



ICCMSE 2022

18th International Conference of Computational Methods in Sciences and Engineering

ICCMSE 2022 CONFERENCE



CONFERENCE PROGRAM.

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Registration Desk Hours:

Date	Hours:
26/10	09.00-14.00, 15.00-19.00
27/10	09.00-12.00

Please note that Greek timezone is :(GMT+3) : **Time now in Greece (Click Here)**

**26 October 2022****Room 1 – Virtual Room 1**

Session Name:	Quantum Science Physical Session (1)	No:	1
Chair Name:	Hirokazu Tada, Hisashi Okumura		
Hours	Paper Title	Author	
09:00-09:30	Magnetoresistance in Single Molecules and Molecular Aggregates	Hirokazu Tada	
09:30-10:00	Disaggregation of amyloid- β aggregates observed by nonequilibrium molecular dynamics simulations	Hisashi Okumura	
10:00-10:30	Computational Insights on the Mechanism of Dual Ni/Photo-catalyzed Cross-Coupling Reaction	Akhilesh K. Sharma	
Session Name:	Quantum Science Physical Session (2)	No:	1
Chair Name:	Jan M.L. Martin, Joe Sato		
10:30-11:00	Improved and More Economical Variants of Double-Hybrid Density Functional Theory: The XYG9 “Triple Hybrid” and B2GP-PLYP-PNO-F12	Jan M.L. Martin	
11:00-11:30	Aiming for Unification of L_{μ} - L_{τ} and the standard model gauge group	Joe Sato	
11:30-12:00	Complex Absorbing Potential Based Coupled Cluster Method for Resonance and Decay	Sourav Pal	

Room 1 – Virtual Room 1

Session Name:	Quantum Science Physical Session (3)	No:	1
Chair Name:	Joe Sato, Masako Takasu		
Hours	Paper Title	Author	
22:00-22:30	Molecular Dynamics Simulation of Starch Branching Enzyme with Ancestral Sequence	Masako Takasu	
22:30-23:00	Thermal relic density of super heavy dark matter	Masato Yamanaka	

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Room 2 – Virtual Room 2			
Session Name:	Digital Health Interventions Big Data for Personalized Cancer Survivorship	No:	5
Chair Name:	dr. Izidor Mlakar, dr. Umut Arioiz		
Hours	Paper Title	Author	
09.00-09.25	Artificial Intelligence-Based Detection of Cancer Survivors' Depression Cues: A Narrative Review	Urška Smrke**, Izidor Mlakar, Umut Arioiz, and Nejc Plohl,	
09.25-09.50	Dialog Management System for Pepper Robot on HoSmartAI Platform	Daniel Hari, Izidor Mlakar**	
09.50-10.15	Multimodal E2E Framework for Depression Classification: Preliminary Results	Umut Arioiz**, Izidor Mlakar, Valentino Safran	
10.15-10.40	HL7 FHIR Healthcare Digital System for Patient Data Incorporation & Visualization	Valentino Šafran**, Umut Arioiz, Izidor Mlakar	
10.40-11.05	A Short Review of Factors Associated with Acceptance of Social Robots in Healthcare and Lessons or Their Implementation in Oncological Settings	Nejc Plohl**, Izidor Mlakar, Bojan Musil, and Urška Smrke	
11.05-11.30	Multichannel Fluorescence Microscopy Images CTC Detection: A Deep Learning Approach	Shaila Calvo-Almeida, Ignacio Serrano-Llabrés**, Victoria M. Cal-González, Paulina Piai, Liliana R. Pires, Lorena Diéguez and Lorena González-Castro	
Session Name:	Deep Learning and Data Science in Simulation and Computational Modelling	No:	13
Chair Name:	Roelof Coetzer		
Hours	Paper Title	Author	
11.40-12.00	Exploring the multiple conformational states of RNA Genome through network analysis	Debashree Chakraborty	

