

Contents

List of Contributors XIII

Preface XVII

1	Introduction: Multiscale Analysis – Modeling, Data, Networks, and Nonlinear Dynamics	1
	<i>Misha (Meyer) Z. Pesenson</i>	
1.1	Multiscale Modeling	5
1.1.1	Domain-Specific Modeling	6
1.1.2	Analysis	7
1.1.3	Model Interpretation and Verification: Experimental/Simulation Data	9
1.2	Multiresolution Analysis and Processing of High-Dimensional Information/Data	10
1.3	Multiscale Analysis, Networks, and Nonlinear Dynamics	11
1.4	Conclusions	14
	References	14

Part One Multiscale Analysis 19

2	Modeling Across Scales: Discrete Geometric Structures in Homogenization and Inverse Homogenization	21
	<i>Mathieu Desbrun, Roger D. Donaldson, and Houman Owhadi</i>	
2.1	Introduction	21
2.2	Homogenization of Conductivity Space	23
2.2.1	Homogenization as a Nonlinear Operator	24
2.2.2	Parameterization of the Conductivity Space	26
2.3	Discrete Geometric Homogenization	31
2.3.1	Homogenization by Volume Averaging	32
2.3.2	Homogenization by Linear Interpolation	33
2.3.3	Semigroup Properties in Geometric Homogenization	37
2.4	Optimal Weighted Delaunay Triangulations	39
2.4.1	Construction of Positive Dirichlet Weights	40

2.4.2	Weighted Delaunay and Q -Adapted Triangulations	43
2.4.3	Computing Optimal Weighted Delaunay Meshes	44
2.5	Relationship to Inverse Homogenization	47
2.6	Electrical Impedance Tomography	49
2.6.1	Numerical Tests	52
2.6.1.1	Harmonic Coordinate Iteration	53
2.6.1.2	Divergence-Free Parameterization Recovery	55
	References	61
3	Multiresolution Analysis on Compact Riemannian Manifolds	65
	<i>Isaac Z. Pesenson</i>	
3.1	Introduction	65
3.2	Compact Manifolds and Operators	66
3.2.1	Manifolds without Boundary	66
3.2.2	Compact Homogeneous Manifolds	67
3.2.3	Bounded Domains with Smooth Boundaries	68
3.3	Hilbert Frames	69
3.4	Multiresolution and Sampling	70
3.5	Shannon Sampling of Band-Limited Functions on Manifolds	72
3.6	Localized Frames on Compact Manifolds	73
3.7	Parseval Frames on Homogeneous Manifolds	76
3.8	Variational Splines on Manifolds	79
3.9	Conclusions	81
	References	81
Part Two	Nonlinear Dynamics: Genelets and Synthetic Biochemical Circuits	83
4	Transcriptional Oscillators	85
	<i>Elisa Franco, Jongmin Kim, and Friedrich C. Simmel</i>	
4.1	Introduction	85
4.2	Synthetic Transcriptional Modules	86
4.2.1	Elementary Activation and Inhibition Pathways, and Simple Loops	87
4.2.2	Experimental Implementation	88
4.3	Molecular Clocks	89
4.3.1	A Two-Node Molecular Oscillator	90
4.3.2	Analysis of the Oscillatory Regime	91
4.3.3	Experimental Implementation and Data	95
4.4	Scaling Up Molecular Circuits: Synchronization of Molecular Processes	96
4.4.1	Analysis of the Load Dynamics	97
4.4.1.1	Quasisteady State Approximation of the Load Dynamics	99
4.4.1.2	Efficiency of Signal Transmission	99
4.4.2	Perturbation of the Oscillator Caused by the Load	100
4.4.2.1	Consumptive Coupling	100

