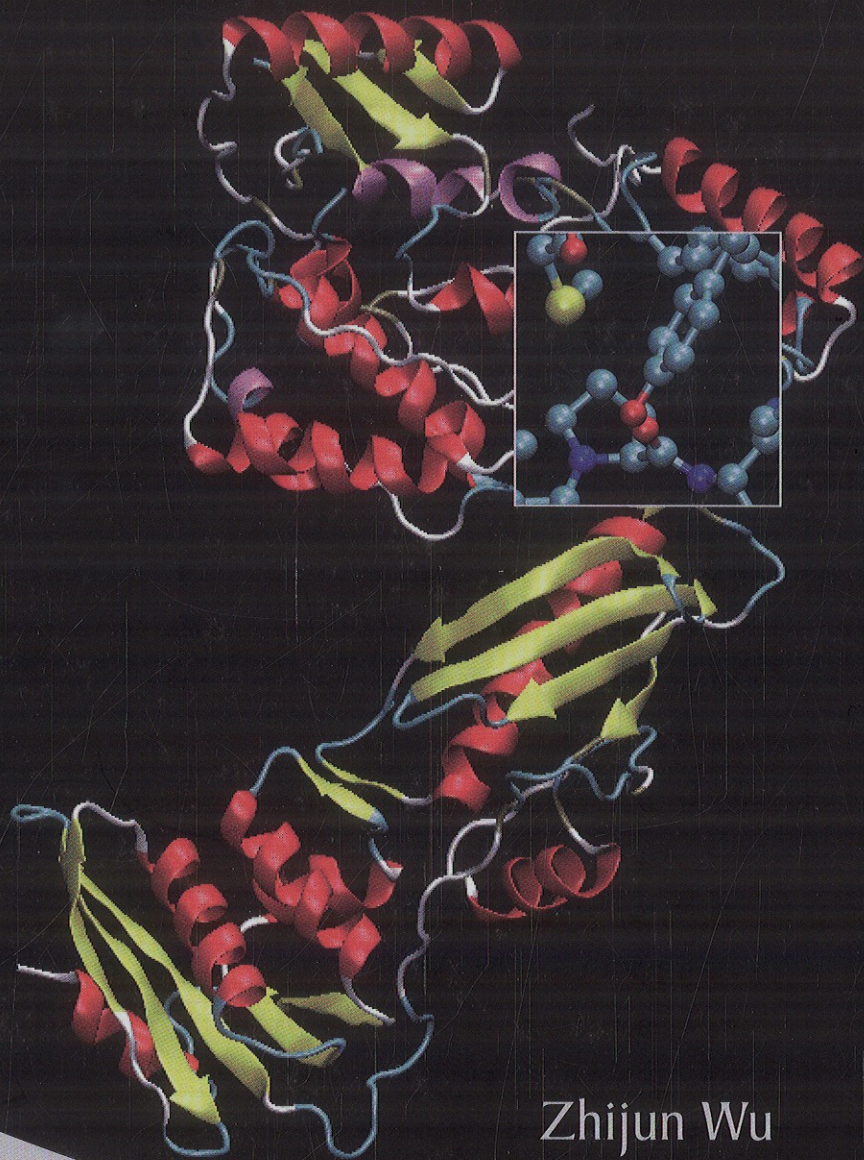


Lecture Notes on Computational Structural Biology



Zhijun Wu

Contents

Preface	vii
1 Introduction	1
1.1 Protein Structure	1
1.2 Structure Determination	9
1.3 Dynamics Simulation	13
1.4 The Myth of Protein Folding	18
2 X-ray Crystallography Computing	27
2.1 The Phase Problem	27
2.2 Least Squares Solutions	37
2.3 Entropy Maximization	46
2.4 Indirect Methods	54
3 NMR Structure Determination	63
3.1 Nuclear Magnetic Resonance	63
3.2 Distance Geometry	73
3.3 Distance-based Modeling	81
3.4 Structural Analysis	87
4 Potential Energy Minimization	99
4.1 Potential Energy Function	100
4.2 Local Optimization	107
4.3 Global Optimization	111
4.4 Energy Transformation	116
5 Molecular Dynamics Simulation	125
5.1 Equations of Motion	125

5.2	Initial-Value Problem	129
5.3	Boundary-Value Problem	138
5.4	Normal Mode Analysis	145
6	Knowledge-based Protein Modeling	156
6.1	Sequence/Structural Alignment	156
6.2	Fold Recognition/Inverse Folding	165
6.3	Knowledge-based Structural Refinement	169
6.4	Structural Computing and Beyond	173
Appendix A	Design and Analysis of Computer Algorithms	182
A.1	Evaluation of Algorithms	183
A.2	Intractability	188
A.3	Lists, Arrays, Graphs, and Trees	192
A.4	Sorting, Searching, and Optimization	195
Appendix B	Numerical Methods	202
B.1	Numerical Linear Algebra	202
B.2	Numerical Optimization	210
B.3	Numerical Solutions to Initial-Value Problems	218
B.4	Numerical Solutions to Boundary-Value Problems	222
	Index	229