Room 2			
Session Name:	Methodologies for process monitoring and fault detection in complex industrial processes	No:	8
Chair Name:	Roelof Coetzer		
Hours	Paper Title	Author	
12.00-12.20	Advanced thermohydraulic multivariate statistical data analysis for improved boiler efficiency and carbon dioxide reduction	<u>Philip Venter</u>	
12.20-12.40	Modelling the Resolution Time of Defaulted Loans using a Promotion Time Cure Model with Gamma Frailty	<u>Janette Larney,</u> Gerrit Grobler, James Allison, Marius Smuts	

Virtual Room 1			
Session Name:	Quantum Science Virtual Session (1)	No:	1
Chair Name:	Taku Onishi		
Hours	Paper Title	Author	
15:00-15:10	Quantum Science - The frontier of Physics and Chemistry	Taku Onishi	
15:10-15:20	Electrons Released from Photoexcited Organic Molecules in Solution Recorded with Femtosecond Time-resolved Near-infrared Spectroscopy	Koichi Iwata	
15:20-15:50	Imaging and controlling ultrafast Dissociation Dynamics	Heide Ibrahim	
15:50-16:20	Chiral recognition of thiaheterohelicene molecules studied by STM and TERS	Takuma Hattori	

Virtual Room 2			
Session Name:	Digital Health Interventions Big Data for Personalized Cancer Survivorship	No:	5
Chair Name:	dr. Izidor Mlakar		
Hours	Paper Title	Author	
16.00-16.30	PERSIST Project: Data collection and usability clinical study results	Matej Horvat**, Maja Ravnik, Dina Bēma, Inese Poļaka, Krista Arcimoviča, Anna Marija Leščinska, Marcela Chavez, Maja Molan , Liliana Pires, Patrick Duflot, Valérie Bleret, Urška Smrke, Ariadna Mato Montero, Beatriz Calderón Cruz.	
16.30-17.00	Breast Lesion Detection from DCE-MRI using YOLOv7	Bahadir Kulavuz**, Mustafa Cavusoglu, Bulent Bayram, Tolga Bakirman, Sinan Sahin, Nusret Araz, Gozde Orhan, Hulusi Emre Surmeli, Tuna Cakar	
17.00-17.30	mHealth Application for Cancer Care Delivery	Kadir Üğüdücü**, Tunç Cerit, Amine Gonca Toprak, Gazihan Alankuş	

Virtual Room 3			
Session Name:	Virtual Symposium on Information, Intelligent, Education and Engineering Application	No:	16
Chair Name:	Chia-Liang Lin and Theodore E. Simos		
Hours	Paper Title	Author	
14.00-14.20	Research on Motion Graphics Design using Kansei Engineering Methods	Xi-Ting Huangx	
14.20-14.40	Research on Aging-friendly Retrofitting of Mobile Apps Interface Design based on Kansei Engineering Methods	Qing-Yun Lian	
14.40-15.00	Path Space Analysis of Chinese Classical Gardens Based on Topological Graph Theory A Case Study of Guo Zhuang Garden in Hangzhou City	Jia-Ni Liu	

Virtual Room 3			
Session Name:	Third Symposium on Fuzzy Logic with Engineering Applications	No:	17
Chair Name:	Avrilia Konguetsof, Basil Papadopoulos		
Hours	Paper Title	Author	
17:00-17:20	Confidence Intervals of a Function of Random Variables using Fuzzy Estimators	Nikos Mylonas, Basil Papadopoulos	
17:20-17:40	Transformation and Generalization of Fuzzy Implication Using Disjunction	Athina Daniilidou, Avrilia Konguetsof, Georgios Souliotis, Basil Papadopoulos	
17:40-18:00	Pragmatic Quantum Computing for Science and Engineering	Apostolos Syropoulos	

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Virtual Room 1

Session Name:	Quantum Science Virtual Session (2)	No:	1
Chair Name:	Taku Onishi, Minoru Tanaka, Osamu Seto		
Hours	Paper Title	Author	
09:00-09:30	Isotope shift as a probe of new physics	Minoru Tanaka	
09:30-10:00	The type-II seesaw mechanism in alternative gauged U(1)X and dark sector	Osamu Seto	
10:00-10:30	Quantification of the hadronic CP violation contribution to the atomic EDMs	Nodoka Yamanaka	
10:30-11:00	Renormalization group improvement of thermally resummed effective potential	Eibun Senaha	
11:00-11:20	Contribution of the Weinberg-type Operator to atomic and nuclear electric dipole moments	Naohiro Osamura	

