Symmetry
2023

The 4th International Conference on Symmetry

21–23 June 2023 | Barcelona, Spain

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Symmetry 2023 - The 4th International Conference on Symmetry

AXA Convention Centre
Barcelona, Spain
21 – 23 June 2023

Conference Chairs

Prof. Dr. Emilio Elizalde
Prof. Dr. Sergei D. Odintsov
Prof. Dr. Juan Luis García Guirao

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The 4th International Conference on Symmetry
21 – 23 June 2023, Barcelona, Spain

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Conference Program

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Thursday 22 June 2023

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09:25 – 09:50 **María Rosa Duran** - Applied Mathematics in Acute Lymphoblastic Leukemia: Works in Progress

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12:15 – 12:30 **Stephen Anco** - Generalization of Noether's First and Second Theorems in Modern Form to Non-Variational PDEs

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12:45 – 13:00 **Alberto Sevilla** - Fine-Tuning of Colloidal Polymer Crystals by Molecular Simulation

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*Please note that the program described in this book is subject to change. To access the most up-to-date version with the latest updates, kindly scan the QR code provided below.

Welcome from the Chairs

Dear Colleagues,

We are delighted to announce that "**Symmetry 2023 — The 4th International Conference on Symmetry**" will be back in person in 2023. The event is supported by MDPI's open access journal ***Symmetry*** and will be held on **21–23 June 2023 in Barcelona**, Spain.

As expressed by Hermann Weyl, who was responsible for important progress in the field of symmetry in math and physics: "Symmetry is a fundamental phenomenon in nature and all sciences". Additionally, paraphrasing Frank Wilczek, "powerful symmetry principles have guided physicists in their quest for nature's fundamental laws". Although one should add, at the same time, that many of the most interesting situations happen to occur when some fundamental symmetry principle is broken. It thus seems as if nature abhors perfect symmetry.

It is this interplay between symmetry and its breakdown, in the many different domains and situations where they appear, which we want to address in the 4th Symmetry Conference in Barcelona. Specifically, we will foster interaction between scholars working in different fields of science.

We welcome scholars, engineers, students, and non-academic colleagues to join Symmetry 2023, and we kindly ask you to save the date. The aim is to make this event a forum for discussion, knowledge exchange, and fruitful interactions among stakeholders working in the different symmetry-related fields: Computer Science, Mathematics, Physics, Chemistry, Biology, and Engineering Science. Both oral and poster contributions are welcome.

We are very enthusiastic about this 4th Symmetry Conference and are relying on you to make it a successful event.

We look forward to meeting you in Barcelona!

Kind regards,

Prof. Dr. Emilio Elizalde

Prof. Dr. Sergei Odintsov

Prof. Dr. Juan Luis García Guirao

General Information

Symmetry 2023 - The 4th International Conference on Symmetry will be held at the AXA Covention Centre, Barcelona, Spain, on 21 – 23 June 2023.

This conference seeks to bring together leading researchers in the interplay between symmetry and its breakdown, in the many different domains and situations where they appear. The event aims to foster interaction between worldwide scholars working in different fields of science.

Conference Venue

AXA Covention Centre
Carrer de Déu i Mata, 111, 08029 Barcelona

Registration Desk

The desk for registration, information and distribution of documents will be open from 13:00h on 21 June 2023.

Certificate of Attendance

Participants of the event will be able to downlod an electronic Certificate of Attendance by accessing their dashboards on Sciforum.net once the event is concluded. The certificates will be found under the “My Certificates" category.

Disclaimer

Delegates will receive a name-badge at the Information Desk, upon registration. The badge must be worn prominently in order to gain access to the congress area during the event. Admission will be refused to anyone not in possession of an appropriate badge.

Insurance

The organizers do not accept liability for personal accident, loss, or damage to private property incurred as a result of participation in *Symmetry 2023 - The 4th International Conference on Symmetry*. Delegates are advised to arrange appropriate insurance to cover travel, cancellation costs, medical, and theft or damage of belongings.

Barcelona and Catalonia

Barcelona is the capital and largest city of Catalonia and is Spain's second largest city, with a population of over one and half million people.

Located on the northeastern Mediterranean coast of Spain, this city has a rich and diverse history, with its roots dating back to Roman times. The fruitful medieval period established Barcelona's position as the economic and political centre of the Western Mediterranean. The city's Gothic Quarter bears witness to the splendour enjoyed by the city from the 13th to the 15th centuries.

The 20th century ushered in widespread urban renewal throughout Barcelona city, culminating in its landmark Eixample district, which showcases some of Barcelona's most distinctive Catalan art-nouveau, or modernista, buildings. The Catalan Antoni Gaudí, one of the most eminent architects, designed buildings such as La Pedrera, the Casa Batlló and the Sagrada Família church, which have become world-famous landmarks.

In 1992, Barcelona gained international recognition by hosting the Olympic games which brought about a massive upturn in its tourism industry. For visitors, this has translated into the very modern, yet incredibly old city you see now in the 21st century, where new elements work to both preserve and celebrate both the city's heritage and origins.

Barcelona is plenty of outdoor markets, restaurants, shops, museums, and churches. The city is also very walkable, with an extensive and reliable Metro system for more far-flung destinations.

For a complete overview, see wikitravel.org or visit barcelonaturisme.com.

The AXA Convention Centre

Address: Carrer de Déu i Mata, 111, 08029 Barcelona

The conference will be held at the AXA Convention Centre in Barcelona, Spain. The AXA Convention Centre is located in a vibrant modern zone of the city, next to the main road and with easy access from the airport, as well as the urban and suburban areas.

It is part of "L'Illa Diagonal", a modern complex which include a shopping centre, two 4-stars hotels, several offices, a sports centre, a public park and a parking with 2500 places.

Conference Dinner

Thursday 22 June, 20:30
Price: 45€ *Tickets must be purchased in advance, but you can ask for availability at the Registration Desk.*

We invite you to join us at the Conference Dinner at **Abrassame**, a cutting-edge restaurant specialised in Mediterranean cuisine which, in addition to its location at the pictouresque terrace of Arenas de Barcelona, will make of your evening at the restaurant an experience to remember.

Abrassame is located at the top of **Arenas de Barcelona** (Address: Gran Via de les Corts Catalanes 373 – 385), only a few minutes away from one of Barcelona's most emblematic must-sees, Montjüic. You can easily reach the restaurant from the conference venue either by foot, taxi, or public transport (buses number D40 or V7). To reach the terrace, you could either use the exterior elevator (adults 1€; children, seniors over 65 years old, and people with reduced mobility are free) or climb through the stairs/elevators inside the shopping centre (free).

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Symmetry (ISSN ISSN 2073-8994) is an international, peer-reviewed, open access journal covering research on symmetry/asymmetry phenomena wherever they occur in all aspects of natural sciences. *Symmetry* is published monthly online by MDPI. It has received an increased Impact Factor of 2.940, and an increased 5-Year Impact Factor of 2.834 in the latest edition of the Journal Citation Reports, published by Clarivate Analytics in June 2022.

Symmetry publishes reviews and regular research papers. Our aim is to encourage scientists to publish their experimental and theoretical research in as much detail as possible. Full experimental and/or methodical details must be provided, so that results can be reproduced.

Journal Webpage: https://www.mdpi.com/journal/symmetry

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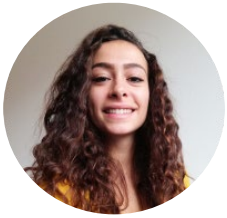

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Abstracts

Talks

Einstein, Barcelona, Symmetry & Cosmology

Emilio Elizalde

IEEC-CSIC and IEEC, Barcelona, Spain

One hundred years ago Albert Einstein visited Barcelona as well as other places in Catalonia and Spain. Also around that time, very interesting solutions to his field equations of the General Theory of Relativity, which he had formulated in 1915 and applied to the cosmos in 1917, were found by Alexander Friedmann; among which, the family that corresponds to our universe. They laid the basis for the construction of Modern Cosmology. Remarkably, the postulates giving rise both to the theory and to the cosmological solution faithfully reflect the far-reaching ideas of naturalness and symmetry, leading to a unique theory and a unique solution, a most precious achievment. The relativity principle itself may also be understood as a symmetry breaking issue. In view of recent observations, however, modifications of general relativity theory are being seriously considered.

On the Abel Differential Equations and the Polynomial Differential Systems

Jaume Llibre

Departament de Matemàtiques, Universitat Autònoma de Barcelona, 08193 Bellaterra, Barcelona, Catalonia, Spain

We study the realtionships between the Abel differential equations dρ/dθ = a(θ)ρ^3 + b(θ)ρ^2 + c(θ)ρ where the functions a(θ), b(θ) and c(θ) are rational functions in the cos θ and sin θ, and the polynomial differential systems of the form x'=-y^m+ Pn(x,y), y'= x^m+ Qn(x,y), being Pn and Qn homogeneous polynomials of degree n>m>0 with m odd.
For these polynomial differential systems we provide sufficient conditions that show that at most two limit cycles can bifurcate in a Hopf bifurcation at the singular point localized at the origin of coordinates. Moreover we show that this upper bound is reached for some of these polynomial differential systems. We also provide sufficient conditions for the integrability of such polynomial differential systems.
Finally we study for this class of polynomial differential systems the existence of algebraic limit cycles, i.e. the existence of limit cycles that live on algebraic curves.

Noether Symmetries in Non-local Gravity Cosmology

Salvatore Capozziello

Dipartimento di Fisica "E. Pancini", Università di Napoli "Federico II", Italy

Recently the so-called Non-Local Gravity acquired a lot of interest as an effective field theory towards the full Quantum Gravity. In this talk, we sketch its main features, discussing possible infrared effects at astrophysical and cosmological scales. In particular, we focus on general non-local actions, including curvature or torsion invariants. In all cases, characteristic lengths emerge at cosmological and astrophysical scales. Furthermore, it is possible to fix the form of the Lagrangian and to study the cosmological evolution considering the existence of Noether symmetries. We discuss also possible astrophysical and cosmological applications for non-local gravity models considering late time cosmic expansion, the structure of galaxy clusters, the S2 orbit around the Galactic Center, the possibility of further modes in gravitational waves. As a final comment it is worth saying that non-locality can be tested in various infrared regimes bringing together physics of short and large scales. Clearly, the possibility to find further gravitational wave modes could be an important test bed for the theory.

