

D.W. Heermann A.N. Burkitt

# Parallel Algorithms in Computational Science

With 46 Figures

Springer-Verlag  
Berlin Heidelberg New York  
London Paris Tokyo  
Hong Kong Barcelona

# Contents

<b>1. Introduction . . . . .</b>	<b>1</b>
<b>2. Computer Simulation Methods . . . . .</b>	<b>5</b>
2.1 Essential Features of Simulation Methods . . . . .	5
2.1.1 Ensemble Averages on a Computer . . . . .	6
2.1.2 Simulation Algorithms . . . . .	6
2.2 The Monte Carlo Algorithm . . . . .	8
2.2.1 Simple Sampling . . . . .	8
2.2.2 Importance Sampling . . . . .	9
2.2.3 Interpretation of the Monte Carlo Process as a Dynamical Process . . . . .	11
2.3 Molecular Dynamics . . . . .	13
2.3.1 The Microcanonical Ensemble . . . . .	14
2.3.2 Discretization and Systematic Effects . . . . .	15
2.3.3 Molecular Dynamics Algorithms . . . . .	17
2.4 Hybrid Molecular Dynamics . . . . .	18
2.5 Accuracy Considerations and Finite-Size Problems . . . . .	21
2.5.1 Choosing the Boundary Conditions . . . . .	21
2.5.2 Effects of Finite Simulation Time . . . . .	22
2.5.3 Statistical Errors and Self-Averaging . . . . .	23
2.5.4 Finite-Size Scaling: Using Finite-Size Effects . . . . .	24
2.6 Monte Carlo Algorithm for the Ising Model . . . . .	25
2.6.1 The Ising Model . . . . .	26
2.6.2 Implementing the Monte Carlo Algorithm for the Ising Model . . . . .	27
2.6.3 The Swendsen-Wang Algorithm and the Equivalence Between the Ising Model and Percolation . . . . .	28
2.6.4 Cluster Identification . . . . .	32
2.6.5 Other Cluster Update Algorithms . . . . .	33
<b>3. Physics and Parallelism . . . . .</b>	<b>37</b>
<b>4. Concepts of Parallelism . . . . .</b>	<b>43</b>
4.1 Some Basic Definitions . . . . .	43
4.2 The Complexity of Computation . . . . .	45

4.3	More on Models and Methods . . . . .	46
4.4	Performance Measurements . . . . .	49
<b>5.</b>	<b>Parallel Machines and Languages . . . . .</b>	<b>51</b>
5.1	General Purpose Parallel Computers . . . . .	51
5.1.1	Processor Concepts . . . . .	51
5.1.2	Communication Networks . . . . .	53
5.2	Parallel Machines for Special Physics Problems . . . . .	58
5.2.1	Monte Carlo Machines . . . . .	59
5.2.2	Molecular Dynamics Computers . . . . .	63
5.3	Languages for Parallel Computers . . . . .	64
5.4	The Matching Problem . . . . .	66
<b>6.</b>	<b>Replicatioh Algorithms . . . . .</b>	<b>71</b>
<b>7.</b>	<b>Geometrically Parallel Algorithms . . . . .</b>	<b>75</b>
7.1	Geometrie Parallelization . . . . .	76
7.2	Strips, Squares and Checker-Boards . . . . .	79
7.2.1	Detailed Balance and the Checker-Board . . . . .	79
7.2.2	Strips . . . . .	80
7.2.3	Squares . . . . .	82
7.2.4	Communication Procedures . . . . .	83
7.2.5	Timing and Efficiency Considerations . . . . .	84
7.2.6	Geometrie Parallelism in Higher Dimensions . . . . .	85
7.3	Non-local and Cluster Algorithms . . . . .	87
7.3.1	Parallel Algorithms for Cluster Identification . . . . .	87
7.3.2	The Public Stack Cluster Algorithm . . . . .	88
7.3.3	The Binary Tree Cluster Algorithm . . . . .	89
7.3.4	Performance Measurements . . . . .	90
7.4	Parallel Molecular Dynamics Algorithms . . . . .	91
7.4.1	Short-Range vs Long-Range Interactions . . . . .	91
7.4.2	A Geometrically Parallelized Algorithm for Molecular Dynamics . . . . .	93^
7.5	Hybrid Molecular Dynamics . . . . .	94
7.6	Polymers on the Lattice . . . . .	95
7.6.1	Single Polymers . . . . .	96
7.6.2	Dense Polymer Systems . . . . .	97
7.7'	Off-Lattice Polymers . . . . .	100
7.8	Hybrid Molecular Dynamics for Polymers . . . . .	101
7.9	Limits of Geometrie Parallelization . . . . .	101
<b>8.</b>	<b>Data Parallel Algorithms . . . . .</b>	<b>105</b>
8.1	Data Parallel Algorithm for Long-Range Interactions . . . . .	105
8.2	-Polymers . . . . .	106

<b>9. Introduction to a Parallel Language . . . . .</b>	.111
9.1 Transputer-Based Parallel Machines . . . . .	.111
9.2 Parallel Programming in Occam . . . . .	.113
9.2.1 The Process and the Channel Concepts . . . . .	.115
9.2.2 Two Elementary Processes . . . . .	.119
9.2.3 A Trivial Example . . . . .	.120
9.2.4 Repetition and the Conditional . . . . .	.121
9.2.5 An Occam Program for the Ising Model . . . . .	.127
9.2.6 More on Choices and Selection . . . . .	.133
9.2.7 Further Language Elements . . . . .	.136
9.2i8 Arithmetic . . . . .	.140
9.2.9 Placements . . . . .	.144
<b>Appendices . . . . .</b>	.149
A. A Parallel Ising Model Program . . . . .	.149
B. Random Number Generator . . . . .	.156
C. A Parallel Molecular Dynamics Program . . . . .	.159
<b>References . . . . .</b>	.171
<b>Subject Index . . . . .</b>	.179

