# Program of the Conferences CMMSE and CHPC 2023

Costa Ballena, Cádiz, Spain July 3 – 8, 2023

- There will be no "reception desk". Participants who attend live can collect their identifier at the entrance of Room 1. There will be a small conference gift, do not leave without it. Questions: J. Vigo-Aguiar jvigo@usal.es
- You can download from your web user the certificate of participation. Participants who attend **online** will receive their certificate of participation via email at the end of the presentation day. Questions: <a href="mailto:joseantonio@ual.es">joseantonio@ual.es</a>
- In Room 1 and 2 are for oral presentations and it is recommended to keep 1.5 meters distance between the participants' seats. The same for the 4 social activities programed.
- Poster, session of July 4<sup>th</sup> (Room 2) concentrates on **Quantum Algorithms** and **High Performance Computing** Poster session of July 5<sup>th</sup> (Room 2) contains more general topics.
- Room 3 will be for online presentations (you can bring your computer or follow the room's live stream).
- Contributed talks are 20 min long with Q&A included, for example (17 + 3).

PRESENCIAL SESSIONS: Sunday 2	
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#### **PROGRAM:**

PRESENCIAL SESSIONS: Monday 3\_\_\_\_\_\_

Opening: 9:20 – 9:30 Room 1 Chair: Peter Schwerdtfeger & J. Vigo-Aguiar

#### **PRESENCIAL SESSIONS:**

**Session I: Mathematical Models for Computer Science** 

9:30 Room 1 Chair: Juan Aledo

Aragón Necessity operators to obtaining independent formal sub-contexts				
	A non-deterministic procedure to query answering with generalized			
Medina	quantifiers.			
Ojeda-				
Aciego	Improvement in MRZ reading using validation methods in passports			
Ojeda-Her-				
nandez	A study of Dengue fever via Formal Concept Analysis			
Pérez	Pérez Next Closure algorithm for partial formal contexts			
Aledo	A consensus set for the aggregation of partial rankings			
Fuzzy Linguistic Hypersoft Set with Application to Public Policies re-				
Muhammad Saqlain garding Improvement in Health Services at Rural Areas				
Fueyo	Levelled Partially Ordered Sets			
	PLENARY TALK 50 min 12:15			
	Ezio Venturino University Torino (Italy)			
-	An Industrial Application: Modeling			
	Biodigester Operations			
	Medina Ojeda- Aciego Ojeda-Her- nandez Pérez Aledo Saqlain Fueyo			

**Session II: Numerical Methods for Solving Nonlinear Equations** 

9:30 Room 2 Chair: A. Cordero & J.R. Torregrosa

Alicia	Cordero	A class of optimal fourth-order methods for nonlinear systems				
Francisco	Chicha-	\$(2K+1)\$-step predictor-corrector methods for solving nonlinear prob-				
Israel	rro López	lems				
Ángel Al-	Magre-					
berto	ñán Ruiz	A procedure to obtain quadratic convergence from the secant method				
		An adaptive Steffensen-like families for solving nonlinear systems using				
Litika	Rani	frozen divided differences				
	Sarría	An efficient iterative scheme for estimation of all roots simultaneously of				
Iñigo	Martínez	non-linear equation				
	Torre-	A procedure for designing high-order iterative schemes for solving non-				
Juan R.	grosa	linear systems				
	Triguero-					
Paula	Navarro	Solving multiple roots simultaneously				
Higinio	Ramos	A Robust Iterative Family for multiple roots of Nonlinear Equations				