Alexander Shelupanov

Department of Complex Information Security of Computer Systems, University of Control Systems and Radioelectronics, Tomsk, Russia

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Symmetry in Regression Analysis - Perpendicular Offsets - The Case of a Photovoltaic Cell

Lorentz Jäntschi

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2 Babeş-Bolyai University, Institute for Doctoral Studies, Kogălniceanu Street no. 1, 400084 Cluj-Napoca, Romania

It is known that for paired measurements subjected to experimental error, better-suited linear regression is obtained using perpendicular offsets. Even so, the vast majority of statistical software still uses classical vertical offsets for reasons of convenience. The same convenience picks the least squares method in favor of maximum likelihood estimation. The treatise for perpendicular offsets for simple linear regression is a little more tricky than the correspondent for vertical offsets. However, to date, there is no general treatise for perpendicular offsets for nonlinear cases. In this work, a typical case of nonlinear dependence—the potential versus intensity of current produced by a photovoltaic cell—is subjected to study; a series of paired potential-intensity data were collected from a commercial photovoltaic device and served for introducing the perpendicular offsets approach, in the case, of nonlinear regression. Photovoltaic cell parameters—internal resistance, short circuit current intensity, the potential of open circuit and the maximum power point—were determined by using the perpendicular offsets approach.

Optically Acive Organophosphorus Compounds With Phosphonate, Phosphinate and Phosphine Oxide Functions: Preparation, Characterization and Utilization

Prof. Dr György Keglevich[1], Dr Péter Bagi[1], Prof. Dr Mátyás Czugler[1], Prof. Dr Konstantin Karaghiosoff[2], Petra Regina Varga[1], József Schindler[1]

1 Budapest University of Technology and Economics, Hungary
2 University of Müenchen, Germany

These days, optically active P-species have been valorized, on the one hand, due to their application as chiral P-ligands in transition metal catalyst complexes and, on the other hand, as pharmaceutical agents. We have had continuing results in the synthesis of different organophosphorus compounds including five- and six-membered P-heterocycles (phospholene, phospholane and dihydro-, tetrahydro- and hexahydrophosphinine derivatives) and a series of phosphonates (alfa-hydroxy- and alfa-aminophosphonates). These species are of interest as intermediates, after deoxygenation, as P-ligands in Pt complexes, and as biologically relevant compounds. The optically active forms were also made available via resolution procedures utilizing TADDOL- or tartaric acid derivatives. In a few cases, the absolute configuration of the P atom was determined by single-crystal X-ray measurement. The Pt complexes of cyclic P-ligands were tested in hydroformylation reactions. The X-ray crystal structure of certain alfa-hydroxy- and aminophosphonates revealed a dimeric structure.

References:

1. Bagi P., Ujj V., Czugler M., Fogassy E., Keglevich G.: Resolution of P-stereogenic P-heterocycles via the formation of diastereomeric molecular and coordination complexes (a review). *Dalton Trans.* **45**, 1823-1842 (2016).
2. Rádai Z., Kiss N. Z. Czugler M., Karaghiosoff K., Keglevich G.: The typical crystal structures of a few representative a-aryl-a-hydroxyphosphonates. *Acta Cryst C*, **75**, 283-293 (2019).
3. Rádai Z., Bagi P., Czugler M., Karaghiosoff K., Keglevich G.: Optical resolution of dimethyl α-hydroxy-arylmethylphosphonates via diastereomer complex formation using calcium hydrogen *O*,*O*'-dibenzoyl-(2*R*,3*R*)-tartrate. *Symmetry-Basel* **12**, 758 (2020).

Some Exact Solutions for a Lotka-Volterra Diffusive Model Applied for High-Grade Brain Tumors

Maria Rosa Duran, Salvador Chulian, Ana Nino, Alvaro Martinez-Rubio, Maria Luz Gandarias

University of Cadiz, Spain

High-grade gliomas are tumors of the glial cells found in the brain and spinal cord. They are called "high-grade" because these tumors are fast-growing and spread quickly through brain tissue, making them hard to treat.
Here, we consider a reduced continuous model describing the evolution of high-grade gliomas in response to hypoxic events through the interplay of different cellular phenotypes. This model was studied in [1] to show how hypoxic events may have a role in accelerating the growth speed of high-grade gliomas.
The model is based on a pair of diffusive Lotka–Volterra equations, including a coupling term accounting for the decay of hypoxic cells into the normoxic phenotype.
We consider this model, generalized to three dimensions, where the force driving phenotype changes depending on the local oxygen pressure.
The coupling term corresponds to the migratory phenotype switch, changing from the proliferative type to a hypoxic one, where there is a lack of oxygen.
Taking into account the classical symmetries admitted by the system [2], we reduce the equations to ordinary differential equations. Then, we focus on exact analytical solutions that present several relevant applications in the field of mathematical biology.
Due to the interest in the phenotypic switch in normoxic and hypoxic cells, we focus on the simulation of such scenarios. In our case, we consider a linear and quadratic phenotypic switch and a limited decrease in hypoxic cells to track the interpretability of the parameters used.

References:
[1] Pardo, R., et al Mart\'inez-Gonz\'alez, A., P\'erez-Garc\'ia, V. M. Nonlinear ghost waves accelerate the progression of high-grade brain tumors. Comm. in Nonlin. Science & Num. Simul 39, 2016, 360--380.
[2] Cherniha R \& King JR. Lie symmetries of nonlinear multidimensional reaction-diffusion systems: I. Journal of Physics A: Mathematical and General 33, 2000, 267-282.

On the Axisymmetric Stokes Flow

Nino Khatiashvili

Iv.Javakhishvili Tbilisi State University, Georgia

Axial symmetry occurs in various physical processes such as fluid flow in pipes, atmospheric vortices, and astrophysical fluids. We study the axisymmetric homogeneous incompressible Newtonian fluid flow of large viscosity for a small Reynolds number over the axis of symmetry in the infinite area. Such flows are called Stokes flows or creeping flows. Creeping fluids (such as some oils and polymers) are widely used in industrial processes and microelectromechanical systems (MEMS).

Velocity components of the flow satisfy the Stokes system (STS) with the equation of continuity and suitable initial-boundary conditions. The Stokes system is the Stokes approximation of the Navier–Stokes Equations (NSE) for the creeping flows and represents the linear system of parabolic equations. We consider STS in the cylindrical polar coordinates under the action of certain pressure. The existence of the bonded solutions of this system is proved.

By the separation of variables, the novel exact solutions of the Stokes system for the specific pressure are obtained in the unsteady case. The profiles of the velocity and the vortex are constructed by means of “MAPLE”.

Curvature Properties of Rotating Objects

Martin Tamm

Dept of Mathematics, University of Stockholm, 106 91 Stockholm, Sweden

An interesting difference between Euclidean geometry and Lorentz geometry is studied. As it turns out, rotating a metric in Euclidian geometry will in general make it more curved (as measured by the scalar curvature). However, surprisingly enough, this is not true in Lorentz geometry, where rotating metrics in certain situations instead tend to be less curved than non-rotating ones. Although the concept of rotation is more complicated in the latter case, the result can, in terms of symmetry, be interpreted as saying that when minimizing curvature, a symmetry that holds in the Euclidian case tends to be broken in the Lorentz case. This also leads to interesting questions in the shadowlands between general relativity and quantum physics. Even if it is still not clear what the answers will be, asking the right questions may give us valuable hints about how the unification of these two theories could be carried out. At the same time, we are led to difficult problems in differential geometry, most of which are still open.

Calculation of Forces on the High Granularity Calorimeter Stainless Steel Absorber Plates in the Compact Muon Solenoid Magnetic Field

Vyacheslav Klyukhin

1 Skobeltsyn Institute of Nuclear Physics, Lomonosov Moscow State University, Russia
2 CERN, Switzerland

The general-purpose Compact Muon Solenoid (CMS) detector at the Large Hadron Collider (LHC) at CERN includes the hadronic calorimeter to register the energies of the charged and neutral hadrons produced in the proton-proton collisions at the LHC at a centre of mass energy 13.6 TeV. The calorimeter is located inside the superconducting solenoid of 6 m in diameter and 12.5 m in length creating the central magnetic flux density of 3.8 T. After finishing the present run of data taken, the existing CMS hadronic endcap calorimeter will be replaced with a new high granularity calorimeter (HGCal) containig in two endcaps the 44 stainless steel absorber plates with a relative permeability value well below 1.05. The volume occupied by 22 plates in each endcap is about 21 m3. The calculation of the axial electromagnetic forces on the absorber plates is a crucial element in designing the mechanical construction of the device. With a three-dimensional computer model of the CMS magnet, the axial forces on each absorber plate are calculated and the dependence of forces on the central magnetic flux density value is presented. The method of calculation and the obtained results are discussed.

Rhodanine Derivatives as Model for New Electrochemical and Colorimetric Sensors Based on Azulene

Eleonora-Mihaela Ungureanu[1], Ovidiu-Teodor Matica[1], Cornelia-Elena Musina[1], Alina Giorgiana Brotea[1], Raluca Isopescu[2], Alexandru C. Razus[3]

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Electrochemical characterization of 2-thioxo-thiazolidin-4-one (**R**), (Z)-5-(azulen-1-ylmethylene)-2-thioxo-thiazolidin-4-one (**R1**), and 5-(4 diethylamino-benzylidene)-2-thioxo-thiazolidin-4-one (**R2**) by cyclic voltammetry, differential pulse voltammetry and rotating disk electrode voltammetry was performed to establish the common properties of these structures. Parallel studies on heavy metal (HM) ion complexation in solution were carried out using UV–Vis.
Since azulenic compounds require special conditions for synthesis, the analogy between the azulenic derivative of rhodanine **R1** and the aromatic rhodanine **R2** creates the premise for an easier selection of azulenic compounds with interesting properties for a certain application. Comparison of the electrochemical studies of these compounds revealed the similarity between the electrochemical processes of their oxidation and reduction, which confirmed their similar chemical properties, which are expected considering the similar electron-donating character of these structures.
The preparation of modified electrodes based on **R1** and **R2** and their electrochemical characterization in view of their application for Pb ion analysis revealed the superiority of the azulene-based monomer. Evidence for film formation by scanning and controlled potential electrolysis was furnished, and HM recognition experiments using their film were carried out. The performance of the chemically modified electrodes was evaluated to establish detection limits for HMs. The azulene monomer **R1** proved to be the best candidate for Pb(II) detection, being about ten times more sensitive than **R2**. However, in solution, **R2** proved to be a good choice for optical measurements, having a higher absorption coefficient. These results support the two ligands having different behaviours in homogeneous and heterogeneous systems.

The Role of Chiral and Achiral Related Structures on the Enantiomer Recognition

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In chemistry, the most widespread method applied for the separation of compounds with a similar structureor mixtures of isomers is the following: the dissolved mixture is reacted with a third compound and the product thus formed will precipitate from the solution. The solid phase contains one compound, and the liquid the other or their derivatives. This method was first employed by Pasteur, who separated the enantiomers of racemic tartaric acid. He added the racemic tartaric acid to the aqueous solution of the d-quinotoxine and the crystals of d-quinotoxine-d-tartaric acid hexa hydrate could be separated via filtration. He recognised that the discrimination of enantiomers could only be carried out with an optically active compound with foreign structures.