Virtual Room 2

Session Name:	Methodologies for process monitoring and fault detection in complex industrial processes	No:	8
Chair Name:	Roelof Coetzer		
Hours	Paper Title	Author	
09.00-09.20	Energy Graph-based Approach To Process Monitoring	JH Smith, G van Schoor, KR Uren	
09.20-09.40	Variable contributions based on pairwise PCA	Andre Mostert, Roelof Coetzer, <u>Sugnet Lubbe</u>	
09.40-10.00	Integrating a fundamental process-driven index and a data-driven production unit index for the multivariate monitoring of multiple production units	<u>NJ le Roux</u> , RF Rossouw	
10.00-10.20	Multivariate Statistical Process Monitoring of a Chemical Process Using Singular Spectrum Analysis	<u>S Krishnannair</u> , Roelof Coetzer, RF Rossouw	

Virtual Room 3

Session Name:	6th Symposium on Computational simulation and experimental analysis of hygrothermal phenomena in historical building envelopes	No:	12
Chair Name:	Peter Hlaváč, Dana Koňáková		
Hours	Paper Title	Author	
09.00 - 09.15	Design of Blended Plasters for Building Renovation with Improved Thermal Insulating Ability	J. Maděra , E. Vejmelková, V. Pommer, K. Šádková, P. Rovnaníková, D. Koňáková	
09.15 - 09.30	On Hygric Properties of Blended Plasters for Building Renovation	J. Maděra, E. Vejmelková, V. Pommer, K. Šádková, P. Rovnaníková, D. Koňáková	
09.30 - 09.45	Degradation of Basalt Based Reinforcement Elements in Salt Solution	M. Keppert , E. Vejmelková, V. Šána, J. Litoš, R. Černý	
09.45 - 10.00	Analysis of Porosity and Abrasion Resistance of Composite Material Based on Flax Fiber and Bioepoxy Resin with Corundum Additive	V. Brejcha, K. Kobetičová, D. Koňáková, M. Böhm	
10.00 - 10.15	Impact of Waste Materials on Hygric Transport Parameters of Low-cement Heat-resistant Composites	E. Vejmelková, V. Pommer , K. Šádková, A. Parashar, R. Černý, P. Konvalinka, D. Koňáková	
10.15 - 10.30	Preliminary Study of Thermal Activation of Brick Clays used as Supplementary Cementitious Materials	E. Vejmelková , V. Pommer, K. Šádková, D. Koňáková	
10.30 - 10.45	Effect of Water Removal Techniques on the Composition of Gypsum-based Composites	L. Scheinherrová , A. Monnot, R. Černý	

Virtual Room 2

Session Name:	Mathematical Models and Investigations Methods for Strongly Nonlinear Systems	No:	15
Chair Name:	Alexey A. Kireenkov		
Hours	Paper Title	Author	
11.00-11.20	Dynamics of generalized Lagrange Top	<u>Sergey V. Sokolov, Sergey M. Ramodanov</u>	
11.20-11.40	A constructive algorithm for building rectifiable curves on proximally smooth sets	<u>Mariana Lopushanski</u>	
11.40-12.00	On the incremental intrinsic equations for thin shape memory alloy shells undergoing austenite-to-martensite thermoelastic transition	<u>Sergey I. Zhavoronok, Alexey S. Kurbatov</u>	
12.00-12.20	On the Dynamics of an elastic rod, one end of which rests on a rotating rough plane	<u>Alexey A. Kireenkov</u>	
12.20-12.40	Transient inverse problems for thin-walled structural elements	<u>Gregory Fedotenkov, Yana Vahterova</u>	
12.40-13.00	Sliding and spinning friction for humanoid robot with four cleats at foot	<u>Sergey Semendyaev</u>	

