

Contents

1	Overview – Parallel Computing: Numerics, Applications, and Trends	1
	Marián Vajteršic, Peter Zinterhof and Roman Trobec	
1.1	Introduction	1
1.1.1	Parallel Numerics	2
1.1.2	Parallel Architectures	4
1.1.3	Scalability	6
1.1.4	Supercomputers	7
1.1.5	Grid Computing	8
1.1.6	Parallel Programming Languages	9
1.1.7	Parallel Compilers	11
1.2	Book Chapters	13
1.2.1	Introduction to Parallel Computation	13
1.2.2	Tools for Parallel and Distributed Computing	14
1.2.3	Grid Computing	15
1.2.4	Parallel Structured Adaptive Mesh Refinement	16
1.2.5	Applications and Parallel Implementation of QMC Integration	17
1.2.6	Parallel Evolutionary Computation Framework for Single- and Multiobjective Optimization	18
1.2.7	WaLBerla: Exploiting Massively Parallel Systems for Lattice Boltzmann Simulations	20
1.2.8	Parallel Pseudo-Spectral Methods for the Solution of the Time Dependent Schrödinger Equation	21
1.2.9	Parallel Approaches in Molecular Dynamics Simulations	23
1.2.10	Parallel Computer Simulation of Heat Transfer in Bio-Tissue	24
1.2.11	SVD Computing in LSI Applications for Data Retrieval	25
1.2.12	Short-Vector SIMD Parallelization in Signal Processing	27
1.2.13	Financial Applications: Parallel Portfolio Optimization	29
1.2.14	Future of Parallel Computing	30

1.3	Conclusions	32
	References	36
2	Introduction to Parallel Computation	43
	Selim G. Akl and Marius Nagy	
2.1	Introduction	44
2.2	Parallel Versus Sequential Computation	45
2.3	Parallel Computational Models	46
	2.3.1 Shared-Memory Models	46
	2.3.2 Interconnection Network Models	48
	2.3.3 Circuit Models	49
	2.3.4 Clusters	49
	2.3.5 Grids	51
2.4	Parallel Algorithm Design Methods	52
2.5	Theoretical Underpinnings	55
	2.5.1 Speedup	55
	2.5.2 Slowdown	57
	2.5.3 Quality-Up	57
	2.5.4 Computations that Seem Inherently Sequential	58
2.6	Parallel Algorithms for Conventional Computations	60
	2.6.1 Parallel Prefix and Suffix Computations on a Linked List	60
	2.6.2 Sorting on a Model with Buses	63
2.7	Parallel Algorithms for Unconventional Computations	66
	2.7.1 Computations that Can be Simulated Sequentially	67
	2.7.2 Computations that Cannot be Simulated Sequentially	73
2.8	Non-Universality in Computation	77
2.9	Conclusion	79
	References	80
3	Tools for Parallel and Distributed Computing	81
	Thomas Fahringer	
3.1	Introduction	82
3.2	Related Work	83
3.3	ASKALON Architecture	85
	3.3.1 Data Repository	87
	3.3.2 ASKALON Visualization Diagrams	88
3.4	SCALEA	88
	3.4.1 Instrumentation	88
	3.4.2 Overhead Analyzer	89
	3.4.3 Performance Analyzer	90
3.5	ZENTURIO	91
	3.5.1 ZEN Experiment Specification Language	91
	3.5.2 Experiment Generator	92
	3.5.3 Experiment Executor	93
3.6	AKSUM	93
	3.6.1 Search Engine	94