Since then, it has become well-known that a supramolecular organisation is characteristic of these crystalline diastereomeric structures, which is stabilised in some cases via infiltration of the solvent molecules.

It has been recognised, furthermore, that this chiral molecule can be also obtained from the enantiomers of the racemic compounds, and this can be the most advantageous resolving agent.

Dutch researchers recognised that the common use of mixtures of several resolving agents with similar structure can be advantageous for separation.

Others observed that a racemic compound, which is inseparable using a resolving agent, became separable by mixing it with an analogous but separable racemic compound.

In conclusion, as regards enantiomer discrimination, chiral–chiral recognition can be most efficient if a chiral compound with a similar structure (either to that of the racemic compound or that of the resolving agent) is also present in addition to the resolving agent.

Boussinesq's Problem for a Power-Law Graded Elastic Half-Space on Elliptical and General Contact Domains

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The indentation of a power-law graded elastic half-space by a rigid counter body is considered in the framework of linear elasticity. Poisson's ratio is assumed to be constant over the half-space. For indenters with an ellipsoidal power-law shape, an exact contact solution is derived, based on the generalizations of Galin's theorem and Barber's maximum normal force principle for the inhomogeneous half-space. As a special case, the elliptical Hertzian contact is revisited. Generally, elastic grading with a positive grading exponent reduces the contact eccentricity. Fabrikant's approximation for the pressure distribution under a flat punch of arbitrary planform is generalized for power-law graded elastic media and compared to rigorous numerical calculations based on the Boundary Element Method (BEM) for a flat punch with a square planform. Very good agreement between the analytical asymptotic solution and the numerical simulation is obtained for the contact stiffness and the contact pressure distribution, except for the corner stress singularity at the corners of the contact square. A recently published approximate analytic solution for the indentation of a homogeneous half-space by a counter body, whose shape only slightly deviates from axial symmetry, is generalized for the power-law graded half-space. The approximate procedure for the elliptical Hertzian contact exhibits the same asymptotic behavior as the exact solution. The asymptotic solution for the indentation by a pyramid with a square planform is in very good agreement with a BEM-based numerical solution of the same problem.

Construction of Pt@BiFeO3/O-g-C3N4 Heterojunction for Efficient Rhodamine B. Photodegradation Driven by Visible-Light

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Photocatalytic degradation of toxic aquatic micropollutants is considered a proficient and green technology for environmental fortification and sustainable economic development. Efficient fabrication of heterojunction systems involving plasmonic metal co-catalysts significantly enhances the activity of semiconductor catalysts for photocatalytic applications. Herein, we report the construction of a Pt@$BiFeO_3$/O-g-C_3N_4 (Pt@BFO/O-CN) heterojunction photocatalyst via an ultrasonic–hydrothermal approach for the degradation of aqueous Rhodamine B (RhB) under visible light illumination. All the as-prepared samples were characterized by physicochemical characterization techniques. The as-constructed Pt@BFO/O-CN heterojunction exhibited an excellent visible-light-driven photodegradation efficiency of RhB of 100% in 50 min with an apparent pseudo-first-order rate constant of about 4.63 x 10^{-2} min^{-1}, which is superior to those of pristine BFO, O-CN, and binary BFO/O-CN. The as-constructed Pt@BFO/O-CN heterojunction demonstrated outstanding stability and recyclability with an efficiency of about 98% after the fourth degradation cycle. The free-radical trapping test results revealed that superoxide ($^{\bullet}O_2^-$) radicals and photogenerated (h^+) took a leading role in the photodegradation reaction of RhB, and the transfer process of photogenerated charge carriers is proposed. This work offers a potential way to construct high-performance heterojunction photocatalytic systems for the decontamination of aquatic micropollutants in industrial wastewater treatment.

F(R) Gravity at Present

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F(R) gravity is one of the modified gravity theories and the most popular of the theories. Here R is the scalar curvature and F(R) is a function of R. The F(R) gravity can describe the accelerating expansion of the present universe and the inflation in the early universe in a unified way. The F(R) gravity may solve the recent problem of Hubble tension.
In order that the F(R) gravity theory could be a realistic theory, the theory must be consistent with the formation of black holes and the recent observational data of the neutron star.
In this talk, I will start by reviewing the basic properties of F(R) gravity and explain how the theory describes cosmological expansion. In the F(R) gravity, there appear the additional scalar degrees of freedom, which becomes a key to keeping the consistencies with the observations.
After that, I will present the application to the static and spherical symmetric compact star configuration like neutron star based on recent work, 2302.03951. Here, especially, we consider the problem of scalar hair.

Applied Mathematics in Acute Lymphoblastic Leukemia: Works in Progress

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Worldwide, almost 280.000 children between 0 and 19 years old are diagnosed with cancer every year, this being one of the main causes of mortality in this group. The most common pediatric tumors are acute lymphoblastic leukemia (ALL). The survival rate of patients with ALL has increased significantly in recent decades, but a small group of patients, around 15-20%, do not respond to standard treatment regimens. Patients are stratified by risk and are treated accordingly. Risk assignment criteria is determined by cytomorphology, molecular biology, cytogenetics, and immunology. The improvement in risk classification is essential for the early identification of relapsing patients, as their prognosis is significantly worse. New strategies are necessary to identify and select patients who do not respond to standard chemotherapy and who are at higher risk of relapse. The use of mathematical models can provide new perspectives that allow progress in the 'war against cancer'. In fact, there is a notable increase in the number of publications and review articles on the use of mathematics in oncology. Advances in this interdisciplinary field of research can provide substantial benefits to both mathematics and medicine.

In short, this work exemplifies the application of mathematical tools applied to the diagnosis, prognosis, and response to the treatment of ALL in children. The study involves the development, theoretical analysis, simulation, and optimization of mathematical models of differential equations and other mathematical techniques to describe the behavior of ALL and the response to treatments. These models are validated using real-world data and predictive variables for recurrence and response to therapies are identified. Additionally, various mathematical methods can be applied to exploit and explore this type of data, with the ultimate goal of providing immediate clinical application results, as well as establishing new prognostic biomarkers.

Primordial Black Holes May Be Dark Matter of the Universe

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Primordial black holes (PBHs) are black holes which are believed to have formed in the very early Universe. Recently an idea that PBHs may be dark matter of the Universe is attracting a lot of attention. In this talk, I first briefly review our knowledge about dark matter and black holes, then introduce the idea of PBHs as dark matter of the Universe, and discuss how it can be observationally tested. It turns out that gravitational waves are the key to observational tests of the idea.

Noether’s Theorem for Nonlocal Lagrangians

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It is well known that the essence of Noether's theorem is the connection between symmetries and conservation laws. For this reason, this talk proposes an extension of Noether's theorem for nonlocal theories, focusing on nonlocal Lagrangians with a finite number of degrees of freedom. In particular, the non-locality describing this type of Lagrangian will be given by integrodifferential operators. Furthermore, we will study Noether's symmetry for them through the concept of the nonlocal total derivative. We will analyze its consequences on the integrodifferential equations that appear in the Euler–Lagrange equations when added to the Lagrangian function. Next, we will focus on invariance under time translations to define the (conserved) energy function. Moreover, using this conserved quantity obtained through this extension, we will infer a suitable definition for momenta, which could open up the possibility of developing a Hamiltonian formalism for such theories.

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The talk is based on three works: [arXiv] 2002.12725 – 2105.10442 – 2203.02206.

Comparing Equivalent Gravities: Common Features and Differences

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We discuss equivalent representations of gravity in the framework of metric-affine geometries, pointing out basic concepts from where these theories originate. In particular, we take into account tetrads and the spin connection to describe the so-called Geometric Trinity of Gravity. Specifically, we consider General Relativity, constructed upon the metric tensor and based on the curvature R; the Teleparallel Equivalent of General Relativity, formulated in terms of torsion T and relying on tetrads and spin connection; and the Symmetric Teleparallel Equivalent of General Relativity, built on non-metricity Q, constructed from metric tensor and affine connection. General Relativity is formulated as a geometric theory of gravity based on metric, whereas teleparallel approaches configure as gauge theories, where auge choices permit us not only to simplify calculations but also to give deep insight into the basic concepts of gravitational fields. Specifically, we point out how the foundation principles of General Relativity (i.e., the Equivalence Principle and the General Covariance) can be seen from a teleparallel point of view. These theories are dynamically equivalent, and this feature can be demonstrated under three different standards: (1) the variational method, (2) the field equations, (3) and the solutions. Regarding the second point, we provide a procedure starting from the (generalised) second Bianchi identity and then deriving the field equations. Referring to the third point, we compare spherically symmetric solutions in vacuum, recovering the Schwarzschild metric and the Birkhoff theorem in all the approaches. It is worth stressing that, in extending the formalisms to f(R), f(T), and f(Q) gravities, respectively, the dynamical equivalence is lost, opening the discussion on the different number of degrees of freedom intervening in the various representations of gravitational theories.

L(2,C) Algebraic Processing of Singularities at the Genome Scale: Transcription Factors and microRNAs

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The decoding of a gene and the regulation of its function widely depend on a small DNA segment—the consensus sequence—in a transcription factor and/or small RNA segment—the seed—in a microRNA. Taking the consensus sequence or the seed as the generator of an infinite group π, we gain access to the symmetries underlying gene decoding. We found a correlation between the closeness of π (defined on r generators A, T/U, G and C , $r = 2$ to 4) to the free group F_r and the absence of a disease [M. Planat et al., CIMB 44, 1417 (2022); IJMS 23, 13290 (2022); 10.20944/preprints202212.0256.v1]. A potential disease occurs either if π is away from F_r or the $SL(2,\mathbb{C})$ (multivariate polynomial) representations of π correspond to a singular scheme spectrum (M. Planat et al., 10.20944/preprints202301.0529.v1). There are algebraic surfaces resulting from isolated singularities of the A-D-E type and surfaces with a non-zero-dimensional subset of singular points. In the latter case, the formal desingularization needs the language of prime divisors of the corresponding scheme. In both cases, we attempt to correlate the nature of the potential disease and the spectrum of the scheme. A small catalogue of singular surfaces for transcription factors and microRNAs is established.

