Transform	
Method	72
Example 2.6. Laplace Solution of Example 2.1 Equations	73
Example 2.7. Laplace Solution for Second Order System with	
Dirac forcing Function	76
2.1.8 Solving Linear ODEs Using Maple's 'dsolve' Command	80
Example 2.8. Solving Linear ODEs Using Maple	80
Example 2.9. Heat Transfer in a Series of Tanks, 'dsolve'	81
2.1.9 Summary	83
2.1.10 Problems	84
2.2 Nonlinear Ordinary Differential Equations	87
2.2.1 Introduction	87
Example 2.2.1. Simultaneous Series Reactions	88
2.2.2 Solving Nonlinear ODEs Using Maple's 'dsolve'	
Command	94
2.2.3 Series Solutions for Nonlinear ODEs	98
Example 2.2.2. Fermentation Kinetics	99
Example 2.2.3	101
2.2.4 Stop Conditions	103
Example 2.2.4. Stop Conditions	103
2.2.5 Stiff ODEs	107
Example 2.2.5. Stiff Ordinary Differential Equations	107
2.2.6 Differential Algebraic Equations	112
Example 2.2.6. Differential Algebraic Equations	112
2.2.7 Multiple Steady States	116
Example 2.2.7. Multiple Steady States	117
2.2.8 Steady State Solutions	124
Example 2.2.8. Steady State Solutions	124
Example 2.2.9. Phase Plane Analysis	139
2.2.9 Summary	148
2.2.10 Problems	149
Appendix A: Matrix Exponential Method	155
Appendix B: Matrix Exponential by the Laplace Transform	
Method	161
References	167
3 Boundary Value Problems	169
3.1 Linear Boundary Value Problems	169
3.1.1 Introduction	169
3.1.2 Exponential Matrix Method for Linear Boundary Value	
Problems	169
Example 3.1	171
Example 3.2	175
3.1.3 Exponential Matrix Method for Linear BVPs with	
Semi-infinite Domains	180

Example 3.3	181
3.1.4 Use of Matrizant in Solving Boundary Value Problems	184
Example 3.4	185
Example 3.5	187
Example 3.6	189
3.1.5 Symbolic Finite Difference Solutions for Linear Boundary Value Problems	195
Example 3.7	196
Example 3.8. Cylindrical Catalyst Pellet	203
3.1.6 Solving Linear Boundary Value Problems Using Maple's 'dsolve' Command	208
Example 3.9. Heat Transfer in a Fin	208
Example 3.10. Cylindrical Catalyst Pellet	209
Example 3.11. Spherical Catalyst Pellet	210
3.1.7 Summary	212
3.1.8 Exercise Problems	213
3.2 Nonlinear Boundary Value Problems	217
3.2.1 Introduction	217
3.2.2 Series Solutions for Nonlinear Boundary Value Problems	218
Example 3.2.1. Series Solutions for Diffusion with a Second Order Reaction	218
Example 3.2.2. Series Solutions for Non-isothermal Catalyst Pellet – Multiple Steady States	223
3.2.3 Finite Difference Solutions for Nonlinear Boundary Value Problems	229
Example 3.2.3. Diffusion with a Second Order Reaction	229
3.2.4 Shooting Technique for Boundary Value Problem	233
Example 3.2.4. Nonlinear Heat Transfer	233
Example 3.2.5. Multiple Steady States in a Catalyst Pellet	238
3.2.5 Numerical Solution for Boundary Value Problems Using Maple's 'dsolve' Command	244
Example 3.2.6. Diffusion with Second Order Reaction	245
Example 3.2.7. Heat Transfer with Nonlinear Radiation Boundary Conditions	247
Example 3.2.8. Diffusion of a Substrate in an Enzyme Catalyzed Reaction – BVPs with Removable Singularity	250
Example 3.2.9. Multiple Steady States in a Catalyst Pellet	253
Example 3.2.10. Blasius Equation – Infinite Domains	256
3.2.6 Numerical Solution for Coupled BVPs Using Maple's 'dsolve' Command	259
Example 3.2.11. Axial Conduction and Diffusion in a Tubular Reactor	259
3.2.7 Solving Boundary Value Problems and Initial Value Problems	262
Example 3.2.12. Diffusion with a Second Order Reaction	262

