

Contents

1	Introduction	1
2	Known graph models from scientific computing	3
2.1	Determining nonzeros of sparse Jacobian matrices	3
2.1.1	Full Jacobian computation	3
2.1.2	Partial Jacobian computation	8
2.2	Combining partial Jacobian computation and ILU	9
2.2.1	Scientific computing problem	10
2.2.2	Combinatorial model	11
3	New coloring heuristics	15
3.1	Maximizing the set of additionally required elements	17
3.1.1	Restricted distance-2 coloring	17
3.1.2	Restricted star bicoloring	29
3.2	Application in geoscience	35
3.3	Coloring restricted to diagonal elements	40
3.4	Implementation details of PreCol	43
4	Interactive educational modules	45
4.1	Concept and design	45
4.2	Gamification	47
4.3	Available modules	48
4.3.1	Column compression	48
4.3.2	Full and partial Jacobian computation	50
4.3.3	Nested dissection ordering	53
4.3.4	Parallel matrix-vector product	60
4.4	New features in EXPLAIN 2.0	64
4.5	Implementation details of EXPLAIN	66
4.5.1	Version 1.0	66
4.5.2	Version 2.0	67
5	Conclusion and future work	73
Bibliography		75
Appendix		83
A.1	Comparing the computations of Algorithm 3.1 and Algorithm 3.2	83

Contents

A.2	Comparing the computations of Algorithm 3.2 and Algorithm 3.4	88
A.3	Comparing the computations of Algorithm 3.5 with different block sizes	90