Do Cointegration Tests Produce Symmetric Results? A Monte-Carlo-Simulation- And Real-Data-Based Comparison of the Null of No Cointegration Tests

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A huge variety of cointegration tests have been developed in time series literature, and researchers often face the problem of selecting an appropriate test. This study tries to solve this problem by assessing sixteen tests with a null of no cointegration on the basis of size, stringency criterion and real economic data. The questions this study tries to answer are whether the performances of tests are symmetric/asymmetric with respect to the use of critical values (asymptotic/simulated), whether the stringencies of these tests are symmetric or asymmetric, and whether these tests provide symmetric/asymmetric results for real data. The study uses Monte Carlo simulations to compare the performance of tests on the basis of the type of critical values (asymptotic/simulated) and stringency criterion. The stringencies of the tests are estimated over the whole alternate space. For real data, the study uses the annual consumption and income of 100 countries from 1960 to 2021 and compares the tests on the basis of empirical size distortion and empirical power gain. The study finds that the tests show asymmetric behavior with respect to the use of critical values (asymptotic/simulated) except for two tests (Engle–Granger test and Phillips and Ouliaris' $\hat{Z}_{\alpha}$ test). Moreover, the stringencies are extremely asymmetric as three tests (Phillips and Ouliaris' $\hat{P}_{\mu}$, $\hat{Z}_{\alpha}$, and Choi Durbin–Hausman) always have lesser stringencies as compared to the rest for all the three specifications of the deterministic part and at all four time dimensions of 30, 60, 120 and 240. Furthermore, on the basis of real data, the tests are again extremely asymmetric in performance. Five tests (the t-test of cointegration in a single equation Error Correction Model, Boswijk Wald test, Phillips and Ouliaris test, Phillips and Ouliaris' test and Choi Durbin–Hausman test) are the leading performers as they have lesser empirical size distortions and larger empirical power gains.

Generalization of Noether's First and Second Theorems in Modern Form to Non-Variational PDEs

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Noether's first theorem is commonly known as producing conservation for each symmetry of a variational principle for a PDE or system of PDEs. Noether's second theorem shows that each such symmetry that involves an arbitrary function of all independent variables produces a differential identity holding for a PDE system. Both of these theorems have converses, which are lesser known. There is a modern formulation of Noether's theorem that applies directly to the PDE or system of PDEs, using only the existence of a variational principle but not its explicit form.

This formulation has a natural generalization to non-variational PDEs and systems of PDEs, in which symmetries are replaced by adjoint symmetries, and the condition of invariance of a variational principle is replaced by a Helmholtz-type condition on adjoint symmetries. With this generalization, for any given PDE or system of PDEs (without requiring that a variational formulation exists), all conservation laws can be derived in an algorithmic way, which is similar to Lie's method for finding all symmetries. Likewise, all differential identities holding for a PDE system can be derived.

The main steps in the generalization will be outlined and examples of finding conservation laws and differential identities for non-variational PDEs and systems of PDEs will be illustrated.

Symmetry of Topological Features in the Band Structure of Rare-Earth Monoantimonides

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The band structures of the rare-earth monoantimonides RSb, R = Gd, Tb, and Dy weretheoretically modeled in this work. First-principles calculations were employed within the GGA+U method to obtain and analyze the spin-polarized band structure. Strong electron correlations in the 4f shell of R were accounted for in this method. The effect of spin–orbit coupling on the electronic structure was considered. In GdSb, TbSb, and DySb, the electron–hole compensated semimetallic states are found to have similar electronic structures and small pseudogaps in the densities of electronic states. The asymmetric electron pocket in the G–X–W direction and symmetric hole pockets in the L–G–X direction were found to be in good agreement with the previous experimental ARPES results. The optical conductivity contribution caused by interband transitions was also calculated and used to interpret the energy dependency of experimental optical conductivity spectra obtained by spectroscopic ellipsometry in [Solid State Sciences 136, 107085 (2023)]. The total magnetic moment of the considered semimetals is fully determined by magnetic moments of the R ions, and the calculated effective magnetic moments are compared to the published experimental values for all compounds

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Fine-Tuning of Colloidal Polymer Crystals by Molecular Simulation

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Through a hierarchical modeling scheme, we determine a phase diagram of attractive, flexible polymer chains in two and three dimensions. A surprisingly rich collection of distinct crystal polymorphs appears, which can be finely tuned through the range of attraction. In three dimensions, these include the face-centered cubic, close-packed hexagonal, simple hexagonal and body-centered cubic crystals and the Frank–Kasper phase. A simple geometric model is proposed, based on the concept of cumulative neighbours of ideal crystals, which can accurately predict most of the observed structures and the corresponding transitions. A geometrical analysis is provided on the characteristics of the self-assembled polymer clusters and crystals under conditions that correspond to vacuum conditions. The present work demonstrates, at a fundamental level and utilizing a highly idealized model, how fine-tuning a single interaction parameter can be used for the design of polymer crystals with tailored morphologies. The proposed simulation scheme is currently extended to study the effect of chain flexibility on the phase behavior with emphasis placed on rod-like polymers.

Super Restoration of Explicit and Spontaneous Breaking of Chiral Symmetry in Four-Fermion Interaction Models

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The phase structures of four-fermion interaction models are investigated in the presence of explicit and spontaneous chiral symmetry breaking by varying the temperature and chemical potential. The four-fermion interaction models composed of the N-component of fermions are employed as simple models to induce spontaneous chiral symmetry breaking. In the model, the chiral symmetry is broken explicitly by fermion mass terms and spontaneously by a non-vanishing expectation value of the composite operators constructed by the fermion and anti-fermion.
It is expected that the broken chiral symmetry is restored on the ground state under extreme conditions. We assume that the ground state is homogeneous. In this case, the ground state is determined by observing the minimum of the effective potential. We evaluate the behavior of the effective potential in the leading order of the 1/N expansion and find that the explicitly and spontaneously broken chiral symmetry is restored at high temperature and/or with a large chemical potential. We also show the analytical expression for the phase boundary where the chiral symmetry is completely restored in low-dimensional models.

Novel Podand Ligand With Superhalogen Nature as Effective Molecular Trap

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A novel tripodal podand ligand tris(2-methoxyethyl) fluoroborate anion (TMEFA) based on the $BF4^-$ superhalogen anion was proposed and investigated theoretically using CBS-QB3, MP2 and OVGF quantum chemical methods together with aug-cc-pVDZ and 6-311++G(3df,2pd) basis sets. TMEFA molecule comprises three 2-methoxyethoxy groups (-O-CH2-CH2-O-CH3) connected to the central boron atom, which results in the C3-symmetry of the compound. The resulting anion was stable against selected fragmentation paths, while its vertical electron detachment energy (VDE) was found to be 5.72 eV (which confirmed its superhalogen nature). Due to its equilibrium structure resembling that of classical tripodal ligands, TMEFA is capable of binding metal cations and can thus form strongly bound ionic compounds with Li^+ and Mg^{2+} ions. The binding energies predicted for such complexes (180.1 and 457.3 kcal/mol, respectively) far exceed those of the similar classical podands (either tetradentate or tridentate), which makes TMEFA a more effective molecular trap or steric shielding agent with respect to selected metal cations.

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On Classification of Symmetry Reductions for Some P(1,4)-Invariant Partial Differential Equations

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Earlier, we suggested [1], for the classification of symmetry reduction (invariant solutions) of PDEs with non-trivial symmetry groups, the investigation of the relationship between the structural properties of nonconjugate subalgebras of the same rank of the Lie algebras of the symmetry groups of the equations under consideration and the properties of the reduced equations corresponding to them.

At the present time, we have investigated the relationship between the structural properties of three-dimensional nonconjugate subalgebras of the Lie algebra of the generalized Poincaré group P(1,4) and the types of symmetry reduction for the following (1+3)-dimensional PDEs:

- Eikonal equation;
- Euler–Lagrange–Born–Infeld equation;
- Homogeneous Monge–Ampère equation;
- Inhomogeneous Monge–Ampère equation.

More details on this theme can be found in [2,3,4,5]. In our talk, we plan to present some of the results obtained.

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Near-Miss Polyhedral Cages: A Geometry for Artificial Protein Nano-Cages

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Recently, an artificial protein structure, referred to as TRAP-cage, was discovered experimentally. The structure was made out of 24 nearly regular hendecagons, each having five neighbours with which to share an edge. The remaining six edges per face define the boundaries of 38 holes. The hendecagons were nearly regular but had edges and angles that were slightly different from a regular polygon with a deformation below 0.5%, making the non-symmetry undetectable with the naked eye.

We describe how such regular and nearly regular geometries, which we call polyhedral cages, can be constructed from Cayley graphs if we impose invariance of the p-cage under a congruent automorphism. The symmetries of the graph/regular solid impose some constraints on the number of edges that each face can contribute to each hole. The symmetries of these symmetric p-cages are the symmetries of the regular solids, and one must first find the most general parametrisation of one of the faces, called the representative face, and then use the solid symmetry to determine the coordinates of the other faces. Some of the p-faces have perfectly regular faces and can be derived analytically. We call them regular p-cages. For the non-regular p-cages, which we call near-miss p-cages, a simulated annealing method varying the coordinates of the representative face is then
used to minimise the amount of deformation of the representative face. We found 2371 p-cages, including 224 regular p-cages, built from P-gon
for P=6 to 20 with a deformation not exceeding 10%, and we present some of them here. One of the aims was to characterise the geometries that nano-bio-engineers could consider to create new artificial protein cages.

Consistent Theories of Dirac Particle Derived From Invariance and Covariance Principles

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The quantum theory of a spin 1/2 particle formulated by Dirac in 1928 suffered several problems. For instance, according to Dirac theory, each component of the quantum velocity has an absolute value equal to the speed of light; moreover, the solutions of the free Dirac equation predict violent oscillations of the expectation value of the particle position, a phenomenon called zitterbewegung.
In the present work, we follow an alternative approach that deductively derives the theory from the principles of relativistic invariance of the theory and covariance of the position.
The results ascertain that Dirac theory is just one of the consistent theories for a free Dirac particle. The class of possible quantum theories for a free Dirac particle is explicitly determined. A special subclass is identified whose theories are free from singular features, such as luminal velocity for massive particles and zitterbewegung.
Each theory is characterized by a particular transformation property of a position with respect to boosts. Dirac theory is entirely characterized by its peculiar transformation property.
An ideal experimental test is designed for a free Dirac particle, such that the predictions of the results by Dirac theory and by one of the alternative theories are different, so that the problem of which theory is valid in nature can be experimentally settled, at least in principle.