4.4.2.2	Nonconsumptive Coupling and Retroactivity	100
4.4.3	Insulation	102
4.4.3.1	Reduction of Perturbations on the Oscillator Dynamics	103
4.4.3.2	Signal Transmission to the Insulated Load	104
4.5	Oscillator Driving a Load: Experimental Implementation and Data	105
4.6	Deterministic Predictive Models for Complex Reaction Networks	105
4.7	Stochastic Effects	107
4.8	Conclusions	110
	References	110
5	Synthetic Biochemical Dynamic Circuits	113
	<i>Raphaël Plasson and Yannick Rondelez</i>	
5.1	Introduction	113
5.2	Out-of-Equilibrium Chemical Systems	114
5.2.1	A Short Historical Overview	114
5.2.1.1	Discovery of Nonlinear Chemical Systems	114
5.2.1.2	Unexpected Oscillating Chemical Systems	115
5.2.2	Building Nonequilibrium Systems	116
5.2.2.1	Energetic Requirements	116
5.2.2.2	System Closure	116
5.2.2.3	Instabilities and Dynamic Stability	118
5.2.3	Design Principles	119
5.2.3.1	Dynamism	119
5.2.3.2	Interacting Feedbacks Processes	121
5.2.3.3	Modularity	122
5.3	Biological Circuits	123
5.3.1	Biological Networks Modeled by Chemistry	123
5.3.2	Biosystems: A Multilevel Complexity	124
5.3.3	A First Example of a Biological Reaction Circuit	124
5.3.4	Biological Networking Strategy	125
5.3.4.1	GRNs Are Templated Networks	125
5.3.4.2	Regulation and Feedback Loops	125
5.3.4.3	Nonlinearities in Genetic Regulation	127
5.3.4.4	Delays	128
5.3.4.5	Titration Effects	129
5.3.5	Higher Level Motifs and Modularity of Biochemical Networks	129
5.4	Programmable <i>In Vitro</i> Dynamics	130
5.4.1	Enzymatic Systems	130
5.4.1.1	DNA–RNA Sequence Amplification	131
5.4.1.2	The Genelet System	131
5.4.1.3	The PEN Toolbox	132
5.4.2	Nonenzymatic Networks: Strand Displacement Systems	134
5.4.3	Numerical Modeling	135
5.4.3.1	Mathematical Descriptions	135
5.4.3.2	LSA and Bifurcation Analysis for Design	137

5.4.3.3	Time Evolutions	138
5.4.3.4	Robustness Analysis and <i>In Silico</i> Evolutions	138
5.5	Perspectives	139
5.5.1	DNA Computing	140
5.5.2	Self Organizing Spatial Patterns	140
5.5.3	Models of Biological Networks	141
5.5.4	Origin of Life	141
	References	142

Part Three Nonlinear Dynamics: the Brain and the Heart 147

6	Theoretical and Experimental Electrophysiology in Human Neocortex: Multiscale Dynamic Correlates of Conscious Experience	149
	<i>Paul L. Nunez, Ramesh Srinivasan, and Lester Ingber</i>	
6.1	Introduction to Brain Complexity	149
6.1.1	Human Brains and Other Complex Adaptive Systems	149
6.1.2	Is “Consciousness” a Four-Letter Word?	150
6.1.3	Motivations and Target Audiences for this Chapter	151
6.1.4	Brain Imaging at Multiple Spatial and Temporal Scales	151
6.1.5	Multiple Scales of Brain Dynamics in Consciousness	153
6.2	Brief Overview of Neocortical Anatomy and Physiology	154
6.2.1	The Human Brain at Large Scales	154
6.2.2	Chemical Control of Brain and Behavior	155
6.2.3	Electrical Transmission	156
6.2.4	Neocortex	156
6.2.5	The Nested Hierarchy of Neocortex: Multiple Scales of Brain Tissue	158
6.2.6	Corticocortical Connections Are Nonlocal and “Small World”	159
6.3	Multiscale Theory in Electrophysiology	160
6.3.1	Characteristic EEG and Physiological Time Scales	160
6.3.2	Local versus Global Brain Models and Spatial Scale	161
6.3.3	A Large-Scale Model of EEG Standing Waves	162
6.3.4	Relationships between Small, Intermediate, and Large Scales: A Simple Mechanical Analog	164
6.4	Statistical Mechanics of Neocortical Interactions	166
6.4.1	SMNI on Short-Term Memory and EEG	166
6.4.1.1	SMNI STM	167
6.4.1.2	SMNI EEG	168
6.4.2	Euler–Lagrange Equations	168
6.4.2.1	Columnar EL	169
6.4.2.2	Strings EL	170
6.4.2.3	Springs EL	171
6.4.3	Smoking Gun	171