#### Session III: Integral Methods in Science and Engineering 16:00 Room 1 Chair: Christian Constanda

		PLENARY TALK 50 min Christian Constanda, University of Tulsa (USA)
Appro	ximation c	of Solution for Bending of an Elastic Plate: Interior vs Exterior Cases
Ricardo	Barros	Pn Synthetic Acceleration for the Source Iteration Scheme in Slab-Geometry Discrete Ordinates Transport Calculations
Josef	Bodmann	On Spectroscopy of Sampled Signals Using the Hilbert Transform
Paul	Harris	A model of the spread of a disease through a population with different age .
Scott	Holmstrom	Integral Solutions for Optical Waveguiding and Diffraction
Dorina	Mitrea	Singular Integral Operators on Spaces of Vanishing Mean Oscillations
Marius	Mitrea	Integral Operators and Boundary Value Problems for Weakly Elliptic Systems
Maria Eugenia	Perez- Mar- tinez	Boundary homogenization in some nonlinear problems: extreme cases
Massimo	Lanza de Cristoforis	A survey on the boundary behavior of the double layer potential in Schauder spaces in the frame of an abstract approach
Adolfo	Pires	Mathematical Modelling of Low-Salinity Waterflooding Including Wettability Alteration
Akbota	Abylayeva	Boundedness and compactness of integral operators, the limits of which are functions
Barbara	Zubik-Kowal	Convergence of dynamic iterations applied to linear and nonlinear differential systems (STREAMING Room 3)

#### Session IV: High Performance Computing 9:30 Room 1 Chair P. Alonso-Jorda

Carl- Johannes	Johnsen	Hierarchical Image Processing with Parallel Out-of-core optimization (HIPPO)
Antonio Jesús	Díaz Honru- bia	A parallel quadtree partitioning algorithm for the VVC standard
Pablo Antonio	Martínez	POAS: A Framework for Exploiting Accelerator Level Parallelism in Heterogeneous Environments
Antonio	Morán Mu- ñoz	An FPGA-based prototype for a high-performance interconnection network using Corundum and NetFPGA
Horacio	Pérez-Sán- chez	Integrating High Performance Computing and Interpretable Machine Learning with Large Language Models for Personalized Medicine: A Novel Decision-Making Tool - SIBILA
Silvia	Rodriguez Alcaraz	Performance evaluation of heterogeneous CPU+iGPU and CPU+FPGA schemes using Intel OneAPI on the cloud
Jonas	Dornonville de la Cour	Massively Lockstep Parallel Algorithms for Full Isomer space Optimization
Gabriel	Gómez	Building a hybrid network topology in an HPC Infiniband-based cluster
Jesús	Jover	A platform for UTM service design and evaluation

#### Session V: Algorithms based on Fixed Point Theory 9:30 Room 2 Chair J. Moreno

Kon- rawut	Kham- mahawong	Best Proximity Point for Generalized Cyclic Enriched Contractions					
Kunquan	Lan	xistence of solutions of nonlinear Cauchy type problems for first order					
		fractional differential equations					
Supak	Phiangsungnoen	Fixed Point Results for Generalized Multivalued contraction in the class of					
		Hausdorff controlled metric spaces					
Sani	Salisu	Golden Ratio Approaches to a Solution of Monotone-type Variational Ine-					
		quality Problem In Certain Geodesic Spaces					
Deepak	Singh	Proximal Contractions and Applications to Engineering Problems					
Phumin	Sumalai	Some Darbo type fixed point theorems in the modular space and exist-					
		ence of solution for fractional ordered 2019-nCoV mathematical model					
Juan	Martinez-	Iterative methods for solving the multiple-set split monotone variational					
	Moreno	inclusion problem in Hilbert spaces					

**Session VI: Computational Chemistry** 

16:00 Room 1 Chair: Maria Stepanova

#### **PLENARY TALK 50 min**

#### Peter Schwerdtfeger Massey University Auckland (New Zealand)

From Lennard-Jones to Max Born, Erwin Madelung, Adolf Hurwitz, and Paul Epstein: A Mathematical Journey through Lattices, Lattice Sums and Phase Transitions

