

---

# Contents

<b>1</b>	<b>Introduction to Computational Science . . . . .</b>	<b>1</b>
1.1	Objectives . . . . .	1
1.2	Definitions . . . . .	1
1.3	Introductory Example . . . . .	2
1.4	Another Example . . . . .	4
1.5	What Is Computational Science? . . . . .	6
1.6	Related Modules . . . . .	8
	References . . . . .	8
<b>2</b>	<b>Types of Visualization and Modeling . . . . .</b>	<b>9</b>
2.1	Objectives . . . . .	9
2.2	Definitions . . . . .	9
2.3	Motivation . . . . .	9
2.4	Introduction . . . . .	10
2.5	Agent-Based Chemical Kinetics . . . . .	11
2.6	Systems Dynamics Chemical Kinetics . . . . .	15
	2.6.1 Simple First Order Reaction . . . . .	15
	2.6.2 Reversible First Order Reactions . . . . .	18
2.7	Computing Questions . . . . .	19
2.8	Related Modules . . . . .	19
	References . . . . .	20
<b>3</b>	<b>Data Types: Representation, Abstraction, Limitations . . . . .</b>	<b>21</b>
3.1	Objectives . . . . .	21
3.2	Definitions . . . . .	21
3.3	Motivation . . . . .	22
3.4	Abstraction . . . . .	22
3.5	Limitations and Space Issues . . . . .	24
3.6	Limits and Errors . . . . .	26
3.7	Order of Operation . . . . .	28
3.8	Accuracy and Speed . . . . .	29
3.9	Collecting Groups of Similar Data . . . . .	32
3.10	Adding Structure to the Homogeneous: Trees . . . . .	35

3.11	Adding Structure to the Homogeneous Collections: Graphs . . . .	36
3.12	Adding Structure to Homogeneous Collections: Stacks and Queues . . . . .	37
3.13	Related Modules . . . . .	38
	References . . . . .	38
<b>4</b>	<b>Scientific Data Acquisition . . . . .</b>	<b>39</b>
4.1	Objectives . . . . .	39
4.2	List of Terms . . . . .	39
4.3	Motivation . . . . .	39
4.4	A First Problem – Introduction . . . . .	40
4.5	Sensor Considerations . . . . .	41
4.6	Computing Issues . . . . .	42
4.7	A Second Problem – Design . . . . .	43
4.8	A Third Problem – Bonus . . . . .	44
4.9	Computing Questions . . . . .	44
4.10	Related Modules . . . . .	44
<b>5</b>	<b>Procedures: Algorithms and Abstraction . . . . .</b>	<b>45</b>
5.1	Objectives . . . . .	45
5.2	Definitions . . . . .	45
5.3	Motivation . . . . .	45
5.4	Procedures . . . . .	46
5.5	Control Structure Example . . . . .	47
5.6	Procedural Abstraction . . . . .	48
5.7	Theater Lights Part 1 . . . . .	48
5.8	Theater Lights Part 2 . . . . .	51
5.9	Leaves on the River Part 1 . . . . .	52
5.10	Leaves on the River Part 2 . . . . .	55
5.11	Related Modules . . . . .	57
	References . . . . .	57
<b>6</b>	<b>Solving Equations . . . . .</b>	<b>59</b>
6.1	Objectives . . . . .	59
6.2	List of Terms . . . . .	59
6.3	Motivation . . . . .	59
6.4	Discussion . . . . .	60
6.5	Computing Questions . . . . .	62
6.6	Related Modules . . . . .	63
	Web Resources . . . . .	63
<b>7</b>	<b>Iterative Solutions . . . . .</b>	<b>65</b>
7.1	Objectives . . . . .	65
7.2	List of Terms . . . . .	65
7.3	Motivation . . . . .	65
7.4	An Example: Have a Hang-Up . . . . .	66