3.6.2	Reinforcement Learning for Performance Analysis	97
3.7	Grid-Prophet	98
3.7.1	Prediction Techniques	99
3.8	Experiments	103
3.8.1	Performance Analysis with SCALEA	103
3.8.2	Performance and Parameter Studies of a Three-Dimensional Particle-In-Cell Application with ZENTURIO	105
3.8.3	Performance Analysis for a Backward Pricing Application with AKSUM	106
3.8.4	Workflow Performance Prediction with the Grid-Prophet	108
3.9	Conclusions	111
	References	111
4	Grid Computing	117
	Uroš Čibej, Anthony Sulistio and Rajkumar Buyya	
4.1	Introduction	117
4.1.1	Grid Categorization	119
4.1.2	Comparison Between Clusters and Grids	122
4.1.3	Putting It All Together	122
4.2	Challenges in Grid Computing	123
4.2.1	Resource Sharing	124
4.2.2	Guaranteed Quality of Service	124
4.2.3	Resource Regulation	126
4.2.4	Data Management	127
4.3	Tools and Applications	129
4.3.1	Middleware	130
4.3.2	Tools for Computationally Intensive Applications	133
4.3.3	Tools for Workflow Composition and Execution	134
4.3.4	Tools That Support Advance Reservation	135
4.3.5	G-Lambda Grid Scheduling System	137
4.3.6	Application Fields	137
4.4	Conclusions and Future Trends	139
	References	140
5	Parallel Structured Adaptive Mesh Refinement	147
	Jarmo Rantakokko and Michael Thuné	
5.1	Introduction	148
5.2	An Introduction to SAMR	150
5.2.1	Approaches to Structured Adaptive Mesh Refinement	150
5.2.2	SAMR in a Computer Science Perspective	153
5.2.3	Software Frameworks for SAMR	154
5.3	Details of SAMR	155
5.3.1	Advancing the Solution on a Structured Adaptive Grid Hierarchy	155
5.3.2	The Algorithmic Key Components of SAMR	157

5.4	Computer Science Aspects of SAMR	158
5.4.1	Data Dependencies	158
5.4.2	Dynamic Load Balancing	159
5.4.3	Parallelization Models	163
5.5	Some Results	164
5.5.1	An Integrated Decomposition and Partitioning Approach for Irregular Block-Structured Applications	164
5.5.2	A Hybrid Dynamic MPI-OpenMP Model	165
5.5.3	Geographical Locality	166
5.5.4	A Hybrid Patch/Domain-Based Partitioner Framework	168
5.5.5	A Meta-Partitioner for Structured Grid Hierarchies	168
5.6	Conclusions and Future Work	169
	References	170
6	Applications and Parallel Implementation of QMC Integration	175
	Peter Jez, Andreas Uhl and Peter Zinterhof	
6.1	Introduction	176
6.2	Monte Carlo and Quasi Monte Carlo Methods in Numerical Integration Over $[0, 1]^s$	177
6.2.1	Application of Reproducing Kernel Hilbert Spaces	181
6.3	QMC Methods for Integrals over \mathbb{R}^s with a Weight Function	182
6.3.1	Feynman's Path Integrals	185
6.3.2	Application in Financial Engineering	186
6.4	QMC Integration on Parallel Systems	188
6.5	Numerical Experiments	191
6.5.1	Sequential Computations	191
6.5.2	Parallel Case	194
6.5.3	Experimental Results	195
6.5.4	Overall Comparison	206
6.6	Application of the Diaphony in Parallel Computation	208
6.7	Conclusion	211
	References	213
7	Parallel Evolutionary Computation Framework for Single- and Multiobjective Optimization	217
	Bogdan Filipič and Matjaž Depolli	
7.1	Introduction	218
7.2	Optimization Problems	219
7.3	Evolutionary Algorithms	222
7.3.1	Multiobjective Evolutionary Algorithms	224
7.4	Parallel Single- and Multiobjective Evolutionary Algorithms	224
7.4.1	Parallelization Types	224
7.4.2	Calculation of Speedups	226
7.5	Casting Process Optimization Task	229
7.6	Parallel Evolutionary Computation Framework	230
7.6.1	Speedup Estimation	231