		Thase Transitions				
James	Avery	Folding Carbon: A Calculus for Molecular Origami				
Arjan	Berger	Quantum chemistry on a Clifford torus				
Jerzy	Cioslowski	atural Orbitals: Old Concepts, New Developments				
Nelaine	Mora-Diez	Computational studies of biological antioxidant activity				
Dennis	Salahub	Towards ML-Accelerated Discovery of Noncatalytic Materials and Mechanisms				
Nicolas	Salles	Modelling the ionic diffusion under electric field				
Udo	Schwingenschögl	Predicting the gas sensing performance of 2D materials				
Silvija	Shewaga	Ethanol oxidation via hydrogen atom transfer in ethanol-copper cluster complexes: A density functional theory study				
Frank	de Morrée	Unfolding Carbon: Algorithmic Generation of Planar Fullerene Precursor Molecules Using Intrinsic Geometry				
Rafal	Abdank-Kozubski	Atomic-Migration-Controlled Processes in nanostructured intermetal- lic: Experimental and Simulation Studies				
Jaakko	Akola	Reaction path modelling of hydrogen evolution reaction on MoS2: voltage and solvation effects				
Maria	Stepanova	Toward the Prediction of Misfolded Protein Assemblies				
Andreas	Hauser	Metallic Nanoparticles of Increasing Size: Computational Approaches on a Mesoscopic Scale				
Christop- her	Ehlert	Metal-Free Molecular Catalysts for the Oxygen Reduction Reaction				

Poster Session 1: 16:00-17:00 Room 2 Chair: Peter Alonso.

Social activities I: Tuesday 4 (22:30 Garden):

Sherry Degustation (sponsor EVIDEN, QAPTI-VATM sales and Quantum Engineer department).

Session VII: Quantum Algorithms and High-Performance Computing (QHPC) 9:30 Room 1 Chair Ester M. Garzón (15 min talks)

		PLENARY TALK 50 min			
	Andre	és Bravo Montes, Quantum Engineer in EVIDEN Ltd.			
Impleme	ntation of a co	ombinatorial optimization problem with cardinality constraint through QAOA in the QAPTIVA Quantum Simulator			
Jose A.	Belloch	On the use of Embedded Multi-core System-on-Chip for audio signal processing			
Pablo A.	Martínez	Automatic code detection using Large Language Models			
Carlos	Garcia	arly Assessments of Using SYCL for Edge Computing			
Carlos	Garcia	Portability Analysis for Biological Sequence Alignment in Heterogeneous Computing			
Carlos	Reaño	Parallelizing the Detection of Differentially Methylated Regions on Heterogeneous HPC Clusters			
Luis Felipe	Romero-Ca- parrós	Accelerating Epilepsy Diagnosis and Prediction on EEG Signals with GPU-Based Frequency Domain Analysis and Resampling.			
Laura M.	Salvador	Improving fault tolerance in QUANTUM comparator circuits			
Jorge	Vázquez	QPU Integration in OpenCL for heterogeneous programming			
Luis Felipe	Romero	SkewEngine: Enhancing Performance of Intensive Calculations on Regular Mesh Data			

Session VIII: Trends in the analysis and simulation of nonlinear partial differential equations 9:30 Room 2 Chair Luigi Brugnano

		PLENARY TALK 50 min			
	Luigi Burganao Università di Firenze (Italy)				
Recent A	ldvances	in the Geometric Integration of Differential Equations			
Ana C.	Carapito	Reset state switched systems and a boundedness property			
Beltrán	de la Flor	Lambda-Structures for Liènard I-type equations.			
Kordan &	Ospanov	he maximal regularity of the third-order differential equation and its ap-			
Myrzagali		plications			
OmKalthoum	Wanassi	Power Series Solutions to Fractional Variational Problems			
Roderick	Melnik	Nonlocal Dynamic Models in Neurodegenerative Disease Analyses and			
		Ecological Applications: Exploring Nonequilibrium Phenomena			
Kailash C.	Patidar	Construction and analysis of a novel numerical scheme for solving AVL-			
		HIV co-infection model			
Bashir	Al-Hdai-	Bifurcation Analysis for a System of Rational Difference Equations			
	bat				

Alberto	Simões	Stabilities of Ulam-Hyers type for a Boundary Value Problem with Higher			
		Order Fractional Derivatives			
Mihai	Dupac	A nonlinear timeseries analysis on the effect of lower leg injury on the			
		gait dynamics			
Jorge	Macías	The design of the Spanish Tsunami Warning System using Machine Learn-			
	Sánchez	ing techniques. The Atlantic component			

