Contents

Preface		ix
To the Instructor		
Behind	the Scenes: Design of a Modern and Integrated Course	xiii
Снарт	ER 1 - Analytical & Numerical Solutions	1
1.1	NUMERICAL EXPLORATION	1
1.2	A COMPUTATIONAL DISCOVERY: UNIVERSALITY OF PERIOD DOUBLING	4
Снарт	ER 2 - A Few Concepts from Numerical Analysis	9
2.1	ROOT FINDING: FAST AND UNRELIABLE	9
2.2	ERROR PROPAGATION	13
2.3	NUMERICAL INSTABILITIES	15
Снарт	ER 3 - Roundoff & Number Representation	19
3.1	NUMBER REPRESENTATION	19
3.2	IEEE STANDARDIZATION	22
3.3	ROUNDOFF SENSITIVITY	25
Снарт	ER 4 • Programming Languages & Tools	29
4.1	HIGH-LEVEL PROGRAMMING LANGUAGES	29
4.2	INTERACTIVE COMPUTATIONAL ENVIRONMENTS	32
4.3	RELEVANT LANGUAGE AND IMPLEMENTATION	
	FEATURES	34
4.4	DATA VISUALIZATION	38
CHAPTER 5 - Sample Problems; Building Conclusions		41
5.1	CHAOTIC STANDARD MAP	41

V

5.2	GRAVITATIONAL 3-BODY PROBLEM	45
CHAPT	ER 6 • Approximation Theory	51
6.1	DIFFERENTIATION: FINITE DIFFERENCES	51
6.2	VERIFYING THE CONVERGENCE OF A METHOD	53
6.3	NUMERICAL INTEGRATION: ILLUSIONS ABOUT WHAT LIES BETWEEN	55
6.4	NOTIONS OF ERROR AND CONVERGENCE*	57
6.5	POLYNOMIAL INTERPOLATION	58
Снарт	ER 7 • Other Common Computational Methods	63
7.1	FITTING GRAPHS TO DATA IN THE AGE OF COMPUTATION	63
7.2	FOURIER TRANSFORMS	65
7.3	ORDINARY DIFFERENTIAL EQUATIONS	68
7.4	SYMBOLIC COMPUTATION	70
Chapt	CHAPTER 8 - Performance Basics & Computer Architectures	
8.1	EXECUTION SPEED AND LIMITING FACTORS OF COMPUTATIONS	77
8.2	MEMORY AND DATA TRANSFER	79
8.3	A PROGRAMMER'S VIEW OF COMPUTER HARDWARE	82
8.4	COMPUTER ARCHITECTURES AND TECHNOLOGICAL CHANGE	85
CHAPT	ER 9 High-Performance & Parallel Computing	89
9.1	CODE OPTIMIZATION	89
9.2	PARALLEL COMPUTING	93
9.3	PROGRAMMING AND UTILIZING PARALLEL HARDWARE	95
9.4	HARDWARE ACCELERATION	99
Снарт	ER 10 - The Operation Count; Numerical Linear Algebra	103
10.1	INTRODUCTION	103
10.2	OPERATION COUNTS IN LINEAR ALGEBRA	103
10.3	OPERATION COUNTS FOR A FEW COMMON	104
10.4	DATA MOVEMENT AND DATA LOCALITY	107
10.1	UCALITY AND DATA LOCALITY	109

Снарт	TER 11 - Random Numbers & Stochastic Methods	113		
11.1	GENERATION OF PROBABILISTIC DISTRIBUTIONS	113		
11.2	MONTE CARLO INTEGRATION: ACCURACY THROUGH			
	RANDOMNESS	114		
11.3	SAMPLE PROBLEM: ISING MODEL*	116		
CHAPTER 12 - Algorithms, Data Structures, and Complexity				
12.1	AN EXAMPLE ALGORITHM: HEAPSORT	123		
12.2	DATA STRUCTURES	125		
12.3	COMPUTATIONAL COMPLEXITY & INTRACTABLE PROBLEMS	127		
12.4	APPROXIMATIONS CAN REDUCE COMPLEXITY	129		
CHAPTER 13 Data 1				
13.1	DATA FILES AND FORMATS	136		
13.2	TEXT PROCESSING UTILITIES	140		
13.3	NETWORK AND STORAGE TECHNOLOGIES	143		
13.4	WEB SCRAPING AND DATA ARCHIVING	145		
CHAPTER 14 Building Programs for Computation and Data				
	Analysis	149		
14.1	PROGRAMMING	149		
14.2	SCRIPTING LANGUAGES	152		
14.3	DATA-INTENSIVE PROBLEMS	153		
Снарт	ER 15 - A Crash Course on Partial Differential Equations	5 157		
15.1	INITIAL VALUE PROBLEMS BY FINITE DIFFERENCES	157		
15.2	NUMERICAL STABILITY REVISITED	162		
15.3	BOUNDARY VALUE PROBLEMS BY FINITE	162		
1E /		165		
15.4	OTHER METHODS FOR FDLS	105		
CHAPT	CHAPTER 16 • Reformulated Problems			
16.1	THREE AND A HALF FORMULATIONS OF			
	ELECTROSTATICS	169		
16.2	SCHRÖDINGER EQUATION*	171		
16.3	OUTLINE OF DENSITY FUNCTIONAL METHOD*	173		

APPENDIX A • The Unix Environment	177
APPENDIX B • Numerical Libraries	181
APPENDIX C - Answers to Brainteasers	183
Bibliography	185
Index	187