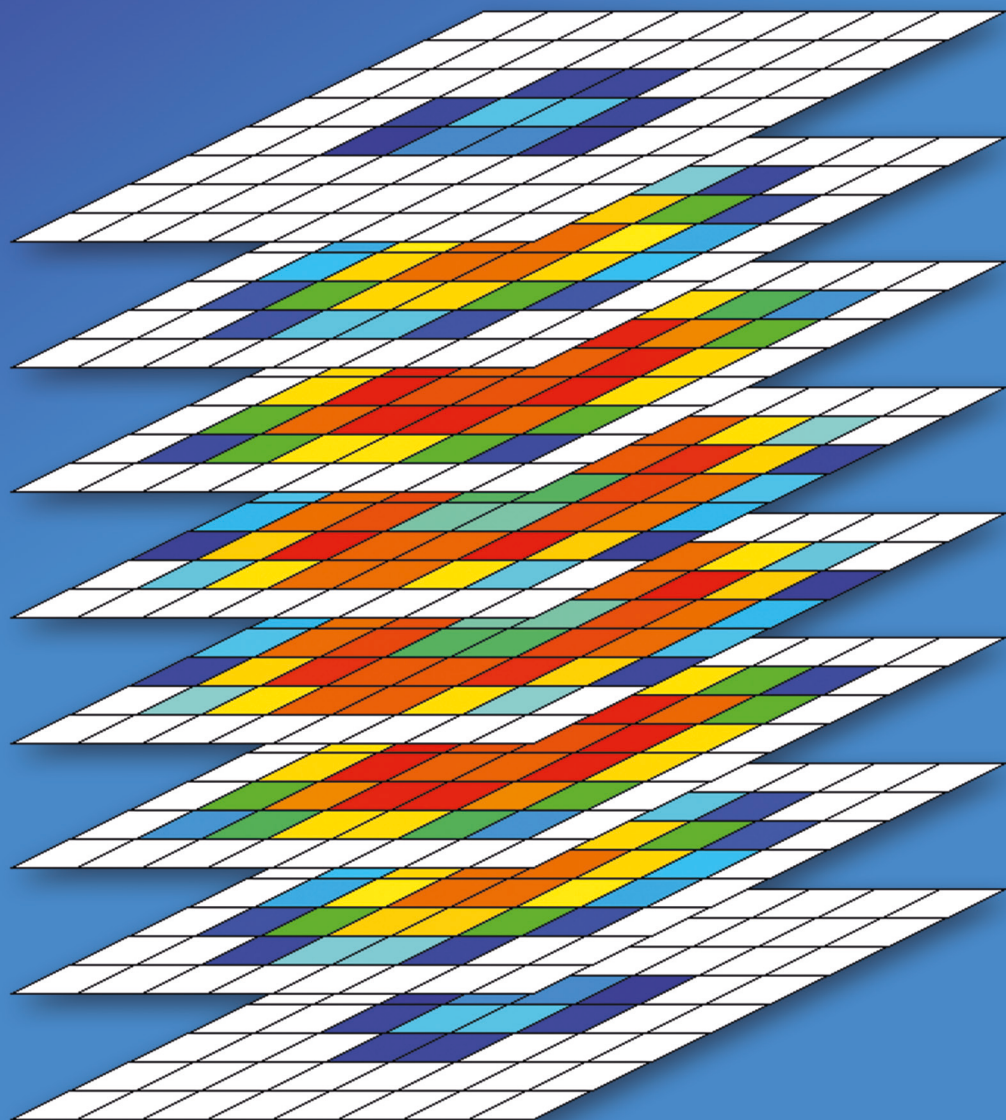




Real-Space Finite-Difference PAW Method for Large-Scale Applications on Massively Parallel Computers

Paul Ferdinand Baumeister

Forschungszentrum Jülich GmbH
Peter Grünberg Institut (PGI)
Quanten-Theorie der Materialien (PGI-1/IAS-1)

Real-Space Finite-Difference PAW Method for Large-Scale Applications on Massively Parallel Computers

Paul Ferdinand Baumeister

Schriften des Forschungszentrums Jülich
Reihe Schlüsseltechnologien / Key Technologies

Band / Volume 53

ISSN 1866-1807

ISBN 978-3-89336-836-5

1	Introduction	1
2	Density Functional Theory	13
2.1	The Many-Body System	13
2.2	Foundation of Density Functional Theory	16
3	Projector Augmented-Wave Method	21
3.1	Basics of PAW	24
3.2	PAW Transformed Operators	28
3.3	Comparison PAW and APW	33
3.4	Total Energy	34
3.5	Hamiltonian	43
3.6	Forces	45
3.7	Preparations for a PAW Calculation	47
3.8	Initial Wave Functions	48
3.9	The Self-consistency Cycle	49
3.10	Summary	49
4	Cartesian Real-Space Grid	51
4.1	Finite Differences	52

4.2	Lagrange Interpolation	57
4.3	Filtering Methods	59
4.4	Algorithms	69
5	Parallelization	75
5.1	Introduction to Parallel Efficiency	75
5.2	Spin- and k-point Parallelization	79
5.3	Real-Space Domain Decomposition	81
5.4	Band Parallelization	98
5.5	Size Scaling	102
5.6	Summary	111
6	Application to GeSbTe	113
6.1	Introduction	113
6.2	Classification of Te in $\text{Ge}_{125}\text{Sb}_{250}\text{Te}_{500}$	116
6.3	Large System: $\text{Ge}_{512}\text{Sb}_{1024}\text{Te}_{2048}$	127
6.4	Summary	133
7	Conclusions	135
A	PAW Data Generation	139
B	Grid vs. Basis	155
C	Implementation Details	161
C.1	Accuracy Benchmark	161
D	User Manual	195
	Bibliography	203

Schlüsseltechnologien / Key Technologies
Band / Volume 53
ISBN 978-3-89336-836-5