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Virtual Room 1

Session Name:	Quantum Science Virtual Session (3)	No:	1
Chair Name:	Masahiko Takahashi, Tetsuya Taketsugu		
Hours	Paper Title	Author	
09:00-09:30	Electron-Atom Compton Scattering: A New and Unique Tool for Imaging Intramolecular Atomic Motion	Masahiko Takahashi	
09:30-10:00	New chemical reaction analysis approaches: Reaction Space Projector (ReSPer) and Natural Reaction Orbital (NRO)	Tetsuya Taketsugu	
10:00-10:30	FUNDAMENTALS OF CHIRAL MATERIALS FROM FREE-ENERGY SIMULATION APPROACHES	Adriana Pietropaolo	
10:30-11:00	Metal ion directed organization of functional supramolecules	Joe Otsuki	
11:00-11:30	Solvato- and Piezofluorochromism of Organoboron Complexes with the [2.2]Paracyclophane Moiety	Hiroshi Ikeda	

Virtual Room 2

Session Name:	Third Symposium on Fuzzy Logic with Engineering Applications	No:	17
Chair Name:	Georgios Souliotis		
Hours	Paper Title	Author	
09:00-09:20	Generalized Fuzzy Dishkant Implications	Dimitrios Grammatikopoulos, Basil Papadopoulos	
09:20-09:40	Construction Fuzzy Implications via Symmetric Copulas	Georgios Souliotis, Avriilia Konguetsof, Basil Papadopoulos	
09:40-10:00	Estimation of Postseismic Structural Damage with the use of Multiple Linear Regression and Fuzzy Linear Regression Methods	Fani Gkountakou, Anaxagoras Elenas, Basil Papadopoulos	

Virtual Room 1			
Session Name:	Control of Cyber-Physical Systems	No:	9
Chair Name:	Grzegorz Bazydło, Remigiusz Wiśniewski		
Hours	Paper Title	Author	
15.00-15.20	Bounded and Place Invariant-Covered Petri Nets for Cyber-Physical Systems Specification	<u>Marcin Wojnakowski</u> , Remigiusz Wiśniewski, Mateusz Popławski	
15.20-15.40	Initial Verification of Liveness Property in the Control Part of Cyber-Physical Systems modelled by Petri nets	<u>Mateusz Popławski</u> , Marcin Wojnakowski, Remigiusz Wiśniewski, Grzegorz Bazydło	

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Virtual Room 1

Session Name:	Third Symposium on Fuzzy Logic with Engineering Applications	17
Chair Name:	Apostolos Syropoulos	
Hours	Paper Title	Author
09:00-09:20	Parametric Fuzzy Implications Produced via Classes of Strong Negations	Stefanos Makariadis, Avriilia Konguetsof, Basil Papadopoulos
09:20-09:40	A New Constructed Method of Copulas from Fuzzy Implication and Fuzzy Negation	Maria Rapti, Basil Papadopoulos
09:40-10:00	Novel Archimedean Copula Aggregation Operator of Fuzzy Credibility Numbers in Multiple Attribute Decision Making	Stylianios Giakoumakis, Avriilia Konguetsof, Basil Papadopoulos

Virtual Room 1

Session Name:	General Session		GS
Chair Name:			
Hours	Paper Title	Author	
10:30-11:00	EGS-SMS Programming Shell for Medical Physics Radiation Simulations Based on the EGS5 Code System	Itzhack Darras, Jon Feldman and Itzhak Orion	
11:00-11.30	Graph Theoretical Analysis as an Aid in the Elucidation of Structure-Property Relations of Perovskite Materials	Vasilios Raptis and Andreas Kaltzoglou	
11:30-12:00	Mathematical Modeling of a Swirling Fuel-Air Jet in Applications to Low-Emission Fuel Combustion	Vladislav N. Kovalnogov, Ruslan V. Fedorov, Usama Mizher, Sergey V. Bysigin, Dmitry A. Generalov	
12.00-12.30	Investigation of Diffusion During Combustion in Porous Media	Vladislav N. Kovalnogov, Tamara V. Karpukhina, Yuri E. Chamchiyan	
12.30-13.00	Mathematical Modeling of the System Atmospheric Boundary Layer - Wind Generator	Yuri A. Khakhalev, Larisa V. Khakhaleva, Vladislav N. Kovalnogov, Ekaterina V. Tsvetova, Andrei V. Chukalin	
13.00-13.30	Development and Research of Atmospheric Boundary Layer's Digital Twin in the Surroundings of Wind Farms	Vladislav N. Kovalnogov, Ekaterina V. Tsvetova, Larisa V. Khakhaleva, Maria V. Karpukhina, Aksinya A. Ometova	
13.30-14.00	Exploring Numerical Techniques and Formulations in Relativistic Hydrodynamics	Sheldon Rhameez Herbst	