3.2.8	Multiple Steady States	266
	Example 3.2.13. Multiple Steady States in a Catalyst Pellet - η vs. Φ	266
3.2.9	Eigenvalue Problems	272
	Example 3.2.14. Graetz Problem–Finite Difference Solution	272
	Example 3.2.15. Graetz Problem–Shooting Technique	278
3.2.10	Summary	286
3.2.11	Exercise Problems	288
References		293
4	Partial Differential Equations in Semi-infinite Domains.....	295
4.1	Partial Differential Equations (PDEs) in Semi-infinite Domains	295
4.2	Laplace Transform Technique for Parabolic PDEs	295
	Example 4.1. Heat Conduction in a Rectangular Slab	296
	Example 4.2. Heat Conduction with Transient Boundary Conditions	301
	Example 4.3. Heat Conduction with Flux Boundary Conditions	305
	Example 4.4. Heat Conduction with an Initial Profile	308
	Example 4.5. Heat Conduction with a Source Term	311
4.3	Laplace Transform Technique for Parabolic PDEs – Advanced Problems	314
	Example 4.6. Heat Conduction with Radiation at the Surface	314
	Example 4.7. Unsteady State Diffusion with a First-Order Reaction	318
4.4	Similarity Solution Technique for Parabolic PDEs	324
	Example 4.8. Heat Conduction in a Rectangular Slab	325
	Example 4.9. Laminar Flow in a CVD Reactor	328
4.5	Similarity Solution Technique for Elliptic Partial Differential Equations	333
	Example 4.10. Steady State Heat Conduction in a Plate	333
	Example 4.11. Current Distribution in an Electrochemical Cell	336
4.6	Similarity Solution Technique for Nonlinear Partial Differential Equations	339
	Example 4.12. Variable Diffusivity	340
	Example 4.13. Plane Flow Past a Flat Plate – Blasius Equation	342
4.7	Summary	348
4.8	Exercise Problems	348
References		352
5	Method of Lines for Parabolic Partial Differential Equations.....	353
5.1	Semianalytical Method for Parabolic Partial Differential Equations (PDEs)	353
	5.1.1 Introduction	353
	5.1.2 Semianalytical Method for Homogeneous PDEs	353
	Example 5.1. Heat Conduction in a Rectangular Slab	356

5.1.3	Semianalytical Method for Nonhomogeneous PDEs.....	365
	Example 5.2.....	366
	Example 5.3.....	374
	Example 5.4.....	382
	Example 5.5.....	390
	Example 5.6. Semianalytical Method for the Graetz Problem.....	401
	Example 5.7. Semianalytical Method for PDEs with Known Initial Profiles.....	414
5.1.4	Semianalytical Method for PDEs in Composite Domains	425
	Example 5.8.....	425
5.1.5	Expediting the Calculation of Exponential Matrix	437
	Example 5.9.....	438
	Example 5.10.....	442
	Example 5.11.....	448
5.1.6	Summary.....	451
5.1.7	Exercise Problems.....	452
5.2	Numerical Method of Lines for Parabolic Partial Differential Equations (PDEs).....	456
5.2.1	Introduction.....	456
5.2.2	Numerical Method of Lines for Parabolic PDEs with Linear.....	456
	Example 5.2.1. Diffusion with Second Order Reaction.....	458
	Example 5.2.2. Variable Diffusivity	464
5.2.3	Numerical Method of Lines for Parabolic PDEs with Nonlinear Boundary.....	469
	Example 5.2.3. Nonlinear Radiation at the Surface	470
5.2.4	Numerical Method of Lines for Stiff Nonlinear PDEs	474
	Example 5.2.4. Exothermic Reaction in a Sphere.....	474
5.2.5	Numerical Method of Lines for Nonlinear Coupled PDEs	480
	Example 5.2.5. Two Coupled PDEs	480
5.2.6	Numerical Method of Lines for Moving Boundary Problems	491
	Example 5.2.6. The Shrinking Core Model for Catalyst Regeneration	491
5.2.7	Summary.....	501
5.2.8	Exercise Problems.....	502
	References	505
6	Method of Lines for Elliptic Partial Differential Equations.....	507
6.1	Semianalytical and Numerical Method of Lines for Elliptic PDEs	507
6.1.1	Introduction.....	507
6.1.2	Semianalytical Method for Elliptic PDEs in Rectangular Coordinates	507
	Example 6.1. Heat Transfer in a Rectangle	508
	Example 6.2.....	520