#### Session IX: New advances in statistical methodologies 16:00 Room 2 Chair: Felipe Marques

Cristina	Días	Structured Families of Models and Applications			
		Solving Simultaneous Equation Models with Artificial Neural Network			
Carmen	Perea	- echniques			
		Addressing the algebraic structure of a linear mixed model with balanced			
Carla	Santos	design towards model's extension			
Frederico	Caeiro	Adaptive estimation of the Extreme Value Index			
		Rank tests and ANOVA for a two-sided analysis in cocoa plant breeding			
Célia	Nunes	experiments			
	Fres-	PCA and robust regression methods for spatio-temporal estimation of			
	neda-	temperature and soil moisture in agricultural fields using remote sensor			
Carlos	Portillo	network data			
		Testing the block compound symmetric covariance matrix structure with			
Filipe	Marques	block circular diagonal blocks			
	Llpirodja-	Smart Control System of Straw Mushroom Growing in Greenhouse using			
Sumate	napong	NodeMCU-8266, Chombueng Ratchaburi			

Poster Session 2: 16:00-17:00 Room 2 Chair: Peter Alonso.

# Social activities II: Wednesday 5 (22:30)

Flamenco & Cocktail (free, invited by the organization)

PRESENCIAL SESSIONS:	Thursday (	6				

## Social activities III: EXCURSION SEVILLA main door: 7:20

# Session X: Trends in the analysis and simulation of nonlinear partial differential equations 16:00 Room 1 Chair Luigi Brugnano

Medine	Demir	Subgrid Artificial Viscosity Modelling Based Defect-Deferred Correction Method for Fluid-Fluid Interaction
Nuno M.	Brites	Estimation of moments and density of first passage times by lower and upper risk thresholds
Dong	Liang	Energy Law and Conservative Numerical Methods for Electromagnetic Problems in Metamaterials with Noise and Nonlinearity
Miguel M.	Reis	Stochastic Differential Equations Harvesting Models: Simulation and Numerical Solution
Sol	Sáez	Analysis of a general reaction diffusion model using Lie symmetries and conservation laws
Adrian	Amor-Mar- tin	A Priori Verification Method for Curl-Conforming Vector Functions in Simplices
Madi	Muratbe- kov	Separability, estimates for the eigenvalues and singular numbers (s-numbers) of a class of hyperbolic type differential operators
Madi	Muratbe- kov	Nuclearity of the resolvent of a third order singular differential operator and the completeness of its root vectors

Session XI: General Session 16:00 Room 2 Chair José Aleixo

Víctor	Gatón Bustillo	A comparison of spectral based Value and Policy Iteration methods in dif-
		ferential games problems
F. Javier	Toledo Melero	Piecewise linear self-adaptive representation of the characteristic curve
		of the photovoltaic single diode model
Jose	Aleixo	Computational Methods for Periodic Systems - Recent Developments
Manuel	Ceballos	Graph theory tools for battery level management in sensor networks
Blas	Gómez Mora	Energy-Focused Simulation of Multi-Access Edge Computing Architec-
		tures in Cellular and Wireless Networks
José	Martins	The spread of the truth to fight against fake news
Verónica	Requena	Convolutional Codes: From First-Order to Minimal ISO Representations
Rogério	Serôdio	A quasi-minimal and uniform state-space realization algorithm for linear
		periodic input/output quaternionic behavioral systems
Xaro	Soler-Escrivà	Quantum Linear Codes Based On Systematic Generator Matrices
Sergio	Ruiz-Villafranca	A TabPFN-based Intrusion Detection System for the Industrial Internet of
		Things
Noemí	de Castro García	Application of gaussian mixture models for automatic maliciousness as-
		signment of IP addresses

Parin	Chaipunya	A block-coordinate decomposition approach to non-cooperative games
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## Social activities IV: (22:30) Orchestra

Friday 7	
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**Session XIII: Mathematical Methods and Applications in Business** 

10:00 Room 1 Chair: Javier Ramírez Fernandez

Alberto	Pinto	The influence of transfers among agents in the preservation of public goods
Francisco Javier	Ramírez Fernández	A multi-criteria intelligent approach for sustainable supply chain development in the renewable energy sector
Verónica	Requena	Convolutional Codes: From First-Order to Minimal ISO Representations
Francisco	Reyes	COST/UTILITY analysis of therapy for lung cancer in a univesity hospital
Maria Jose	Ruiz Or- tega	Strategic orientations, relational factors and performance: a new approach drawing on structural equations modelling
Pedro	García-Vi-	Knowledge, adversity and strategy orientation in tourism: curvilinear and
Manuel	llaverde	moderating effects
Gloria	Parra Re-	Enter the first to be sustainable: RESILIENCE AND ADVERSITY
	quena	