Quantum Science Symposium

Video Session Program

Session Name:	Quantum Science Video Session (1): Theoretical Chemistry and Physics	1
Paper Title		Author
Time-Dependent Multiconfiguration Approaches for Atoms and Molecules in Intense Laser Fields		K. L. Ishikawa
Theoretical study on laser-induced particle formation of Pd		Yuzuru Kurosaki
Theory of Coherent States in a Heat conduction		E. V. Orlenko
A radiative neutrino mass model with a singlet charged scalar and its phenomenology		Tetsuo Shindou
Chemical Concepts from Density Functional Theory: Influence of a Mechanical Force and an External Electric or Magnetic Field		Frank De Proft
Development of Computational Analysis of Difference Vibrational Spectroscopy		Akihiro Morita
Fully quantum mechanical embedding methods based on localized molecular orbitals		Alessandro Genoni
Collective nuclear coordinates, diabatic free energy surfaces and kinetic equations for multistage nonequilibrium charge transfer in polar media		Serguei Feskov
Enhancement of the parity-violating energy difference in electronic excited states of chiral molecules		Naoya Kuroda

Session Name:	Quantum Science Video Session (2): Materials Science	1
Paper Title		Author
Electronic and protonic behavior of hydrogen in metal oxides		K. Fukutani
Efficient spin-charge conversion using two-dimensional electrons gas systems of all-epitaxial single-crystalline perovskite-oxide heterostructures		Shinobu Ohya
Structure-property relationships in geometrically frustrated magnets $\text{Ln}_2\text{LiFeO}_6$ with unusually high valence Fe^{5+} ion		Masato Goto
First-principles calculations for the etching mechanism of function materials in pure water assisted by Pt catalyst		A. I. Osaka

Session Name:	Quantum Science Video Session (3): Molecular Science	1
Paper Title		Author
Multidimensional Potential Energy Surfaces for Propylene Oxide Interacting with Rare-Gas Atoms and Diatomic Molecules		Federico Palazzetti
Three Examples of Efficient Evaluation of Intermolecular Interactions		Berta Fernández
FUNDAMENTALS OF CHIRAL MATERIALS FROM FREE-ENERGY SIMULATION APPROACHES		Adriana Pietropaolo
Computational Studies of Electric Field Effects in CO ₂ Methanation on Ni Metal Surfaces		Katsuhiro Wakamatsu

Session Name:	Quantum Science Video Session (4): Inorganics	1
Paper Title		Author
Luminescence characteristics of Ce ³⁺ and Ce ³⁺ /Eu ²⁺ co-doped Ca _{1.4} Ba _{0.6} Si ₅ O ₃ N ₆ phosphors for application in white LEDs		Toshihiro Moriga
Lightening Calculations for Schiff base Lanthanide Complexes		Takashiro Akitsu
Non-adiabatic molecular dynamics simulation of excited state dynamics of [Fe(bpy) ₃] ²⁺ using a model electronic Hamiltonian		Satoru Iuchi

Session Name:	Quantum Science Video Session (5): Molecular Biology	1
Paper Title		Author
Rational design of proficient enzymes		S. Osuna
Modeling Enzymes That Target Nucleic Acids: From DNA Repair to RNA Interference		Stacey D. Wetmore
Study on Analysis Approach of Canonical Kohn-Sham Molecular Orbital Calculation in Large-scale Molecular System		Toshiyuki Hirano
Photo-cleavage quantum yield of coumarin-caged luciferin		Miyabi Hiyama
Properties of the Protein-Protein Interface Revealed by Molecular dynamics Simulations		Takefumi Yamashita
Computational investigation of the inhibitor reaction on the free energy surface between SARS-CoV-2 M ^{pro} and N3 complex		Toshio Asada