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A Scalar Product for Computing Fundamental Quantities in Matter

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In classical electrodynamics, there exists a convenient and general way to compute the amounts of fundamental quantities such as linear and angular momentum contained in a given dynamic electromagnetic field [1]. Such an approach exploits the tools of Hilbert spaces. The quantities are computed "a la Dirac" as sandwiches f|G|f>, where |f> is the ket representing the field and G is the Hermitian operator representing the quantity of interest, e.g., an angular momentum operator. Among other advantages, such a methodology allows one to obtain new expressions [2].
In my talk, I will explain how the algebraic approach can be extended to static material systems, allowing one to compute the amounts of fundamental quantities such as helicity and angular momentum contained in static matter, given its charge and magnetization densities [3]. I will also use the framework to show that the electromagnetic helicity of the free electromagnetic field and the static magnetic helicity are two different embodiments of the same physical quantity, the total helicity [4]. The total helicity is the sum of two terms: a term that measures the difference between the power of the left-handed and right-handed polarization components of the free field, and another term that measures the screwiness of the static magnetization density in matter. This unification establishes the theoretical basis for studying the permanent transfer of helicity between light and matter.

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A Virtual Clinical Trial for Leukemia Therapy Using Mathematical Models

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Acute Lymphoblastic Leukemia (ALL) is the most common type of childhood cancer, constituting 80% of leukemias diagnosed in pediatric ages. This disease arises from a disruption of the production in the bone marrow of a type of blood cell called the lymphocyte. While most of such leukemias present a good prognosis, ALL relapses are considerably aggressive. Thus, the mathematical modeling of their therapies is of the utmost importance to overcome a possible future recurrence of this disease.
In this work, we develop a mathematical model, focusing on the bone marrow and its behavior. Firstly, healthy bone marrow is simulated, where the appearance of a leukemic cell disrupts homeostasis. Later, the standard risk patient treatment is applied according to current protocols. The influence of chemotherapy on the disease level depends on the drug type and how much is administrated. Furthermore, we combine this model with immunotherapy, providing a possible combination of both therapies. The aim of this study is then to look for the best option to alternate chemo- and immunotherapy and also minimize toxicity for the patient.

Three-Dimensional Evaluation of Cranio-Cervical Maxillofacial Symmetry Before and After Implant-Assisted Maxillary Expansion

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Transverse deficiency of the maxilla is a fundamental problem that presents itself from infancy, usually as a symmetrical (bilateral) or asymmetrical (unilateral) posterior crossbite, crowding of the anterior teeth, and high arched V-shaped palate, among others. These in turn involve trauma, sagittal repositioning of the mandible, temporomandibular joint disorders, septal deviation, respiratory alterations due to turbinate hypertrophy that could be aggravated by allergic conditions and skeletal alterations typical of OSA (Obstructive Sleep Apnea). Thus, to date, it has been reported that the transverse deficiency of the maxilla is present in approximately 40% of patients with some dentofacial deformity (malocclusion); it has also been reported that this deficiency affects 23% of teen patients and more than 10% of adult patients, and in turn, as it continues, the degeneration of the temporomandibular joint surfaces worsens. According to the abovementioned, maxillary decompression could be considered the **gold standard** for the treatment of transverse deficiency of the maxilla because it could be considered to be the starting point for adequate management of the alterations of the cranio-cervical maxillofacial region. However, due to the fact that the maxilla is articulated with more than seven bones and consequently to the sutures of the facial mass, which are directly related to the structures of the cranio-cervico-maxillofacial region, a question arises that to date has not been answered in a mathematically precise way: **is it possible to perform the expansion of the maxilla assisted by implants maintaining the symmetry of the structures of the cranio-cervico-maxillofacial region?**

Development of Hybrid Symmetric Compact Finite Difference Schemes With High Resolution Characteristics for the Approximation of Derivatives

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Finite difference methods (FDMs) have traditionally been a popular choice for derivative approximations because they are simple and easy to implement. However, in the last fifty years, compact finite difference methods (CFDMs) have gained much popularity due to their higher accuracy and smaller stencil sizes compared to FDMs. In addition to the accuracy and size of the stencil, it is also important to consider the resolution characteristics. The performance of any finite difference scheme used for derivative approximation depends mainly on two factors: one is the accuracy of the scheme so as to obtain the closest approximation to the exact value, and the other is the resolution characteristics of the scheme.

In this work, non-standard symmetric compact finite difference schemes are constructed for the numerical approximation to first- and second-order derivatives. The proposed compact schemes have an eighth order of accuracy and are tri-diagonal in nature. The proposed schemes make use of a stencil smaller than those of conventional tri-diagonal compact finite difference schemes of the same order. They also possess high resolution properties and more resolving efficiency than conventional schemes. Some numerical experiments have been carried out, showing the good performance of the proposed schemes. Furthermore, the proposed schemes can be applied to discretize a given PD, which can be solved with great efficiency with the proposed approach. Some details about the numerical experimentation of our proposed compact schemes in combination with a time marching technique in order to obtain approximate solutions of a well-known PDE, namely the Burgers equation, are presented.

A New Symmetry in Valuation Theory

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Valuation theory studies valued fields, that is, fields equipped with a map onto an ordered abelian group, satisfying certain additional properties (such as the ultrametric triangular law); this is called valuation. It constitutes an important area of investigation in algebra with many applications. Perhaps the most relevant are in algebraic geometry (resolution of singularities, local uniformization) and number theory (p-adic number systems). In 1957, M. Krasner introduced hyperfields: field-like structures with a multivalued addition. We will present the possibility of generalising the notion of valuation to hyperfields—first as a map onto an ordered abelian group, satisfying some natural properties inspired by analogy with the classical case, then as a homomorphism of hyperfields targeting a particular type of hyperfield. We will finally discuss the equivalence of the two definitions, an equivalence that suggests previously hidden symmetries in valuation theory. This investigation is based on research made by the author during his PhD studies.

On the Transformation Properties of a Sequence of Equations

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The question of obtaining analogues of the Painlevé equations, having properties that mirror those of the Painlevé equations themselves, is a topic that has been of interest for some considerable time now. Such analogues may be higher-order equations, or matrix equations, for example. Of particular use here is the well-known connection between Painlevé equations, and more generally ordinary differential equations with the Painlevé property, and completely integrable systems, with the former often appearing as symmetry reductions of the latter. Properties expected of analogues of the Painlevé equations may include Lax pairs, special integrals and auto-Bäcklund transformations, i.e., mappings between solutions of the same equation. Here we consider the derivation of auto-Bäcklund transformations for a sequence of such analogues of increasing order, that is, a so-called Painlevé hierarchy. Of fundamental importance in obtaining these results are the properties of a related hierarchy of completely integrable equations. Further related equations and other properties are also discussed.

SND@LHC: A New Experiment on Neutrino Physics at the LHC

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SND@LHC is a compact and stand-alone experiment to perform measurements with neutrinos produced at the LHC in a hitherto unexplored pseudo-rapidity region of 7.2 < n < 8.6, complementary to all the other experiments at the LHC. The experiment is located 480 m downstream of IP1 in the unused TI18 tunnel. The detector is composed of a hybrid system based on an 800 kg target mass of tungsten plates, interleaved with emulsion and electronic trackers, followed downstream by a calorimeter and a muon system. The configuration allows efficiently distinguishing between all three neutrino flavours, opening a unique opportunity to probe physics of heavy flavour production at the LHC in the region that is not accessible to ATLAS, CMS and LHCb. This region is of particular interest also for future circular colliders and for predictions of very high-energy atmospheric neutrinos. The detector concept is also well suited to searching for Feebly Interacting Particles via signatures of scattering in the detector target. The first phase aims at operating the detector throughout LHC Run 3 to collect a total of 290 fb$^{−1}$. The experiment was recently installed in the TI18 tunnel at CERN and has seen its first data. A new era of collider neutrino physics has started.

Heterogeneous Crystallization of Flexible Chains of Tangent Hard Spheres Under Confinement

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Results on heterogeneous crystallization of athermal polymers under confinement in one or three dimensions [1,2] are obtained through extensive Monte Carlo simulations employing the simulator-descriptor suite Simu-D [3]. Polymers are modelled as freely jointed chains of tangent hard spheres of uniform size. Confinement is presented as flat, parallel, and impenetrable walls. Heterogeneous crystallization is studied, for a wide range of systems with varied average chain lengths and packing densities, as the summation of two contributions: one in the bulk volume of the system (bulk crystallization), and one on the confining wall surfaces (surface crystallization). Crystal nucleation and growth are analyzed and gauged through the Characteristic Crystallographic Element (norm) descriptor [4,5]. Once a critical volume fraction is met, initially disordered, amorphous hard-sphere chain packings transit to a stable ordered, crystal phase, growing from the confining wall surfaces to the inner volume of the systems. Depending on the simulation conditions, different morphologies are established in the bulk zone ranging from random hexagonal close-packed layers with a unique stacking direction, perpendicular to the walls (confinement in one dimension), to predominantly hexagonal close-packed (confinement in all dimensions) crystals. Alternatively, surface crystals show perfection with a predominantly triangular character. Results are compared with the bulk, homogeneous crystallization to identify the similarities and differences.

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An Analytic Formula to Calculate the Reheating Temperature via Gravitational Particle Production in Quintessential Inflation

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In this talk, I present an analytic formula for smooth non-oscillating backgrounds that calculates the energy density of massive and massless particles created via gravitational particle production at the end of inflation, thus giving the corresponding reheating temperature at the end of the kination phase. It can be applied to models of quintessential inflation such as alpha-attractors, and shows that for masses larger than the Hubble rate at the end of inflation, namely H_{END}, the reheating temperature is exponentially suppressed. On the contrary, for masses of the order of H_{END}, one obtains a maximum reheating temperature in the order of 10^7 GeV. Finally, to overcome the constraints caused by the overproduction of gravitational waves in quintessential inflation and the gravitino problem, I have shown that the viable masses which ensure the Big Bang nucleosynthesis success are in a range between 2×10^{10} GeV and $ 4\times 10^{13}$ GeV, leading to a maximum reheating temperature in the order 10^5-10^7 GeV.

Effect of Electrode Spacing on the Performance of a Membraneless Microbial Fuel Cell with Magnetite as an Additive

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A microbial fuel cell (MFC) is a bioelectrochemical system that can be employed for the generation of electrical energy under microbial activity during wastewater treatment practices. Optimization of the electrode spacing is perhaps the key to enhancing the performance of an MFC. In this study, electrode spacing was evaluated to determine its effect on the performance of MFCs. The experimental work was conducted utilizing batch digesters with electrode spacings of 2.0 cm, 4.0 cm, 6.0 cm, and 8.0 cm. The results demonstrated that the performance of the MFC improved when the electrode spacing increased from 2.0 to 6.0 cm. However, the efficiency decreased after 6.0 cm. The digester with an electrode spacing of 6.0 cm enhanced the efficiency of an MFC, which led to smaller internal resistance and a biogas production rate of 662.4 mL/g VS_{fed}. The electrochemical efficiency analysis demonstrated higher coulombic efficiency (68.7%) and electrical conductivity (177.9 µS/cm) for the 6.0 cm, which is evidence for the enrichment of electrochemically active microorganisms. With regards to toxic contaminant removal, the same digester also performed well, revealing removals of over 83% for chemical oxygen demand (COD), total solids (TS), total suspended solids (TSS), and volatile solids (VS). Therefore, these results indicated that electrode spacing is a factor affecting the performance of an MFC, with the electrode spacing of 6.0 cm revealing the greatest potential to maximize the biogas generation and the degradability of the wastewater biochemical matter.