6.1.3	Semianalytical Method for Elliptic PDEs in Cylindrical Coordinates – Graetz Problem	536
	Example 6.3. Graetz Problem with a Fixed Wall Temperature	536
6.1.4	Semianalytical Method for Elliptic PDEs with Nonlinear Boundary Conditions	547
	Example 6.4. Nonlinear Radiation Boundary Condition	547
6.1.5	Semianalytical Method for Elliptic PDEs with Irregular Shapes	556
	Example 6.5. Potential Distribution in a Hull Cell	556
6.1.6	Numerical Method of Lines for Elliptic PDEs in Rectangular Coordinates	564
	Example 6.6. Numerical Solution for Heat Transfer in a Rectangle	565
	Example 6.7. Numerical Solution for Heat Transfer for Nonlinear Elliptic PDEs	573
6.1.7	Summary	581
	References	585
7	Partial Differential Equations in Finite Domains.....	587
7.1	Separation of Variables Method for Partial Differential Equations (PDEs) in Finite Domains	587
7.1.1	Introduction.....	587
7.1.2	Separation of Variables for Parabolic PDEs with Homogeneous Boundary Conditions	587
	Example 7.1. Heat Conduction in a Rectangle	587
	Example 7.2. Heat Conduction with an Insulator Boundary Condition	599
	Example 7.3. Mass Transfer in a Spherical Pellet	604
7.1.3	Separation of Variables for Parabolic PDEs with an Initial Profile	609
	Example 7.4. Heat Conduction in a rectangle with an Initial Profile.....	609
	Example 7.5. Heat Conduction in a Slab with a Linear Initial Profile.....	613
7.1.4	Separation of Variables for Parabolic PDEs with Eigenvalues Governed by Transcendental Equations	618
	Example 7.6. Heat Conduction in a Slab with Radiation Boundary Conditions	618
7.1.5	Separation of Variables for Parabolic PDEs with Nonhomogeneous Boundary Conditions	623
	Example 7.7. Heat Conduction in a slab with Nonhomogeneous Boundary Conditions	623
	Example 7.8. Diffusion with Reaction.....	629
7.1.6	Separation of Variables for Parabolic PDEs with Two Flux Boundary Conditions	635

