1. Record Nr. UNINA9910869163103321

Titolo	Computational Science – ICCS 2024 : 24th International Conference, Malaga, Spain, July 2–4, 2024, Proceedings, Part VI / / edited by Leonardo Franco, Clélia de Mulatier, Maciej Paszynski, Valeria V. Krzhizhanovskaya, Jack J. Dongarra, Peter M. A. Sloot
Pubbl/distr/stampa	Cham : , : Springer Nature Switzerland : , : Imprint : Springer, , 2024
ISBN	9783031637780
Edizione	[1st ed. 2024.]
Descrizione fisica	1 online resource (434 pages)
Collana	Lecture Notes in Computer Science, , 1611-3349 ; ; 14837
Disciplina	511.3
Soggetti	Computer science Artificial intelligence Computer engineering Computer networks Software engineering Computer science - Mathematics Theory of Computation Artificial Intelligence Computer Engineering and Networks Software Engineering Mathematics of Computing
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Nota di bibliografia	Includes bibliographical references and index.
Nota di contenuto	Intro -- Preface -- Organization -- Contents - Part VI -- Network Models and Analysis: From Foundations to Artificial Intelligence -- Representation Learning in Multiplex Graphs: Where and How to Fuse Information? -- 1 Introduction -- 2 Related Work -- 3 Information Fusion in Multiplex Graphs -- 3.1 Experimental Setup and Evaluation -- 3.2 Baseline Approaches (no Fusion) -- 3.3 Graph-Level Fusion -- 3.4 Prediction-Level Fusion -- 3.5 GNN-Level Fusion -- 3.6 Embedding-Level Fusion -- 4 Conclusions, Research Gaps and Future Work -- References -- Data Augmentation to Improve Molecular Subtype Prognosis Prediction in Breast Cancer -- 1 Introduction -- 2 Related

Works -- 3 Breast Cancer Cohort -- 4 Data Augmentation Methods -- 5 Experiments and Results -- 6 Conclusion and Future Work -- References -- Threshold Optimization in Constructing Comparative Network Models: A Case Study on Enhancing Laparoscopic Surgical Skill Assessment with Edge Betweenness -- 1 Introduction -- 2 Methodology -- 2.1 Needle Passing Task -- 2.2 EMG Data Collection and Pre-processing -- 2.3 NASA-TLX Scores -- 2.4 Nodes and Edges -- 2.5 Edge Betweenness and Modularity for Threshold Selection -- 3 Results -- 3.1 Enrichment Analysis -- 4 Discussion -- 5 Conclusion -- References -- Graph Vertex Embeddings: Distance, Regularization and Community Detection -- 1 Introduction -- 2 Related Work -- 3 Problem Statement -- 4 Method -- 4.1 Embeddings as Solution to Optimization Problem -- 4.2 Regularized Embeddings -- 4.3 Distance Functions -- 5 Experiments -- 5.1 Datasets -- 5.2 Graph Analysis -- 5.3 Graph Drawing -- 5.4 Community Detection in Graphs -- 6 Conclusions -- References -- A Robust Network Model for Studying Microbiomes in Precision Agriculture Applications -- 1 Introduction -- 2 Methods -- 2.1 Overview of Workflow -- 2.2 Data Description -- 2.3 Biological Feature Grouping.
2.4 Co-expression Network Analysis -- 2.5 Characterizing Robust Biological Functions -- 2.6 Comparison of OTUs Pairs Underlying KEGG Modules -- 2.7 Bacterial Functional Enrichment Analysis -- 3 Results and Discussion -- 3.1 A Comparison of Networks in High and Low Biomass Groups -- 3.2 Co-expression Networks Analysis -- 3.3 Characterization of Distinctive KEGG Modules in High and Low Biomass Groups -- 3.4 Comparison of Dynamics of OTUs Pairs Underlying KEGG Modules -- 4 Conclusion -- References -- A Graph-Theory Based fMRI Analysis -- 1 Introduction -- 2 Background -- 2.1 fMRI -- 2.2 Machine Learning -- 2.3 Graph Theory -- 2.4 Network Alignment -- 3 Material and Methods -- 3.1 Dataset Description -- 3.2 Pipeline Description -- 3.3 Proposed Solution -- 4 Results -- 5 Conclusions -- References -- A Pipeline for the Analysis of Multilayer Brain Networks -- 1 Introduction -- 2 Background -- 2.1 Definition of Multilayer Networks -- 2.2 Brain Network Applications -- 3 Materials and Methods -- 3.1 Data Source -- 3.2 Construction and Analysis of Multilayer Networks -- 4 Result and Discussion -- 5 Conclusion -- References -- Numerical Algorithms and Computer Arithmetic for Computational Science -- Modified CORDIC Algorithm for Givens Rotator -- 1 Introduction -- 2 Review of Algorithms and Solutions -- 3 CORDIC Algorithm and Its Modified Version -- 3.1 Realisationation -- 4 Measurements -- 5 Conclusion -- References -- Numerical Aspects of Hyperbolic Geometry -- 1 Introduction -- 2 Hyperbolic Geometry and Representations -- 3 Representation Variants -- 4 Tessellations -- 5 Tests -- 6 Experimental Results -- 7 Comparison Based on Non-numerical Advantages -- 8 Conclusions -- References -- A Numerical Feed-Forward Scheme for the Augmented Kalman Filter -- 1 Introduction -- 2 Problem Settings and Kalman Filter Estimation of the Forcing Term.
3 A Feed-Forward Strategy for the Augmented Kalman Filter -- 3.1 Modeling the Feed-Forward Action -- 3.2 Feed-Forward Reference Extraction -- 3.3 Tuning the Feed-Forward Gain GFF -- 3.4 Regularization Issues -- 4 Numerical Experiments -- 4.1 Inadequacy of the KF Proportional Action with a Diffusive Gain -- 4.2 The Effect of Regularization and Block-Diagonal Reference Extraction -- 5 Discussion and Conclusions -- References -- Calculation of the Sigmoid Activation Function in FPGA Using Rational Fractions -- 1 Introduction -- 2 Artificial Neural Nets and Data Representations -- 3 Rational Fractions and Calculation of the Sigmoid Activation Function