About Lie Symmetry Analysis of Fractional Differential Equations

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The purpose of the fractional calculus is to investigate the fractional order integral and derivative operators over real and complex domains as well as their applications. The fractional calculus has a long history of 328 years. During the last few decades fractional calculus is an emerging field with several important applications in more than 135 fields of science and engineering. Several fractional operators and their applications were deeply investigated, particularly during the last years. Indeed, fractional calculus produced interesting results within the well-established field of Lie symmetries and applications. In my talk I will present finding the exact solutions of a given fractional partial differential equation. Besides, the generalization of Lie symmetries for fractional differential equations will be analyzed. In addition, the nonclassical Lie symmetries will be presented for fractional differential equations. The invariant subspace method will be considered to report some exact solutions of several fractional differential equations. Several illustrative examples will be reported.

Vacuum Polarization Energies of Solitons

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The vacuum polarization energy (VPE) is the leading quantum correction to the classical energy of solitons that are solutions outside the perturbative sector of a non-linear field theory.
Before addressing two topics that are particularly relevant for symmetry aspects I will briefly describe how the VPE is unambiguously computed using spectral methods for the quantum fluctuations about the soliton by renormalizing the ultra-violet divergences with counterterms from the perturbative sector.
As a first symmetry topic I will reflect on the analytic structure of scattering data. These data are obtained for the interaction of the quantum fluctuations with the soliton and feature prominently within spectral methods. I will explain how using this analytic structure considerably simplifies the computation. This is particularly the case when there are multiple fields with different masses: It will make possible to obtain the VPE as a single integral over a differentiable function of complex momenta rather than separately summing the contributions from the various energy intervals between the mass gaps.
Second, the soliton is often constructed from a Bogomolny-Prasad-Sommerfield (BPS) identity. In such a scenario the classical energy only depends on the boundary value(s) of the fields and may possess an invariance with respect to deformations of the soliton profiles. Then the VPE will be decisive on the proper soliton solution with the lowest total energy; one may rephrase that as a symmetry being broken on the quantum level. I will exemplify this for a couple of soliton models. For some models it even turns out that the VPE destabilizes classically stable solutions.

A Geometric Approach to Sundman Transformation and Its Applications in Integrability

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We will start by recalling the geometric approach to Sundman infinitesimal time-reparametrisation for autonomus systems of first-order differential equations and some of its applications are used to illustrate the general theory. Then we analyse how to define Sundman transformations for autonomous systems of second-order differential equations and the necessity of considering alternative tangent bundle structures will be shown. Special emphasis is put on geodesic motions and systems described by mechanical type Lagrangians. The Jacobi-Maupertuis metric appears as a particular case of a Sundman transformation. As an application to integrability the linearisability of scalar second-order differential equations under generalised Sundman transformations is developed.

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Adomian Decomposition Method for Solving Fourth-Order Parabolic Equation Using Maple18

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The Adomian Decomposition Method (ADM) is a powerful numerical technique for solving complex differential equations. In this paper, we present an application of the ADM for solving fourth-order parabolic equations. Specifically, we use Maple18 software to implement the ADM and obtain numerical solutions for the fourth-order parabolic equation. We first introduce the fourth-order parabolic equation and its properties. We then describe the ADM and its implementation using Maple18. Finally, we present our results and conclusions. Our problem statement is to solve the fourth-order parabolic equation using the ADM. This equation is a complex partial differential equation that describes the evolution of a physical system over time. The equation involves fourth-order spatial derivatives and second-order time derivatives, making it difficult to solve using traditional numerical methods. Our strategy is to use the Maple18 program to implement the ADM. A powerful numerical method known as the ADM breaks down a given differential equation into a set of easier equations that can be resolved analytically. The procedure entails building a series solution based on a recursive formula and using that solution to incrementally increase the accuracy of the numerical solution. Our findings show how the ADM can successfully solve the fourth-order parabolic problem. For a variety of parameter values, we are able to produce precise numerical solutions, and our findings are generally consistent with previously published findings. We also show how the ADM outperforms other numerical techniques in terms of computing efficiency.

Polychromatic T-Matrix: Group-Theoretical Perspective and Applications

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One of the deepest connections between mathematics and physics lies in the theory of representation of groups. As was discovered by Wigner, physical fields can be classified according to their transformation properties under isometries of space-time: rotations, translations, and Lorentz boosts, which together constitute the Poincare group. The classical free electromagnetic field falls into the zero mass and helicity $\lambda = \pm 1$ class: it can be decomposed as a sum of parts that transform according to such massless unitary irreducible representations of the Poincare group. The coefficients of this decomposition, which are complex scalar functions, belong to a Hilbert space with a certain scalar product dictated by the representation theory.

Light–matter interactions can be described by means of the scattering operator, or equivalently the transition operator (T-matrix), which maps such Hilbert space onto itself. Recent advances allow one to numerically compute the T-matrices of objects such as molecules, nanoparticles, metasurfaces, and 3D-printed materials. Computations based on the T-matrix allow the efficient and accurate prediction of the electromagnetic response of complicated practical systems, such as nano-structured coatings for suppressing light reflection in solar cells, or optical cavities for the enhanced sensing of molecules.

Many theoretical aspects behind the T-matrix method, however, have been limited to monochromatic scattering. In my talk, I will show how representation theory can be applied to the T-matrix formalism in order to guide its rigorous extension to the polychromatic domain. I will demonstrate how this allows one to formulate and answer questions such as the following: given a time-dependent light pulse, how much momentum, angular momentum and energy are transferred to an object hit by that pulse? Knowing the light-matter interaction properties of an object at rest, what are its optical properties when it moves with relativistic speed?

Predicting Relapse in Leukemia Using Topological Data Analysis and Machine Learning

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Despite high survival rates for children and adolescents with acute lymphoblastic leukemia (ALL), about 15–20% of patients experience a relapse. At diagnosis, the risk of relapse is estimated using biological factors, such as flow cytometry data. Typically, these data are manually assessed by projecting them onto a subset of biomarkers, and qualitative assessment is performed using cell density and empty spaces in 2D projections of the data. In this study, the authors use topological data analysis (TDA) to quantify shapes, including empty spaces, in pre-treatment ALL datasets with known patient outcomes. By combining fully unsupervised TDA analyses with machine learning, the authors identify significant shape characteristics that accurately predict the risk of relapse, particularly for patients previously classified as "low risk." The predictive power of CD10, CD20, CD38, and CD45 as biomarkers for ALL diagnosis is also confirmed independently. Based on their analyses, the authors propose three prognostic pipelines for analyzing flow cytometry data from ALL patients, depending on technical and technological availability. These analyses can also be extended to other types of hematological malignancies.

Integrability and Asymptotic Behaviour of a Matrix Lattice Equation

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In this talk, we consider a matrix lattice equation, both in its autonomous and nonautonomous versions, and show integrability in both cases. These lattice equations were derived by a process of elimination in the auto-Bäcklund transformations of a matrix second Painlevé equation, which arises as a symmetry reduction of a matrix modified Korteweg-de Vries equation. Moreover, we explore the construction of Miura maps that relate two lattices, through intermediate integrable lattice equations, to matrix analogues of autonomous and nonautonomous Volterra equations but in two matrix-dependent variables that, in general, are subject to consistency conditions. For these last Volterra-type systems, we consider certain special classes of matrices and derive coupled systems of integrable equations. We also consider asymptotic reductions to matrix partial differential equations. In addition, in the nonautonomous case, we construct a new nonisospectral matrix Volterra system together with its corresponding Lax pair. It is also interesting that in the nonautonomous case, the relationship between certain lattices even in the scalar case seems to be new.

The Odd Weibull-Inverse Gompertz Distribution: Properties and Applications

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This study aims to introduce a new lifetime distribution called the Odd Weibull-inverse Gompertz distribution (OWIG). The OWIG is derived by combining the inverse Gompertz distribution with the odd Weibull family of distributions. Some statistical properties are discussed, including reliability functions, moments, skewness, kurtosis, and order statistics. The proposed OWIG is particularly significant as its density takes various forms. In addition, the OWIG exhibits various asymmetrical shapes for the hazard rate function. This enables the OWIG to model different hazard behaviors that are more commonly observed in natural phenomena. The maximum likelihood approach is used to estimate the parameters of the proposed OWIG. The OWIG's flexibility and efficiency in predicting unique symmetric and asymmetric patterns are shown by analyzing real-world applications in various industries. The results demonstrate that the proposed OWIG is an excellent candidate as it provides the most accurate fits to the data compared to other competing distributions.

Arithmetic Functions Associated With Hypergroups

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The theory of hypercompositional structures (or hyperstructure theory) originated in 1934 when F. Marty introduced the notion of a hypergroup as a generalization of a group. Hypercompositional algebra is centered on the idea that many group properties remain valid if we permit that a result of an operation becomes a set. Moreover, while factorizing a group by a normal subgroup results again in a group, factorization of a group by an arbitrary subgroup results in a hypergroup. The power of this theory is in the use of multi-valued operations, called also hyperoperations. They are laws of synthesis (composition) of the elements of the underlying set with the result being a subset rather than a singleton as in classical algebraic structures. One of the main topics in the theory of hypergroups that has attracted the attention of numerous researchers is represented by the study of different functions, with a strong combinatorial meaning, associated with hypergroups. To be more specific, in this presentation, we will focus on the following functions: fuzzy grade, commutativity degree, Euler's totient function and degree of influence. After a short description of these functions, the most important results will be recalled and illustrated by different examples of several classes of hypergroups.

A Complete p-Poisson Description of MONDian Gravity

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In order to describe many astrophysical observations without using a hypothetical dark matter component, MOdified Newtonian Dynamics (MOND) gravity has been used over the years. At the non-relativistic limit, the behaviour has been characterised by using an AQUAdratic Lagrangian (AQUAL), which is equivalent to the basic MOND prescription only in systems with sufficient symmetry, e.g., spherical or cylindrical symmetric systems. I will describe how in many aspects this description corresponds to the well-known mathematical generalisations of the Laplacian operator and the Poisson equations, namely the p-Laplacian operator and the p-Poisson equation. Looking at the symmetries of this prescription, I present a more general or complete p-Laplacian operator and its corresponding p-Poisson equation to describe gravitational phenomena. As a consequence, I show exact solutions for a point mass particle and for a spherical symmetric distribution of matter. I also show when and how an external field effect is produced and that this formulation does not present an external field effect in the case of wide open binary stars.

