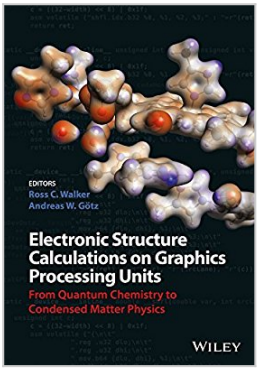

Electronic Structure Calculations on Graphics Processing Units: From Quantum Chemistry to Condensed Matter Physics

From Wiley

Electronic Structure Calculations on Graphics Processing Units: From Quantum Chemistry to Condensed Matter Physics From Wiley

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.

Electronic Structure Calculations on Graphics Processing Units: From Quantum Chemistry to Condensed Matter Physics

From Wiley

Electronic Structure Calculations on Graphics Processing Units: From Quantum Chemistry to Condensed Matter Physics From Wiley

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.

Electronic Structure Calculations on Graphics Processing Units: From Quantum Chemistry to Condensed Matter Physics From Wiley Bibliography

- Sales Rank: #2549118 in eBooks
- Published on: 2016-02-16
- Released on: 2016-02-16
- Format: Kindle eBook

Editorial Review

From the Back Cover

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.

Users Review

From reader reviews:

Richard Cassidy:

Book is written, printed, or descriptive for everything. You can learn everything you want by a guide. Book has a different type. To be sure that book is important matter to bring us around the world. Close to that you can your reading expertise was fluently. A publication Electronic Structure Calculations on Graphics Processing Units: From Quantum Chemistry to Condensed Matter Physics will make you to become smarter. You can feel considerably more confidence if you can know about everything. But some of you think that will open or reading some sort of book make you bored. It is not necessarily make you fun. Why they can be thought like that? Have you looking for best book or acceptable book with you?

Jackie Peters:

Now a day those who Living in the era everywhere everything reachable by connect with the internet and the resources in it can be true or not call for people to be aware of each details they get. How many people to be smart in obtaining any information nowadays? Of course the answer then is reading a book. Studying a book can help persons out of this uncertainty Information specifically this Electronic Structure Calculations on Graphics Processing Units: From Quantum Chemistry to Condensed Matter Physics book as this book offers you rich data and knowledge. Of course the details in this book hundred per-cent guarantees there is no doubt in it you know.

Vickie Kay:

Playing with family within a park, coming to see the sea world or hanging out with friends is thing that usually you might have done when you have spare time, and then why you don't try issue that really opposite from that. Just one activity that make you not sense tired but still relaxing, trilling like on roller coaster you have been ride on and with addition of knowledge. Even you love Electronic Structure Calculations on Graphics Processing Units: From Quantum Chemistry to Condensed Matter Physics, you may enjoy both. It is great combination right, you still would like to miss it? What kind of hangout type is it? Oh seriously its mind hangout people. What? Still don't have it, oh come on its called reading friends.

Jennifer Stephens:

Do you like reading a book? Confuse to looking for your best book? Or your book seemed to be rare? Why so many query for the book? But any people feel that they enjoy to get reading. Some people likes reading through, not only science book and also novel and Electronic Structure Calculations on Graphics Processing

Units: From Quantum Chemistry to Condensed Matter Physics or others sources were given expertise for you. After you know how the good a book, you feel would like to read more and more. Science reserve was created for teacher or even students especially. Those books are helping them to bring their knowledge. In some other case, beside science book, any other book likes Electronic Structure Calculations on Graphics Processing Units: From Quantum Chemistry to Condensed Matter Physics to make your spare time a lot more colorful. Many types of book like this one.

Read Electronic Structure Calculations on Graphics Processing Units: From Quantum Chemistry to Condensed Matter Physics From Wiley for online ebook

Electronic Structure Calculations on Graphics Processing Units: From Quantum Chemistry to Condensed Matter Physics From Wiley Free PDF d0wnl0ad, audio books, books to read, good books to read, cheap books, good books, online books, books online, book reviews epub, read books online, books to read online, online library, greatbooks to read, PDF best books to read, top books to read Electronic Structure Calculations on Graphics Processing Units: From Quantum Chemistry to Condensed Matter Physics From Wiley books to read online.

Online Electronic Structure Calculations on Graphics Processing Units: From Quantum Chemistry to Condensed Matter Physics From Wiley ebook PDF download

Electronic Structure Calculations on Graphics Processing Units: From Quantum Chemistry to Condensed Matter Physics From Wiley Doc

Electronic Structure Calculations on Graphics Processing Units: From Quantum Chemistry to Condensed Matter Physics From Wiley Mobipocket

Electronic Structure Calculations on Graphics Processing Units: From Quantum Chemistry to Condensed Matter Physics From Wiley EPub