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Quantum Chemistry Review; 4.2 Hardware and CUDA Overview; 4.3 GPU ERI Evaluation; 4.4 Integral-Direct Fock Construction on GPUs
4.5 Precision Considerations4.6 Post-SCF Methods; 4.7 Example Calculations; 4.8 Conclusions and Outlook; References; Chapter 5: GPU Acceleration for Density Functional Theory with Slater-Type Orbitals; 5.1 Background; 5.2 Theory and CPU Implementation; 5.3 GPU Implementation; 5.4 Conclusion; References; Chapter 6: Wavelet-Based Density Functional Theory on Massively Parallel Hybrid Architectures; 6.1 Introductory Remarks on Wavelet Basis Sets for Density Functional Theory Implementations; 6.2 Operators in Wavelet Basis Sets; 6.3 Parallelization; 6.4 GPU Architecture
6.5 Conclusions and OutlookReferences; Chapter 7: Plane-Wave Density Functional Theory; 7.1 Introduction; 7.2 Theoretical Background; 7.3 Implementation; 7.4 Optimizations; 7.5 Performance Examples; 7.6 Exact Exchange with Plane Waves; 7.7 Summary and Outlook; 7.8 Acknowledgments; References; Appendix A: Definitions and Conventions; Appendix B: Example Kernels; Chapter 8: GPU-Accelerated Sparse Matrix-Matrix Multiplication for Linear Scaling Density Functional Theory; 8.1 Introduction; 8.2 Software Architecture for GPU-Acceleration; 8.3 Maximizing Asynchronous Progress
8.4 Libcusmm: GPU Accelerated Small Matrix Multiplications8.5 Benchmarks and Conclusions; Acknowledgments; References; Chapter 9: Grid-Based Projector-Augmented Wave Method; 9.1 Introduction; 9.2 General Overview; 9.3 Using GPUs in Ground-State Calculations; 9.4 Time-Dependent Density Functional Theory; 9.5 Random Phase Approximation for the Correlation Energy; 9.6 Summary and Outlook; Acknowledgments; References; Chapter 10: Application of Graphics Processing Units to Accelerate Real-Space Density Functional Theory and Time-Dependent Density Functional Theory Calculations; 10.1 Introduction
10.2 The Real-Space Representation

Sommario/riassunto

"Electronic Structure Calculations on Graphics Processing Units: From Quantum Chemistry to Condensed Matter Physics provides an overview of computing on graphics processing units (GPUs), a brief introduction to GPU programming, and the latest examples of code developments and applications for the most widely used electronic structure methods. The book covers all commonly used basis sets including localized Gaussian and Slater type basis functions, plane waves, wavelets and real-space grid-based approaches. The chapters expose details on the calculation of two-electron integrals, exchange-correlation quadrature, Fock matrix formation, solution of the self-consistent field equations, calculation of nuclear gradients to obtain forces, and methods to treat excited states within DFT. Other chapters focus on semiempirical and correlated wave function methods including density fitted second order Moshlasser-Plesset perturbation theory and both iterative and perturbative single- and multireference coupled cluster methods. Electronic Structure Calculations on Graphics Processing Units: From Quantum Chemistry to Condensed Matter Physics presents an accessible overview of the field for graduate students and senior researchers of theoretical and computational chemistry, condensed matter physics and materials science, as well as software developers looking for an entry point into the realm of GPU and hybrid GPU/CPU programming for electronic structure calculations"--