Covariant Compactification: A Radical Revision of Kaluza-Klein Unification

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We present a geometric field theory in which the action and field equation are constructed from an ultra-high-density vector field and its covariant derivative. **These have full general covariance in a higher-dimensional spacetime**. If the covariant derivative is diagnosable across a neighbourhood under real changes of coordinate basis, spacetime coincides with a product manifold.
This theory constitutes a significant revision of the Kaluza–Klein framework, with the following features:

- **Unlike most post-1960 Kaluza–Klein theories, the additional dimensions are real, physical space dimensions.** However, unitary gauge transformations do not act directly on them; rather, these transformations act directly on spinor fields, inducing transformation of the tensor representations contained in the outer product of a spinor and its conjugate.
- The dimensionalities of the factor spaces are determined by the eigenvalues of the covariant derivative and hence by its algebraic invariants. Tensors decompose into multiplets, which have both Lorentz and internal symmetry indices.
- The field equation is the simplest generalisation of the Poisson equation for gravity consistent with general covariance and the equivalence principle. It is an eigenvalue equation, where the operator is a second-order differential tensor carrying information about the system's geometry. It can be written in a form with the Ricci tensor and metric acting as operators on the vector field.
- This equation has a 'classical vacuum' solution which is a product of Minkowski spacetime and an Einstein manifold (such as a two-sphere in the six-dimensional case).
- Away from this classical vacuum, connection components in appropriate coordinates include SO(N) gauge fields. The Riemann tensor includes their field strength and the unitary gauge fields can be found amongst them.
- **Symmetry restoration does not take place at high energies; it occurs at the zero-curvature 'decompactification limit', in which all dimensions appear on the same footing**.

Understanding the H0 Tension Problem With Machine Learning

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The physics behind the H0 tension problem are intriguing and still need to be understood. To alleviate or solve this problem, different scenarios have been discussed and developed in the recent literature. Some notable results have been obtained using Machine Learning approaches. Moreover, some serious issues with the standard cosmological model have been identified. Among them, the deviation from the cold dark matter paradigm on cosmological scales is the most interesting one.

Bayesian Machine Learning is a simulation-based learning approach allowing us to overcome various data-related issues, among others. It allowed us to study the H0 tension problem using swampland criteria and cosmic opacity showing how they can change our understanding of the problem, among others.

Here, we will discuss some of our recent results in this direction and indicate various directions that need to be explored for a better understanding of the physics behind the H0 tension problem.

Symmetry and Asymmetry in Predicting the Impact of Single Mutations on Protein Stability

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Predicting the impact of single mutations on protein stability is of great importance for protein design, the prognosis of mutation pathogenicity, and testing our understanding of protein folding principles. For successful predictions, one has to consider several symmetry/asymmetry-related issues. Methods manipulating protein structures usually overestimate the effect of mutations due to their inability to find the optimal conformation of the mutant structure. For machine learning approaches, the quality of existing data is crucial: the majority of the existing experimental data describe truncating mutations, most of which are mutations to alanine. Another difficulty is that most of the mutations refer to the natural proteins and are generally destabilizing. Therefore, the training dataset is inevitably biased toward destabilizing mutations. As a result, one has to symmetrize the dataset before training; otherwise, a method tends to predict mutations as destabilizing even on a balanced dataset.

Recently, an experimental dataset was published, which contains estimates of the impact on protein stability for ~400,000 single mutations. This dataset is much less biased than the experimental data measured before. After symmetrizing the dataset, we trained a deep neural network method, ABYSSAL, which has a symmetrical architecture to avoid bias toward destabilizing mutations. ABYSSAL shows good performance on the new data. However, for the conventional data, our method shows significantly lower performance comparable to the best state-of-the-art methods. ABYSSAL is the first symmetrical method to be trained on the new mutation dataset.

Evolution of Structural Systems Through Dynamic Seismic-Resistant Behaviour. A Prospective for the Year 2100

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The ingenuity of human beings has been constantly evolving throughout history, especially in the field of construction. The constant improvement of the techniques and construction systems has allowed the construction works of the past to remain as tangible evidence over several millennia, with orthogonality and symmetry being one of the most important resources for architectural and structural designs of the past and contemporary times. However, with technological advances and new materials, trends in the probable future warn that the new architectural proposals will be completely asymmetrical and curved. Therefore, this study analyses and determines the correlation between the factor of orthogonality and symmetry, as well as the incidence of the construction technique, materials and location of 65 case studies that are most representative of each culture and historical period. With the analysis of the dynamic behaviour of the buildings during an earthquake, the different vibration periods and the variation of the fundamental period, it is possible to determine that in more than 80% of the cases, the massive construction works developed in the ancient and middle ages, as well as their symmetrical composition, allow for greater stability and seismic resistance. Nevertheless, they take up a lot of space and their elaboration is more time-consuming , while in the modern and contemporary age, with the industrialisation of steel and concrete, the structural elements are reduced, taking advantage of the functional spaces, thus improving the seismic behaviour.However, the best performing architectural element continues to be orthogonal and symmetrical. Finally, analyses of curved and asymmetrical architectural projections of the future predict that new materials will be required for the construction and optimal structural performance of buildings in the event of a relevant seismic event. For this reason, it is of vital importance to propose a line of research on new materials and construction systems.

Abstracts

Poster Exhibition

1. Methodology for the Development of Structural and Functional Security Models for Elements of Distributed Information Systems

Vladimir Baranov[1], Alexander Shelupanov[2]

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The report presents the results of a study on ways to solve the problem of building security models for elements of distributed information systems (DIS). During the study, the existing modeling approaches in this area were analyzed. A reasonable conclusion was made that the method of constructing ontological structural–functional models of DIS elements will be the most informative and flexible.

The following methodology is proposed. Three types of information modules are distinguished as part of DIS: local information and computer networks (LICN), data processing centers (DPC) and remote users. Each of these typical information modules (TIM) consists of a finite number of types of elements: routers, switches, workstations, servers and the line between them. All types of these elements were decomposed as concepts of the levels of the OSI/ISO model. These concepts are interfaces, protocols, services, drivers, and other entities. In this case, the structural–functional links between them will be ontological structural–functional links of the functioning model of the element under consideration. These elementary ontological structural–functional schemes are typical for their species and will serve as material for modeling TIM. It is only necessary to lay ontological links between them of a higher level, reflecting the structure of TIM DIS.

The vulnerabilities of the ontological model concepts discussed above, identified from international databases, make it possible to visually determine their location in the structure and role in the process of functioning of the TIM DIS element.

The developed technique makes it possible to form ontological structural–functional models of TIM DIS of varying complexity, to determine the set of vulnerabilities of their concepts and the required protection measures. The paper describes a software product that allows the automation of this process.

2. Methodology for Determining Scenarios for the Implementation of Threats to Information Security

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This report discusses ways to solve the important problem of identifying scenarios for the implementation of threats to information security (IST). In the course of the study, distributed information systems (DIS) were decomposed into three levels of detail: the first is the system level, the second is the level of DIS elements—typical information modules (TIM)—and the third is the level of TIM elements. At each level, typical entry points of IST, transit elements and objects of destructive impact are identified, systematized and classified. Conditions are defined when elements at different levels become penetration points, transit points, or attack targets. A system of rules for their categorization according to the degree of criticality for the functional and structural stability of the DIS as a whole, its elements and individual technological processes, as well as for the confidentiality, integrity and availability of protected information, has been developed.

A technique has been developed that consists of algorithms for the implementation of IST, a mathematical apparatus for determining the preference for their propagation paths and the choice of objects of influence and technological safety maps for DIS at different levels, taking into account the degree of criticality of elements and processes as objects of destructive impact. A description of a software product has been made that makes it possible to automate the calculations of probable scenarios for the implementation of the IST.

It is concluded that the developed methodology is another contribution to the theory and methodology of information security, and its software implementation will find practical application as an element of an information system for decision support in the field of information security management.

3. A Spherically Symmetric Model of a Micropolar Real Gas Flow

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In this work, we present a spherically symmetric 3D flow of a micropolar, viscous, polytropic, and heat-conducting real gas. Namely, we take the subset of R3 bounded by two concentric spheres that present solid thermoinsulated walls as the domain. We also consider the generalized equation of state for the pressure in the sense that the pressure depends on the mass density as a power function. The model is based on the conservation laws for the mass, momentum, momentum moment and energy, as well as the equation of state for a real gas, and is derived first in the Eulerian and then in the Lagrangian description. The use of the symmetry assumption simplifies the mathematical description of the flow and allows a more detailed analysis of the effects of various parameters on the behavior of the gas. By applying the Faedo–Galerkin method, a numerical solution to a corresponding problem is obtained and numerical simulations are performed to demonstrate the behavior of the solutions under various parameters and initial conditions and to validate the method. The results of the simulations are discussed in detail and compared with already-known models. The obtained results have important implications for the understanding of micropolar fluid dynamics and the design of practical systems such as gas turbines and rocket engines that are based on spherically symmetric assumptions.

4. Numerical Simulations for Viscous and Heat-Conducting Micropolar Gas Flow with Cylindrical Symmetry

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This work describes the model for micropolar gas and focuses on the initial boundary value problem describing the behavior of the micropolar viscous and thermally conductive gas in cylinders with solid and thermally insulated walls. The set of variables used in this model includes the mass density, velocity, microrotation velocity, and temperature. It is assumed that the boundary conditions for velocity, microrotation velocity, and heat flux are homogeneous. Since the domain of this system is cylindrical in nature, we assume that the solution should be cylindrically symmetric, and in the Lagrangian description, we obtain a parabolic system that has a globally unique generalized solution. For the described initial boundary value problem, we construct the Faedo–Galerkin approximations and the corresponding numerical method to obtain a numerical solution. The given numerical method was additionally analyzed in terms of the complexity of the initial conditions based on the number of terms in their respective Fourier expansions.