-- 3.1 Rational Fractions -- 3.2 Rational Fractions in Processors -- 3.3 Calculation of the Sigmoid Function -- 4 Experimental Results -- 5 Conclusion -- References -- Parallel Vectorized Algorithms for Computing Trigonometric Sums Using AVX-512 Extensions -- 1 Introduction -- 2 Goertzel and Reinsch Algorithms -- 3 Divide-and-conquer Approach -- 3.1 Goertzel Algorithm -- 3.2 Reinsch Algorithm -- 4 Implementation of the Algorithms -- 5 Results of Experiments -- 6 Conclusions and Future Works -- References -- File I/O Cache Performance of Supercomputer Fugaku Using an Out-of-Core Direct Numerical Simulation Code of Turbulence -- 1 Introduction -- 2 Out-of-Core Direct Numerical Simulation Code -- 2.1 Direct Numerical Simulation Code Implementation -- 2.2 Out-of-Core Implementation Concept -- 3 Fugaku Architecture -- 4 Evaluation of Compute Node (CN)-Cache Performance -- 4.1 Performance Evaluation of the I/O Cache with IOR -- 4.2 Performance Evaluation of the I/O Cache with a Simple Program Similar to the Ooc-DNS Code -- 4.3 Performance Evaluation of I/O Cache with the Ooc-DNS Code -- 4.4 Execution of Ooc-DNS Code with 8,1923 Grid Points -- 5 Conclusions -- References.
A Novel Computational Approach for Wind-Driven Flows over Deformable Topography -- 1 Introduction -- 2 Governing Equations for Wind-Driven Flows over Deformable Topography -- 3 Hybrid Finite Element/Finite Volume Solver -- 3.1 Coupling Conditions at the Interface -- 4 Computational Results -- 4.1 Accuracy Results -- 4.2 Wind-Driven Circulation Flow by Pipe Failure in the Topography -- 5 Conclusions -- References -- Unleashing the Potential of Mixed Precision in AI-Accelerated CFD Simulation on Intel CPU/GPU Architectures -- 1 Introduction -- 2 Related Work -- 3 Floating-Point Data Formats and Mixed Precision in AI-Accelerated CFD Simulation -- 4 Intel CPU and GPU Architectures in Deep Learning Mixed-Precision Computation -- 5 AI-Accelerated CFD Simulation -- 5.1 CFD Simulation of Steady Flow Around a Motorcycle and Rider -- 5.2 Integration of AI Acceleration with CFD Solver -- 5.3 Training Dataset -- 6 Experimental Results -- 6.1 Testing Platforms -- 6.2 Accuracy and Performance Results -- 7 Conclusion -- References -- Quantum Computing -- The Significance of the Quantum Volume for Other Algorithms: A Case Study for Quantum Amplitude Estimation -- 1 Introduction -- 1.1 Quantum Volume -- 1.2 QAE as a Numerical Integration Technique -- 1.3 Related Work -- 1.4 Our Contributions -- 2 Preliminaries -- 2.1 The Noise Model -- 2.2 QAE Without Noise -- 2.3 QAE on Noisy Processors -- 2.4 Dummy QAE Circuits -- 2.5 Fisher Information -- 2.6 A Monte Carlo Example -- 3 Results -- 3.1 Success in a Quantum Volume Experiment -- 3.2 Results for the Error Model -- 3.3 Speed of the QPU -- 3.4 Estimations for the Size of Circuits -- 4 Application of the Noise Model to QAE -- 4.1 General Functions -- 4.2 Shallow Functions -- 5 Conclusions -- References -- KetGPT - Dataset Augmentation of Quantum Circuits Using Transformers -- 1 Introduction.
2 Evolution and Structure of Transformers -- 2.1 Tokenizer -- 2.2 Feed-Forward Neural Network -- 2.3 Self-attention -- 3 KetGPT - Transformers for Quantum Circuit Generation -- 3.1 Input Dataset and Data Preprocessing -- 3.2 Generator: Architecture and Tokenizer -- 3.3 Verification Method: KetGPT Classifier -- 3.4 Implementation Details -- 4 Results and Discussion -- 4.1 Manual Inspection -- 4.2 Classifier-Based Evaluation -- 4.3 Analysis Based on Circuit Structure -- 5 Conclusion and Outlook -- 6 Software Availability -- References -- Design Considerations for Denoising Quantum Time Series Autoencoder -- 1 Introduction -- 2 QuTSAE Design -- 2.1 Design

