

Institute for Advanced Simulation (IAS)
Jülich Supercomputing Centre (JSC)

Performance analysis and comparison of parallel eigensolvers on Blue Gene architectures

Jan Felix Münchhalfen

Inhaltsverzeichnis

1	Introduction	3
2	Mathematical principals	5
2.1	Basic definitions	5
2.2	Eigenvalue problem	7
3	Algorithms	13
3.1	General approach	13
3.2	Tridiagonalization	14
3.3	Solution of the tridiagonal eigenvalue problem	19
3.3.1	Divide and conquer	19
3.3.2	MRRR	22
3.4	Back transformation	28
4	Architectures and libraries	31
4.1	Blue Gene	31
4.1.1	Blue Gene/P (JUGENE)	32
4.1.2	Blue Gene/Q (JUQUEEN)	34
4.2	Libraries	36
4.2.1	ELPA	36
4.2.2	Elemental	39
5	Performance analysis, comparision and optimization	45
5.1	Test Matrices	45
5.2	Correctness of results	46
5.3	Tuning parameters	46
5.3.1	ELPA - JUGENE	47
5.3.2	ELPA - JUQUEEN	48
5.4	Runtime Analysis	50
5.4.1	JUGENE - ELPA one-stage, two-stage and Elemental . .	50
5.4.2	JUQUEEN - ELPA one-stage, two-stage and Elemental .	53
5.4.3	Runtime analysis conclusions	56
6	Scalasca instrumentation	57
6.1	Scalasca	57
6.2	Elemental instrumentation	58

6.3	ELPA one-stage instrumentation	58
6.4	ELPA two-stage instrumentation	59
7	Outlook	61

Jül-4359
Januar 2013
ISSN 0944-2952