7.7	Empirical Evaluation	233
7.7.1	Experimental Setup	233
7.7.2	Experiments and Results	234
7.8	Conclusion	239
	References	240
8	WaLBerla: Exploiting Massively Parallel Systems for Lattice Boltzmann Simulations	241
	Christian Feichtinger, Jan Götz, Stefan Donath, Klaus Iglberger and Ulrich Rüde	
8.1	Motivation	242
8.2	Introduction to the Lattice Boltzmann Method	243
8.3	Domain Partitioning Using Patches	245
8.3.1	Memory Reduction	247
8.4	Communication Concept	247
8.4.1	Process Local Communication	248
8.4.2	MPI Communication	248
8.5	Performance Studies	249
8.5.1	Serial Experiments	250
8.5.2	Parallel Experiments	252
8.5.3	IBM Cell Processor	258
8.6	Conclusion	258
	References	259
9	Parallel Pseudo-Spectral Methods for the Time-Dependent Schrödinger Equation	261
	Tore Birkeland and Tor Sørevik	
9.1	Introduction	261
9.2	Time Stepping and Split Operator Technique	264
9.3	Variable Transformations and Spectral Bases	265
9.3.1	Cartesian Coordinates and Fourier Basis	265
9.3.2	Spherical Coordinates	266
9.4	Parallelizing Many Dimensional FFTs	267
9.5	Creating a Framework for Combining Discretization Methods	271
9.5.1	Wavefunction	272
9.5.2	Operators and Transforms	273
9.5.3	Split-Step Propagator	274
9.5.4	Explicit Propagators	275
9.6	A Numerical Example	275
9.6.1	Physical Model	275
9.6.2	Numerical Considerations	276
9.6.3	Scalability	277
9.7	Conclusion	278
	References	278

10 Parallel Approaches in Molecular Dynamics Simulations	281
Dušanka Janežič, Urban Boršnik and Matej Praprotnik	
10.1 Split Integration Symplectic Method	282
10.1.1 Calculation of Infrared Spectra	288
10.1.2 Enlarging the Integrational Time Step	290
10.2 Parallel Computers	290
10.2.1 Parallel Computing	291
10.2.2 Parallel Computer Types	292
10.2.3 Reducing Computational Complexity in Molecular Dynamics Simulations	293
10.3 Parallel Molecular Dynamics Computer Simulations	294
10.3.1 Methods for Parallel Molecular Dynamics Simulations	295
10.3.2 Specialized Processors	296
10.3.3 Global Communication in Parallel Molecular Dynamics Simulations	298
10.4 Parallelization of SISM	299
10.4.1 The Distributed Diagonal Force Decomposition Method	299
10.5 Conclusions	301
References	302
11 Parallel Computer Simulations of Heat Transfer in Biological Tissues	307
Roman Trobec	
11.1 Introduction	308
11.2 Principal Steps in Computer Simulation	311
11.3 Numerical Solution of Partial Differential Equations	314
11.3.1 Finite Difference Method	315
11.3.2 Finite Element Method	316
11.3.3 Solution Methods of Time-Dependent PDEs	316
11.3.4 Computational and Memory Complexity	320
11.4 Diffusion Equation	321
11.4.1 Analytical Solution	324
11.4.2 Finite Differences with Gradient Term	324
11.4.3 Explicit Finite Difference Scheme	325
11.4.4 Comparison of Results	328
11.5 Bio-Heat Equation	330
11.6 Geometric Modeling of a Knee	333
11.7 Simulation Methods and Parameters	336
11.8 Variation of Simulation Parameters	338
11.9 Simulation Results	340
11.9.1 Washing Out During Arthroscopy	341
11.9.2 Resting After Arthroscopy	342
11.9.3 Postoperative Topical Cooling	342
11.10 Validation of Results	345
11.11 Parallel Implementation	347