Session XIV: CMMSE/CHPC 2024 Conference

10:00 - 12:30 Room 1 Proposal of sessions to cmmse@usal.es

Proposal of new referees and special issues editors to jvigo@usal.es

Session XV: ONLINE SESSION: (videos): All days in Room3. Program:

#### Session P1: Poster Session (Tuesday 4)

#### Tuesday 4: 16:00-17:00 Room 2 (punctuality required) Chair: Peter Alonso

Francisco	Almeida	Peformance and energy efficiency study of a deep learning system optimized with TensorRT
Vicente	Gonzalez	Structure-preserving Denoising of Electron Microscopy Tomograms in Hybrid CPU/GPU Systems
Francisco	Almeida	Parallelization and Perforamance Analysis of Climate Indicators Generation Using Python
Jose Luis	Bosque	IRMaSim: a tool to develop deep reinforcement learning resource managers
Javier	Cuenca	Toward Automatic Selection of the Inter-GPU Communication Library for Solving HPC Applications
Jesús	Cámara Moreno	A Hierarchical Approach for Autotuning Task-based Numerical Libraries on Heterogeneous Architectures
Javier	López Fandiño	Accelerated Extinction Profiles for Anomaly Detection in Fluvial Ecosystems
Juan Antonio	Sicilia Montalvo	Android Malware Analysis using Machine Learning Techniques
Manuel	de Castro	Evaluation of modern high-level FPGA technologies in the context of fluid dynamics applications
Pedro	Alonso-Jordá	Generating Hardware-Aware Code for Matrix Multiplication
Martín	Garzón	IMRT Planning Based on the gEUD Model and Evolutionary Optimization on multicore systems
German	León	Evaluating the soft error sensitivity of LU decomposition on low-power and high-performance GPUs
Francisco José	Orts Gómez	Quantum circuits for computing Hamming distances requiring fewer T gates
Enrique S.	Quintana Ortí	Implementing a Parallel BLIS-like Matrix Multiplication Algorithm over RISC-V
Cristian	Ramirez	Implementing a Parallel BLIS-like Matrix Multiplication Algorithm over RISC-V
Jose	Ranilla	Orthogonal Non-Negative Matrix Factorization for Real-time Respiratory Rate Estimation: A Hybrid Approach for Health Monitoring
Pedro	Vera Candeas	A Hardware Implementation for Sound Source Separation using

		Multichannel Non-negative Matrix Factorization and Direction- of-Arrival Kernels
Francisco	Almeida	Energy Efficiency and Performance Analysis of a legacy scientific application
Francisco	Almeida	Comprehensive Analysis of Energy Efficiency and Performance of ARM and RISC-V SoCs

Session P2: Poster Session (Wednesday 5)

Wednesday 5: 16:00-17:00 Room 2 (punctuality required) Chair: Peter Alonso

Susana	Ferreira	Innovative pedagogical practices in Discrete Mathematics
María Teresa	Trobajo	Online collaborative tools with Latex. Learning experiences of scientific writing of mathematics texts in STEM studies
Ana	Valongo	Neighbourhood, continuity and limit - connecting the dots using AiC framework
Rui	Santos	ROC curve for evaluating pooled sample classification strategies
João Paulo	Martins	Pooled classification based on quantitative variables: a protocol to estimate hypothyroidism prevalence
Miguel	Martins Felgueiras	Pseudo-convex mixtures to model bathtub-shaped hazard rate data
Pedro	Alonso	Gaussian Markov Random Fields and High Relative Accuracy
Miguel	Carriegos	Finite aggregation of cybersecurity data. A data-driven approach
Ana	Portilla	Stability of p-harmonic functions under quasi-isometries
Higinio	Mora	Binary Number Representation and Exact Rational Computing
Christopher	Ehlert	Metal-Free Molecular Catalysts for the Oxygen Reduction Reaction