7.5	Another Design: Out on a Limb . . . . .	70
7.6	The Solution Is at Hand. . . with Solver . . . . .	74
7.7	But Wait, There's More! . . . . .	78
7.8	Integers Are Not Real. . .Numbers . . . . .	80
7.9	Computing Questions . . . . .	80
7.10	Related Modules . . . . .	81
	References . . . . .	81
<b>8</b>	<b>Solving Sets of Equations . . . . .</b>	<b>83</b>
8.1	Objectives . . . . .	83
8.2	Definitions . . . . .	83
8.3	Motivation . . . . .	84
8.4	Problem Definition . . . . .	84
8.5	Boundary Conditions . . . . .	85
8.6	Solution Methods . . . . .	86
8.7	Numerical Aspects . . . . .	86
8.8	An Excel Solution . . . . .	89
8.9	Setting Up Excel for Iterative Calculation . . . . .	90
8.10	A Matrix Solution . . . . .	92
8.11	The Modeling Process . . . . .	94
8.12	Computing Questions . . . . .	95
8.13	Related Modules . . . . .	95
	Further Study . . . . .	95
<b>9</b>	<b>Procedures: Performance and Complexity . . . . .</b>	<b>97</b>
9.1	Objectives . . . . .	97
9.2	Definitions . . . . .	97
9.3	Motivation . . . . .	97
9.4	Simulation Model Performance . . . . .	98
9.5	Example of Computational Complexity: Tick Marks . . . . .	99
9.6	Another Example of Computational Complexity: Color a Square of Patches in NetLogo . . . . .	102
9.7	Example of Computational Complexity: Merge Sort . . . . .	103
9.8	Standard Big-Oh Function Classifications for Comparing Algorithms . . . . .	105
9.9	Related Modules . . . . .	107
	References . . . . .	107
<b>10</b>	<b>Self-Defining Data: Compression, XML and Databases . . . . .</b>	<b>109</b>
10.1	Objectives . . . . .	109
10.2	Definitions . . . . .	109
10.3	Motivation . . . . .	109
10.4	Self-Defining Type 1: Compression . . . . .	110
10.5	Self-Defining Type 2: XML . . . . .	112
10.6	Self-Defining Type 3: Databases . . . . .	112
10.7	Self-Defining Type 3 Part 2: Data Warehouses . . . . .	115

10.8	Self-Defining Type 3 Part 3: Other Database Types . . . . .	117
10.9	Related Modules . . . . .	118
	Reference . . . . .	118
<b>11</b>	<b>Searching . . . . .</b>	<b>119</b>
11.1	Objectives . . . . .	119
11.2	Definitions . . . . .	119
11.3	Motivation . . . . .	120
11.4	Searching Amino Acids . . . . .	120
11.5	BLASTP Algorithm . . . . .	123
11.6	Computing Questions . . . . .	125
11.7	Related Modules . . . . .	126
	Ten Protein Sequences of 99 Amino Acids . . . . .	126
	References . . . . .	127
<b>12</b>	<b>Curve Fitting . . . . .</b>	<b>129</b>
12.1	Objectives . . . . .	129
12.2	Definitions . . . . .	129
12.3	Motivation . . . . .	129
12.4	Fitting “By Hand” . . . . .	130
12.5	Fitting By Hand with Graphing Aid . . . . .	131
12.6	Fitting via Numerical Analysis (Regression) . . . . .	132
12.7	Fitting via Excel . . . . .	133
12.8	Computing Questions . . . . .	134
12.9	Related Modules . . . . .	134
<b>13</b>	<b>Optimization . . . . .</b>	<b>135</b>
13.1	Objectives . . . . .	135
13.2	Definitions . . . . .	135
13.3	Motivation . . . . .	135
13.4	What Makes Up an Optimization Problem? . . . . .	136
13.5	What Is the “Language” of an Optimization Problem? . . . . .	136
13.6	Working Through the Setup of an Optimization Problem . . . . .	137
13.7	Solving an Optimization Problem . . . . .	139
13.8	Simulated Annealing . . . . .	139
13.9	Genetic Algorithm . . . . .	142
13.10	Linear Programming . . . . .	145
13.11	Simplex Method . . . . .	146
13.12	Computing Questions . . . . .	148
13.13	Related Modules . . . . .	149
	References . . . . .	149
<b>14</b>	<b>Data Organization and Analysis . . . . .</b>	<b>151</b>
14.1	Objectives . . . . .	151
14.2	Definitions . . . . .	151
14.3	Motivation . . . . .	152

---

14.4	Spatial Data Representation . . . . .	152
14.5	Joining Data . . . . .	152
14.6	Spatial Joining . . . . .	156
14.7	Computing Questions . . . . .	156
14.8	Related Modules . . . . .	157
	Reference . . . . .	157
<b>Appendix: NetLogo Tutorial . . . . .</b>		<b>159</b>
<b>Appendix: LabQuest Tutorial . . . . .</b>		<b>165</b>
<b>Appendix: GIS Tutorial . . . . .</b>		<b>173</b>
<b>Definitions . . . . .</b>		<b>181</b>
<b>Index . . . . .</b>		<b>189</b>

Concise Guide to Computing Foundations

Core Concepts and Select Scientific Applications

Brewer, K.; Bareiss, C.

2016, XV, 191 p. 76 illus., 41 illus. in color., Hardcover

ISBN: 978-3-319-29952-5