

1. Record Nr.	UNINA9910816354503321
Titolo	Electronic structure calculations on graphics processing units : from quantum chemistry to condensed matter physics // Ross C. Walker and Andreas W. Goetz, editors
Pubbl/distr/stampa	West Sussex, England : , : Wiley, , 2016 ©2016
ISBN	1-118-67070-1 1-118-67071-X 1-118-67069-8
Descrizione fisica	1 online resource (448 p.)
Classificazione	SCI013050
Disciplina	621.39/96
Soggetti	Electronic structure - Computer simulation Electronic structure - Mathematical models Graphics processing units - Programming Mathematical physics
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Description based upon print version of record.
Nota di bibliografia	Includes bibliographical references and index.
Nota di contenuto	Title Page; Copyright; Table of Contents; List of Contributors; Preface; Acknowledgments; Glossary; Abbreviations - Scientific; Abbreviations - Technical; Chapter 1: Why Graphics Processing Units; 1.1 A Historical Perspective of Parallel Computing; 1.2 The Rise of the GPU; 1.3 Parallel Computing on Central Processing Units; 1.4 Parallel Computing on Graphics Processing Units; 1.5 GPU-Accelerated Applications; References; Chapter 2: GPUs: Hardware to Software; 2.1 Basic GPU Terminology; 2.2 Architecture of GPUs; 2.3 CUDA Programming Model; 2.4 Programming and Optimization Concepts 2.5 Software Libraries for GPUs2.6 Special Features of CUDA-Enabled GPUs; References; Chapter 3: Overview of Electronic Structure Methods; 3.1 Introduction; 3.2 Hartree-Fock Theory; 3.3 Density Functional Theory; 3.4 Basis Sets; 3.5 Semiempirical Methods; 3.6 Density Functional Tight Binding; 3.7 Wave Function-Based Electron Correlation Methods; Acknowledgments; References; Chapter 4: Gaussian Basis Set Hartree-Fock, Density Functional Theory, and Beyond on GPUs; 4.1

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 Considerations 4.6 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 Outlook References; 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 Libcumm: GPU Accelerated Small Matrix Multiplications 8.5  
 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 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"--

2. Record Nr.	UNISA996465315803316
Titolo	Information Retrieval Technology : 5th Asia Information Retrieval Symposium, AIRS 2009, Sapporo, Japan, October 21-23, 2009, Proceedings / / edited by Dawei Song, Chin-Yew Lin, Akiko Aizawa, Kazuko Kuriyama, Masaharu Yoshioka, Tetsuya Sakai
Pubbl/distr/stampa	Berlin, Heidelberg : , : Springer Berlin Heidelberg : , : Imprint : Springer, , 2009
ISBN	3-642-04769-6
Edizione	[1st ed. 2009.]
Descrizione fisica	1 online resource (XIII, 446 p.)
Collana	Information Systems and Applications, incl. Internet/Web, and HCI ; ; 5839
Classificazione	DAT 825f SS 4800
Disciplina	004n/a
Soggetti	Data mining Application software Information storage and retrieval Algorithms Data structures (Computer science) Data Mining and Knowledge Discovery Information Systems Applications (incl. Internet) Information Storage and Retrieval Algorithm Analysis and Problem Complexity Data Structures Data Storage Representation
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Bibliographic Level Mode of Issuance: Monograph
Nota di bibliografia	Includes bibliographical references and index.
Nota di contenuto	Regular Papers -- Fully Automatic Text Categorization by Exploiting WordNet -- A Latent Dirichlet Framework for Relevance Modeling -- Assigning Location Information to Display Individuals on a Map for Web People Search Results -- Web Spam Identification with User Browsing Graph -- Metric and Relevance Mismatch in Retrieval Evaluation -- Test Collection-Based IR Evaluation Needs Extension toward Sessions -- A Case of Extremely Short Queries -- Weighted Rank Correlation in Information Retrieval Evaluation -- Extractive Summarization Based on

Event Term Temporal Relation Graph and Critical Chain -- Using an Information Quality Framework to Evaluate the Quality of Product Reviews -- Automatic Extraction for Product Feature Words from Comments on the Web -- Image Sense Classification in Text-Based Image Retrieval -- A Subword Normalized Cut Approach to Automatic Story Segmentation of Chinese Broadcast News -- Japanese Spontaneous Spoken Document Retrieval Using NMF-Based Topic Models -- Finding 'Lucy in Disguise': The Misheard Lyric Matching Problem -- Selecting Effective Terms for Query Formulation -- Discovering Volatile Events in Your Neighborhood: Local-Area Topic Extraction from Blog Entries -- A Unified Graph-Based Iterative Reinforcement Approach to Personalized Search -- Exploiting Sentence-Level Features for Near-Duplicate Document Detection -- Posters -- Language Models of Collaborative Filtering -- Efficient Text Classification Using Term Projection -- IPHITS: An Incremental Latent Topic Model for Link Structure -- Supervised Dual-PLSA for Personalized SMS Filtering -- Enabling Effective User Interactions in Content-Based Image Retrieval -- Improving Text Rankers by Term Locality Contexts -- Mutual Screening Graph Algorithm: A New Bootstrapping Algorithm for Lexical Acquisition -- Web Image Retrieval for Abstract Queries Using Text and Image Information -- Question Answering Based on Answer Trustworthiness -- Domain Specific Opinion Retrieval -- A Boosting Approach for Learning to Rank Using SVD with Partially Labeled Data -- Opinion Target Network and Bootstrapping Method for Chinese Opinion Target Extraction -- Automatic Search Engine Performance Evaluation with the Wisdom of Crowds -- A Clustering Framework Based on Adaptive Space Mapping and Rescaling -- Research on Lesk-C-Based WSD and Its Application in English-Chinese Bi-directional CLIR -- Searching Polyphonic Indonesian Folksongs Based on N-gram Indexing Technique -- Study on the Click Context of Web Search Users for Reliability Analysis -- Utilizing Social Relationships for Blog Popularity Mining -- S-node: A Small-World Navigation System for Exploratory Search -- Efficient Probabilistic Latent Semantic Analysis through Parallelization.

---

#### Sommario/riassunto

This book constitutes the refereed proceedings of the 5th Asia Information Retrieval Symposium, AIRS 2009, held in Sapporo, Japan, in October 2009. The 18 revised full papers and 20 revised poster papers presented were carefully reviewed and selected from 82 submissions. All current aspects of information retrieval - in theory and practice - are addressed; working with text, audio, image, video and multimedia data.

---