

Contents

Part I. Computational Differential Equations	3
1 The SCIRun Computational Steering Software System	5
<i>S. G. Parker, D. W. Weinstein and C. R. Johnson</i>	
1.1 Introduction	5
1.2 Requirements of SCIRun as a Computational Steering System	9
1.3 Components of SCIRun	10
1.4 The Datatypes Library	20
1.5 Dataflow	23
1.6 Steering in a Dataflow System	26
1.7 Modules	27
1.8 Applications of SCIRun in Computational Medicine	34
1.9 Summary	39
1.10 Future Work	40
1.11 References	41
1.12 Software Appendix	44
2 Object-Oriented Solvers for Initial Value Problems	45
<i>H. Olsson</i>	
2.1 Introduction	45
2.2 Overview of the Code	51
2.3 Case Studies: New algorithms	54
2.4 Comparison with Classical Solvers	59
2.5 Conclusions	61
2.6 References	61
3 SPRINT2D Software for Convection Dominated PDEs	63
<i>M. Berzins et al.</i>	
3.1 Introduction	63
3.2 The SPRINT2D Software	64
3.3 Mesh Generation and Adaptivity	67
3.4 A PSE for SPRINT2D	70
3.5 Case Studies	72
3.6 Conclusions	77
3.7 References	79

4	Electrochemical Modelling and Software Genericity	81
	<i>G. Nelissen and P. Vankeirsbilck</i>	
4.1	Introduction	81
4.2	Electrochemical Modelling	84
4.3	A Generalized Approach to Numerical Modelling	87
4.4	Abstractions	89
4.5	Critical Remarks	100
4.6	Conclusions	101
4.7	References	102
5	An Object-Oriented Adaptive Finite Element Code: Design Issues and Applications in Hyperthermia Treatment Planning	105
	<i>R. Beck, B. Erdmann and R. Roitzsch</i>	
5.1	Introduction	106
5.2	Code Structure	107
5.3	Applications in Hyperthermia Treatment Planning	117
5.4	Concluding Remarks	121
5.5	References	121
6	On the Efficient Implementation of Multilevel Adaptive Methods	125
	<i>U. Rde</i>	
6.1	Introduction	125
6.2	Multilevel Implementations	127
6.3	Data Abstraction Concepts for Multilevel Adaptive Methods	130
6.4	Efficiency	132
6.5	Abstract Mesh Data Structures	136
6.6	Patch-Adaptive Multigrid	138
6.7	Conclusions	141
6.8	References	141
7	Finite Element Kernel with Metaobject Protocol	143
	<i>R. Chudoba</i>	
7.1	Introduction	143
7.2	Example Problems	145
7.3	Procedural Approach	146
7.4	Object-Oriented Approach	149
7.5	Algorithm-Oriented Approach	153
7.6	Conclusions	159
7.7	References	161

8	Efficient Management of Parallelism in Object-Oriented Numerical Software Libraries	163
	<i>S. Balay et al.</i>	
8.1	Introduction	163
8.2	The Message Passing Model for Programming Distributed-Memory Parallel Systems	167
8.3	Distributed Computational Objects	172
8.4	Six Guiding Principles	174
8.5	PETSc Design of Fundamental Objects	178
8.6	Sample Performance Results	198
8.7	Conclusion	200
8.8	References	201
9	Object-Oriented Construction of Parallel PDE Solvers	203
	<i>M. Thuné et al.</i>	
9.1	Introduction	203
9.2	The Object-Oriented Approach	207
9.3	Overview of Cogito	209
9.4	Case Study 1: Application of Cogito/Grid	211
9.5	Case Study 2: Application of Cogito/Solver	213
9.6	Cogito for Implicit Methods	215
9.7	Validation of Cogito	218
9.8	Concluding Remarks	224
9.9	References	225
10	Modern Software Techniques in Computational Finance	227
	<i>K. N. Pantazopoulos and E. N. Houstis</i>	
10.1	Introduction	227
10.2	Option Computations	232
10.3	Software Design Issues in Option Valuation	237
10.4	FINANZIA Implementation and Examples	240
10.5	Future Extensions	244
10.6	Conclusions	245
10.7	References	246
11	Increasing the Efficiency and Reliability of Software Development for Systems of PDEs	247
	<i>A. M. Bruaset, E. J. Holm and H. P. Langtangen</i>	
11.1	Introduction	247
11.2	A Plastic Forming Process	249
11.3	The Basic Ideas	252
11.4	Diffpack	254
11.5	Systems of PDEs	257

11.6	Extensions of the Concept	261
11.7	Other Applications	263
11.8	Another Application of the Flexible Design	264
11.9	Concluding Remarks	265
11.10	References	267

Part II. Computational Geometry 269

12 Object Oriented Surface Design 271

R. Bartels

12.1	Overview	271
12.2	Geometrical Abstractions	272
12.3	Data Structures	277
12.4	Splines	278
12.5	Surfaces	280
12.6	Refiners	281
12.7	Applications	282
12.8	Development Environment	284
12.9	References	287

13 Object-Oriented Scattered Data Modelling with Siscat 289

E. Arge and Ø. Hjelle

13.1	Introduction	289
13.2	A Cartographic Model Problem	291
13.3	The Basic Surface Hierarchy in Siscat	293
13.4	Aspects of Basic Methods	295
13.5	Composite Methods	301
13.6	References	307

Part III. Software Development 309

14 Is the Quality of Numerical Subroutine Code Improving? 311

T. R. Hopkins

14.1	Introduction	311
14.2	Software Metrics	312
14.3	A Comparison of Freely Available Packages	314
14.4	CALGO Fortran Codes	319
14.5	Conclusion	321
14.6	References	322

15 Object-Oriented Redesign of a Real-World Fortran 77 Solver	325
<i>M. Weidmann</i>	
15.1 Introduction	325
15.2 The SEMPA Project	327
15.3 The CFD Program	328
15.4 Analysis and Redesign of the Solver	329
15.5 Original and New Module Comparison	333
15.6 Discussion of the Approach	334
15.7 References	336
16 Automating the Debugging of Large Numerical Codes	339
<i>F. Manne and S. O. Andersen</i>	
16.1 Introduction	339
16.2 Comparative Debugging	341
16.3 Examples of Use	345
16.4 The Wizard	346
16.5 Conclusion	349
16.6 References	350
17 The TAMPR Program Transformation System: Simplifying the Development of Numerical Software	353
<i>J. M. Boyle, T. J. Harmer and V. L. Winter</i>	
17.1 Introduction	353
17.2 Some TAMPR Applications	356
17.3 The TAMPR Approach to Program Transformation	361
17.4 Example of the TAMPR Approach to Program Transformation	365
17.5 Conclusion	370
17.6 References	371
List of Contributors	373
Index	377