5. Cartan F(R) Gravity and Cosmological Accelerated Expansion

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We investigate the cosmological accelerated expansion in Cartan F(R) gravity. F(R) modified gravity is the theory replacing Ricci scalar in the Einstein–Hilbert action of general relativity to a general function, F(R). Cartan F(R) gravity is reformulated on Cartan–Riemann geometry described by vierbein and spin connection. Torsion is represented by the derivative of F(R) and vierbein in Cartan F(R) gravity. It does not always vanish in Cartan formalism. The equivalent scalar–tensor theory is derived by extracting the torsion from the Ricci scalar without the conformal transformation. Cartan F(R) gravity is free from the equivalence problem between Jordan and Einstein frames for the scalar–tensor theory derived through conformal transformation in F (R) gravity. We employ the Cartan F(R) gravity to explain the accelerated expansion of the universe. The potential of the scalar field in Cartan F(R) gravity has various types by F(R) correction. The logarithmic model has the potential with a flat part to apply the slow-roll inflation scenario. Additionally, the potential has a gently sloping part with enough small value to explain the dark energy when the coupling parameter is small. The simple logarithmic model in Cartan F(R) gravity is expected to provide a unified explanation for the accelerated expansion of the universe at different energy scales, such as inflation and dark energy.

6. Local and Global Order in Dense Packings of Semi-flexible Athermal Polymers

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We study local and global order at increasing volume fractions in dense packings of linear, semi-flexible chains of tangent hard spheres [1] through extensive Monte Carlo simulations with the suite Simu-D [2]. Chain stiffness is controlled by a tunable harmonic potential for the bending angle. The studied equilibrium angles range from acute to obtuse ones, reaching the limit of rod-like polymers. We analyze the effect of the packing density and chain stiffness on polymer self-organization at the local and global levels. The local order, which corresponds to crystallinity, is gauged by the Characteristic Crystallographic Element (CCE) norm descriptor [3], while the global order (distinct mesophases) is computed through the scalar orientational order parameter [4]. In all cases, we identify the critical volume fraction for the phase transition and gauge the established crystal morphologies as a function of the packing density and equilibrium bending angle, ranging from random hexagonal closed-packed (RHCP) morphologies of mixed character to almost perfect face-centered cubic (FCC) and hexagonal close-packed (HCP) crystal structures. In the case of rod-like polymers and right-angle polymers, the establishment of the long-range nematic order is observed as a function of the packing density. A comparison is also provided against the analogous packings of monomeric and fully flexible chains of hard spheres.

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7. Quasidegeneracy of $(H_2C=B=CH_2)^-$ and $(H_3B–C≡CH)^-$ Systems Induced by an Excess Electron Attachment

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On the basis of ab initio calculations using the MP2, CCSD(T), and OVGF methods with the aug-cc-pVDZ and aug-cc-pVTZ basis sets, we obtained seven neutral and seven anionic isomers matching the BC_2H_4 formula. The $(H_2C=B=CH_2)^-$ isomer belongs to the family of borata-alkene synthons, which can be applied, for example, in retrosynthesis or as a nucleophilic agent. The two most stable anionic isomers, namely D_{2d}-symmetry $(H_2CBCH_2)^-$ and C_{3v}-symmetry $(H_3B\text{-}CCH)^-$, were found to be isoenergetic, having electronic energies within 1 kcal/mol. On the other hand, the $H_3B\text{-}C≡CH$ system was identified as the least stable isomer among the neutrals. Its different ability to bind an excess electron by the BC_2H_4 neutral isomeric structures turned out to cause significant changes in the relative energies of the corresponding anions. Electronic stabilities of the $(BC_2H_4)^-$ anions were predicted by evaluating the vertical electron detachment energy (VDE) values. All of the anionic systems were found to be stable against the detachment of an excess electron as their VDEs span the 1.71–4.32 eV range. It was also found that the actual VDE value characterizing each anion strongly depends on the bonding pattern exhibited by the boron atom involved in the structure.

8. Au/TiO_2 Nanosheets for Photocatalytic Degradation of Methylene Blue Under Simulated Visible Light

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Au/TiO_2 nanosheets (anatase) with facets [001] were synthesized by a hydrothermal method, exhibiting very reactive properties and favoring an increase in the number of superoxide and hydroxyl radicals. The high reactivity of the [001] facets can be attributed to the trapping of the photoelectrons, inhibiting electron–hole recombination. The enhanced efficiency of nanosheets was realized by doping with gold nanoparticles. The results suggested that gold nanoparticles with a size of 2–5 nm were dispersed on the surface of TiO_2 nanosheets. The structure and morphology of the Au/TiO_2 nanosheets were characterized by scanning electron microscopy (FE-SEM), high-resolution transmission electron microscopy (HR-TEM), X-ray photoelectron spectroscopy (XPS) and X-ray diffraction (XRD). The crystallite nanosheet size was in the range of 15–20 nm. The photocatalytic activity was evaluated by the degradation of methylene blue under simulated visible light at 25^0C. The performance of the Au/TiO_2 nanosheet photocatalyst was tested in three cycles. It was observed that after irradiation for 120 min, more than 98% of the methylene blue was decomposed.

9. Studies on Tetrahydroacridines to Investigate Possible Application in Alzheimer's Disease Treatment

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In recent decades, p-conjugated organic compounds have aroused great interest, finding multiple uses in areas such as organic electronics, ion sensing, and solar cell development. With this background, acridines represent a class of heteroatomic p-conjugated compounds that have found applications in fields such as medicinal chemistry, dye industries and metal chemo sensing, in organic electronics, due to their strong electron-donating ability and remarkable optoelectronic properties, but also in the field of organic light-emitting diodes, due to their aza-analogues of anthracene for OLED applications. On the other hand, tetrahydroacridines have received increased attention in medicinal chemistry due to their ability to inhibit topoisomerase enzymes and block DNA transcription. In particular, they have been widely explored for the treatment of Alzheimer's disease, human cancer, and tuberculosis. Even so, there is a lack of knowledge concerning their optoelectronic properties [1]. Recently, considerable attention has been given to acridines in our laboratory, and we have developed new tetrahydroacridines. More recently, we reported the synthesis of novel benzidin-bis-tetrahydroacridine analogues [2]. In continuation of our previous work and as part of our interest in new organic materials, we herein report the synthesis of three unknown bis tetrahydroacridines derivatives: two new 7,7'-(ethane-1,2-diyl)-bis-polymethylenquinoline-bis-carboxamides (***3a-b***) and one 7,7'-(ethane-1,2-diyl)-bis-polymethylenquinoline-bis-carboxylic acids (***4a***) were synthesised by Pfitzinger condensation of 5,5'-(ethane-1,2-diyl) diindoline-2,3-dione (2) with several cyclanones, and their optical and electrochemical properties were investigation by use of UV–VIS and emission spectroscopy, CV measurements and DFT calculations.

10. In Silico Approaches for Rational Design of New Electrochemical Sensors Based on Azulene-Phenyloxazolone

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The in silico study of three azulene-phenyloxazolone derivatives, differently substituted, was conducted in order to reveal key parameters for the assessment of their electrochemical behaviour. Previous DFT calculations using hybrid algorithms on azulenes substituted with thiophen– or furan–vinyl–pyridine azulen-1-ylmethylene-2-thioxothiazolidin-4-one derivatives showed reliable and accurate correlations between oxidation and reduction potentials experimentally measured and calculated using frontier molecular orbital energies. In this work, the variation of computed properties related to the electronic density and charge distribution, obtained using the DFT/B3LYP functional method, is discussed in terms of azulene substitution. The redox potential previously obtained by electrochemical experiments was correlated with energy levels of computationally determined frontier molecular orbitals. Additionally, correlations of electrochemical properties with global and local quantum reactivity parameters are given. The observed findings are useful to predict heavy metal ion recognition from waste industrial waters and proved to be an optimistic strategy to design and evaluate potential ligand candidates for heavy metal ion complexation.

11. Lie Theory: Applications to Mathematical Model Describing HIV-Immune System

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The Lie symmetry method has been successfully used for approximately 100 years and is still used today in a variety of physics problems. However, its use in epidemiology has been uncommon, possibly because the ordinary differential equations studied in this field are typically of first order as opposed to those studied in physics, which are typically of second order. In this study, Lie group analysis is applied to a model which describes an HIV-immune system model. The model is a nonlinear system of three first-order ordinary differential equations. For a particular relationship among the involved parameters, the system employs a three-dimensional solvable Lie symmetry algebra and its general solution is therefore determined. The primary goal of this study is to apply Lie symmetry techniques to the model and provide approximate solutions for the three-dimensional system of first-order ordinary differential equations that characterizes the HIV-immune system. Furthermore, Prelle–Singer techniques are used to establish the integrability of a nonlinear HIV-immune system.

12. Detection of Brain Gene Expression Images Based on Image Processing Techniques

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The brain is organized into neuronal populations that display respective molecular identities, that is, they are characterized by the expression of specific gene combinations. Therefore, it is important to analyze gene expression in the different brain regions taking into account the full genome, as much as possible, as well as the precise expression level of these genes in each brain location.

In our study, we obtained images corresponding to 334 experiments of situ hybridization from the Brain Allen Institute website (http://mouse.brain-map.org/) that belong to diverse gene families. From each experiment, we selected three representative coronal planes of the medulla oblongata, which were used for the subsequent analysis.

To this end, semantic segmentation of the cerebelum region was performed before image registration of the entire dataset. The segmentation was carried out using a Deeplabv3-ResNet18, constructed by a Deeplabv3 model using a ResNet-18 backbone, defining the contour of the selected study area that corresponded to the aforementioned medulla oblongata.

The registration was performed using the Matlab Image Processing Toolbox with a non-rigid technique for each image with respect to respective control images for each coronal plane. Subsequently, clustering was carried out. The clustering consisted of K-means analysis with R software so that the pixels from each of the three representative planes were clustered into areas according to the quantitative expression level for each of the genes. This step was carried out by trying different numbers of clusters, yielding subdivisions of the brain images into areas that were compared to the known classical anatomical subdivisions.

Therefore, we have designed a procedure to retrieve brain images showing gene expression, and performed their segmentation, registration and clustering, allowing us to define brain areas according to their molecular identity, based on the expression level of multiple genes in each precise location.

13. Effects of Competition and Advertisement on Rooftop PV System Installations Using System Dynamics

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This study predicted the effects of competition and advertisement on photovoltaic (PV) system installations and power generated for residential rooftop buildings. Initially, the model factors were identified, including PV installations, generated power, PV cost reduction, competition, and advertisement. The model was then run through a simulation from the year 2022 until 2030. The results showed that the cumulative PV installations and power generated due to competition (advertisement) will reach 19.23 (109.71) MW and 33.22 (189.58) GWh, respectively. Finally, the cost of the PV system will drop from USD 3370 to USD 896 in the year 2030. In conclusion, manufacturers and suppliers of PV products should work closely with the end-users to develop cost-effective and high-quality PV systems and implement effective advertising methods to improve resident awareness of the advantages of PV system installations. In conclusion, the developed model is a valuable assessment tool that can support manufacturers on how to increase the power generated by rooftop PV systems and thereby contribute to reducing the dependency on traditional energy sources.

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