11.11.1	Opportunities for Parallelization	348
11.11.2	Computation and Communication Complexity	349
11.11.3	Measured Speedup	352
11.12	Conclusions	354
	References	356
12	Parallel SVD Computing in the Latent Semantic Indexing Applications for Data Retrieval	359
	Gabriel Okša and Marián Vajteršic	
12.1	Introduction	359
12.2	Two Updating Problems in LSI	361
12.2.1	Updating Documents	361
12.2.2	Updating Terms	362
12.3	Two Downdating Problems in LSI	363
12.3.1	Downdating Documents	364
12.3.2	Downdating Terms	366
12.4	Kogbetliantz Method for Triangular Matrices	366
12.4.1	Butterfly Form of Triangular Matrices	367
12.4.2	Modulus Pivot Strategy	368
12.4.3	Block Version and Parallelism	370
12.5	Parallel Two-sided Block-Jacobi SVD Algorithm with Dynamic Ordering	377
12.6	LSI Implemented on a Grid	383
12.6.1	Storage	383
12.6.2	Updating Documents	384
12.6.3	Updating Terms	385
12.6.4	Downdating Documents	385
12.6.5	Downdating Terms	386
12.6.6	Retrieval of Documents	387
12.7	LSI Implemented on a Distributed System	388
12.7.1	Building a Global Approximation	389
12.7.2	Updating and Downdating	391
12.7.3	Retrieval of Documents	392
12.8	Conclusions	394
	References	395
13	Short-Vector SIMD Parallelization in Signal Processing	397
	Rade Kutil	
13.1	Introduction	397
13.1.1	Signal Processing Algorithms	398
13.1.2	Short-Vector SIMD	399
13.2	General Vectorization Approaches	401
13.2.1	Loop Unrolling	401
13.2.2	Straight Line Code Vectorization	401
13.2.3	Loop Fusion	402
13.2.4	Loop Transposition	402

13.2.5	Algebraic Transforms	403
13.3	Convolution Type Algorithms	404
13.3.1	Simple FIR Filter	404
13.3.2	The Haar Filter	407
13.3.3	Biorthogonal 7/9 Without Lifting	408
13.3.4	Biorthogonal 7/9 With Lifting	414
13.3.5	Conclusion	418
13.4	Recursive Algorithms	419
13.4.1	Sequential IIR Algorithm	420
13.4.2	Scheduling Approach	420
13.4.3	Algebraic Transforms	421
13.4.4	Experimental Results	422
13.5	Block Algorithms	423
13.5.1	Data Layout	424
13.5.2	Basic FFT-Blocks	425
13.5.3	Automatic Tuning and Signal Processing Languages (SPL)	426
13.6	Mixed Algorithms	428
13.6.1	Recursive Convolution – Wavelet Transforms	428
13.6.2	Multi-dimensional Algorithms	429
13.7	Conclusion	431
	References	432
14	Financial Applications: Parallel Portfolio Optimization	435
	<i>Andreas Grothey</i>	
14.1	Introduction	436
14.2	Asset and Liability Management by Stochastic Programming	437
14.2.1	Stochastic Programming	438
14.2.2	Asset and Liability Management Models	440
14.2.3	Model Extensions	444
14.3	Parallel Solution Approaches: Decomposition	446
14.4	Parallel Solution Approaches: Interior Point Based Algorithms	448
14.4.1	IPM Applied to Stochastic Programming Problems	451
14.4.2	Results	457
14.5	Parallel Solution Approaches: Heuristics and Evolutionary Algorithms	458
14.6	Other Approaches	458
14.7	Detailed Comparison of Parallel Interior Point Approaches	459
14.7.1	OOPS (Gondzio and Grothey)	459
14.7.2	Riccati-Based IPM Solver (Blomvall and Lindberg)	461
14.7.3	Tree Sparse IPM Solver (Steinbach)	464
14.8	Conclusions	465
	References	466

15 The Future of Parallel Computation	471
Selim G. Akl and Marius Nagy	
15.1 Introduction	472
15.2 Quantum Computing	475
15.2.1 Quantum Mechanics	475
15.2.2 Mathematical Framework	478
15.2.3 Entanglement	484
15.3 Parallelism in Quantum Computing	485
15.3.1 Quantum Parallelism	485
15.4 Examples	488
15.4.1 Parallelizing the Quantum Fourier Transform	488
15.4.2 Quantum Decoherence	496
15.4.3 Quantum Error-Correction	499
15.4.4 Quantum Distinguishability	502
15.4.5 Transformations Obeying a Global Condition	506
15.5 Looking Ahead	507
References	508
Index	511