Example 7.9. Diffusion in a Slab with Nonhomogeneous Flux Boundary Conditions	635
7.1.7 Numerical Separation of Variables for Parabolic PDEs	643
Example 7.10. Heat Transfer in a Rectangle.....	643
7.1.8 Separation of Variables for Elliptic PDEs	649
Example 7.11. Heat Transfer in a Rectangle.....	649
Example 7.12. Diffusion in a Cylinder	655
Example 7.13. Heat Transfer with Nonhomogeneous Boundary Conditions	660
Example 7.14. Heat Transfer with a Nonhomogeneous Governing Equation	667
7.1.9 Summary.....	672
7.1.10 Exercise Problems.....	672
References.....	678
8 Laplace Transform Technique for Partial Differential Equations.....	679
8.1 Laplace Transform Technique for Partial Differential Equations (PDEs) in Finite Domains.....	679
8.1.1 Introduction.....	679
8.1.2 Laplace Transform Technique for Hyperbolic PDEs.....	679
Example 8.1. Wave Propagation in a Rectangle	679
Example 8.2. Wave Propagation in a Rectangle	682
8.1.3 Laplace Transform Technique for Parabolic Partial Differential Equations – Simple Solutions.....	685
Example 8.3. Heat Transfer in a Rectangle	685
Example 8.4. Transient Heat Transfer in a Rectangle.....	688
8.1.4 Laplace Transform Technique for Parabolic Partial Differential Equations – Short Time Solution	690
Example 8.5. Heat Transfer in a Rectangle	691
Example 8.6. Mass Transfer in a Spherical Pellet	696
8.1.5 Laplace Transform Technique for Parabolic Partial Differential Equations – Long Time Solution.....	701
Example 8.7. Heat Conduction with an Insulator Boundary Condition	703
Example 8.8. Diffusion with Reaction.....	709
Example 8.9. Heat Conduction with Time Dependent Boundary Conditions	714
8.1.6 Laplace Transform Technique for Parabolic Partial Differential Equations – Heaviside Expansion Theorem for Multiple Roots	719
Example 8.10. Heat Transfer in a Rectangle.....	720
Example 8.11. Diffusion in a Slab with Nonhomogeneous Flux Boundary Conditions during Charging of a Battery.....	725
Example 8.12. Distribution of Overpotential in a Porous Electrode	729

Example 8.13. Heat Conduction in a Slab with Radiation Boundary Conditions	736
8.1.7 Laplace Transform Technique for Parabolic Partial Differential Equations in Cylindrical Coordinates	742
Example 8.14. Heat Conduction in a Cylinder	742
8.1.8 Laplace Transform Technique for Parabolic Partial Differential Equations for Time Dependent Boundary Conditions – Use of Convolution Theorem	747
Example 8.15. Heat Conduction in a Rectangle with a Time Dependent Boundary Condition	748
8.1.9 Summary	755
8.1.10 Exercise Problems	755
References	760
9 Parameter Estimation	761
9.1 Introduction	761
9.2 Least Squares Method	762
9.2.1 Summation Form or Classical Form	769
9.2.2 Confidence Intervals: Classical Approach	775
9.2.3 Prediction of New Observations	776
9.2.4 A One Parameter through the Origin Model	777
9.3 Nonlinear Least Squares	778
Example 9.1. Parameter Estimation	783
9.4 Hessian Matrix Approach	789
9.5 Confidence Intervals	795
9.6 Sensitivity Coefficient Equations	797
9.7 One Parameter Model	807
9.8 Two Parameter Model	812
9.9 Exercise Problems	819
References	819
10 Miscellaneous Topics	821
10.1 Miscellaneous Topics on Numerical Methods	821
10.1.1 Introduction	821
10.1.2 Iterative Finite Difference Solution for Boundary Value Problems	821
Example 10.1. Diffusion with a Second Order Reaction	821
Example 10.2. Nonisothermal Reaction in a Catalyst Pellet – Multiple Steady States	825
10.1.3 Finite Difference Solution for Elliptic PDEs	827
Example 10.3. Heat Transfer in a Rectangle	827
Example 10.4. Heat Transfer in a Cylinder	832
10.1.4 Iterative Finite Difference Solution for Elliptic PDEs	833
Example 10.5. Heat Transfer in a Rectangle – Nonlinear Elliptic PDE	833

10.1.5	Numerical Method of Lines for First Order Hyperbolic PDEs	838
	Example 10.6. Wave Propagation in a Rectangle with Consistent Initial/Boundary Conditions.	839
	Example 10.7. Wave Propagation in a Rectangle with inconsistent Initial/Boundary Conditions	844
10.1.6	Numerical Method of Lines for Second Order Hyperbolic PDEs	848
	Example 10.8. Wave Equation with Consistent Initial/Boundary Conditions	848
	Example 10.9. Wave Equation with Inconsistent Initial/Boundary Conditions	852
10.1.7	Summary	855
10.1.8	Exercise Problems	855
	References	856
	Subject Index	857