Choices for QuTSAE Architecture -- 2.2 Design Choices for QuTSAE Input Encoding -- 2.3 Design Choices for QuTSAE Output Decoding/Cost Function -- 2.4 Design Choices for QuTSAE Encoder/Decoder Ansatze -- 3 Experiments -- 3.1 Determining the Optimum Ansatz Size -- 3.2 Impact of Latent Space on Performance -- 3.3 Time Series Denoising -- 4 Conclusions -- References -- Optimizing Quantum Circuits Using Algebraic Expressions -- 1 Introduction -- 2 Proposed Approach -- 3 Representing Quantum Circuits as Algebraic Expressions -- 4 Optimizing the Algebraic Expressions -- 5 Results -- 6 Conclusion -- References -- Implementing 3-SAT Gadgets for Quantum Annealers with Random Instances -- 1 Introduction -- 2 Fundamental Concepts -- 2.1 The 3-SAT and Max-3-SAT Problems -- 2.2 The QUBO Problem and Its Equivalence in Ising Models -- 2.3 Quantum Annealing -- 3 Related Work -- 3.1 Nuesslein2n+m -- 3.2 Nuessleinn+m -- 4 New Approaches -- 4.1 CJ1n+m -- 4.2 CJ2n+m -- 5 Experimental Results -- 6 Conclusion and Future Work -- A Number of Physical Qubits Required per Gadget -- References -- Quantum Annealers Chain Strengths: A Simple Heuristic to Set Them All -- 1 Introduction. 2 Quantum Annealing and Minor Embedding Methods.

Sommario/riassunto

The 7-volume set LNCS 14832 – 14838 constitutes the proceedings of the 24th International Conference on Computational Science, ICCS 2024, which took place in Malaga, Spain, during July 2–4, 2024. The 155 full papers and 70 short papers included in these proceedings were carefully reviewed and selected from 430 submissions. They were organized in topical sections as follows: Part I: ICCS 2024 Main Track Full Papers; Part II: ICCS 2024 Main Track Full Papers; Part III: ICCS 2024 Main Track Short Papers; Advances in High-Performance Computational Earth Sciences: Numerical Methods, Frameworks and Applications; Artificial Intelligence and High-Performance Computing for Advanced Simulations; Part IV: Biomedical and Bioinformatics Challenges for Computer Science; Computational Health; Part V: Computational Optimization, Modelling, and Simulation; Generative AI and Large Language Models (LLMs) in Advancing Computational Medicine; Machine Learning and Data Assimilation for Dynamical Systems; Multiscale Modelling and Simulation; Part VI: Network Models and Analysis: From Foundations to Artificial Intelligence; Numerical Algorithms and Computer Arithmetic for Computational Science; Quantum Computing; Part VII: Simulations of Flow and Transport: Modeling, Algorithms and Computation; Smart Systems: Bringing Together Computer Vision, Sensor Networks, and Artificial Intelligence; Solving Problems with Uncertainties; Teaching Computational Science.