Electronic Structure Calculations on Graphics Processing Units: From Quantum Chemistry to Condensed Matter Physics
Ross C. Walker (Editor), Andreas W. Goetz (Editor)

Hardcover ISBN: 978-1-118-66178-9  April 2016  $182.00

DESCRIPTION

*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 Møller-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.
ABOUT THE AUTHOR

Ross C. Walker, San Diego Supercomputer Center and Department of Chemistry and Biochemistry, University of California San Diego

Dr. Walker is an Assistant Research Professor at the San Diego Supercomputer Center, an Adjunct Assistant Professor in the Department of Chemistry and Biochemistry at the University of California San Diego, and an NVIDIA CUDA fellow. He leads a team of scientists that develop advanced techniques for molecular dynamics (MD) simulations aimed at improving drug and biocatalyst design.

Aspects of his work that are of particular relevance for the proposed book include the development of quantum mechanics (QM) and quantum mechanics/molecular mechanics (QM/MM) methods for MD simulations, and the development of a widely used GPU accelerated MD code with funding from the National Science Foundation program SI2 (Software Infrastructure for Sustained Innovation). These methods, including the GPU accelerated MD code, are integrated into the AMBER MD software package that is used worldwide.

Over the course of the last years Dr. Walker has given presentations and lectured on multiple occasions about GPU acceleration of MD codes and scientific applications. Dr. Walker's research is documented in over 30 peer-reviewed journal articles and multiple collected works. In 2010 Dr. Walker co-authored with Dr. Goetz a book chapter that reviews the use of GPU accelerators in quantum chemistry.

Andreas W. Goetz, San Diego Supercomputer Center, University of California San Diego

Dr. Goetz is an Assistant Project Scientist at the San Diego Supercomputer Center with strong expertise in method and scientific software development for quantum chemistry and molecular dynamics simulations on high performance computing platforms. He is a contributing author of the ADF (Amsterdam Density Functional) software for DFT calculations and the AMBER MD software package.

Over the last years, Dr. Goetz has given various contributed and invited presentations of his work at renowned universities and international conferences. Dr. Goetz has also organized and taught workshops demonstrating the use of the software he develops. His research is documented in 21 peer-reviewed journal articles and 1 book contribution.

For additional product details, please visit https://www.wiley.com/en-us