6.4.3.1	Neocortical Magnetic Fields	172
6.4.3.2	SMNI Vector Potential	172
6.5	Concluding Remarks	173
	References	174
7	Multiscale Network Organization in the Human Brain	179
	<i>Danielle S. Bassett and Felix Siebenhühner</i>	
7.1	Introduction	179
7.2	Mathematical Concepts	181
7.3	Structural Multiscale Organization	182
7.4	Functional Multiscale Organization	187
7.5	Discussion	191
7.5.1	Structure and Function	191
7.5.2	Hierarchical Modularity	193
7.5.3	Power-Law Scaling	194
7.5.4	Network Models of Multiscale Structure	194
	References	195
8	Neuronal Oscillations Scale Up and Scale Down	
	Brain Dynamics	205
	<i>Michel Le Van Quyen, Vicente Botella-Soler, and Mario Valderrama</i>	
8.1	Introduction	205
8.2	The Brain Web of Cross-Scale Interactions	206
8.3	Multiscale Recordings of the Human Brain	208
8.4	Physiological Correlates of Cross-Level Interactions	210
8.5	Level Entanglement and Cross-Scale Coupling of Neuronal Oscillations	212
8.6	Conclusions	213
	References	214
9	Linking Nonlinear Neural Dynamics to Single-Trial Human Behavior	217
	<i>Michael X Cohen and Bradley Voytek</i>	
9.1	Neural Dynamics Are Complex	217
9.2	Data Analysis Techniques and Possibilities Are Expanding Rapidly	218
9.3	The Importance of Linking Neural Dynamics to Behavior Dynamics	219
9.4	Linear Approaches of Linking Neural and Behavior Dynamics	220
9.5	Nonlinear Dynamics and Behavior: Phase Modulations	221
9.6	Cross-Frequency Coupling	224
9.7	Linking Cross-Frequency Coupling to Behavior	226

9.8	Testing for Causal Involvement of Nonlinear Dynamics in Cognition and Behavior	228
9.9	Conclusions	229
	References	229
10	Brain Dynamics at Rest: How Structure Shapes Dynamics	233
	<i>Etienne Hugues, Juan R. Vidal, Jean-Philippe Lachaux, and Gustavo Deco</i>	
10.1	Introduction	233
10.2	Model	234
10.3	Results	236
10.3.1	Neural Dynamics	236
10.3.1.1	Case of Infinite Conduction Velocity	236
10.3.1.2	Case of Finite Conduction Velocity	238
10.3.2	BOLD Dynamics	238
10.4	Comparison with Experimental Data	239
10.5	Discussion	240
	References	242
11	Adaptive Multiscale Encoding: A Computational Function of Neuronal Synchronization	245
	<i>Misha (Meyer) Z. Pesenson</i>	
11.1	Introduction	245
11.2	Some Basic Mathematical Concepts	247
11.3	Neural Synchronization	247
11.3.1	Connections with Some Existing Approaches to MRA	253
11.4	Concluding Remarks	253
	References	254
12	Multiscale Nonlinear Dynamics in Cardiac Electrophysiology: From Sparks to Sudden Death	257
	<i>Zhilin Qu and Michael Nivala</i>	
12.1	Introduction	257
12.2	Subcellular Scale: Criticality in the Transition from Ca Sparks to Ca Waves	258
12.3	Cellular Scale: Action Potential and Ca Cycling Dynamics	260
12.3.1	Intracellular Ca Alternans	260
12.3.2	Fast Pacing-Induced Complex APD Dynamics	262
12.3.3	EAD-Mediated Nonlinear Dynamics at Slow Heart Rates	264
12.4	Excitation Dynamics on the Tissue and Organ Scales	266
12.4.1	Spatially Discordant APD Alternans	266
12.4.2	Spiral and Scroll Wave Dynamics	267
12.4.3	Chaos Synchronization	269
12.5	Conclusions	271
	References	271

13	Measures of Spike Train Synchrony: From Single Neurons to Populations	277
	<i>Conor Houghton and Thomas Kreuz</i>	
13.1	Introduction	277
13.2	Measures of Spike Train Distance	278
13.2.1	Notation	278
13.2.2	The Victor–Purpura Metric	279
13.2.3	The van Rossum Metric	280
13.2.4	The ISI- and the SPIKE-Distance	282
13.2.4.1	The ISI-Distance	284
13.2.4.2	The SPIKE-Distance	285
13.2.5	Entropy-Based Measure	286
13.3	Comparisons	286
13.3.1	The ISI- and the SPIKE-Distance	286
13.3.2	The ISI-Distance and the van Rossum Metric	287
13.3.3	The SPIKE-Distance and the Victor–Purpura Metric	288
13.3.4	Comparison of All Distances on Birdsong Data	289
13.4	Measuring the Dissimilarity within a Population	290
13.5	Measuring the Dissimilarity between Populations	292
13.5.1	The Population Extension of the Victor–Purpura Metric	292
13.5.2	The Population Extension of the van Rossum Metric	293
13.6	Discussion	294
	References	296
	Index	299

