

1st International Conference on Symmetry

Parc Científic de Barcelona

Barcelona, Spain

16 - 18 October 2017

Conference Chair

Sergei D. Odintsov

Conference Co-Chairs

Cino Pertoldi

Kimball A. Milton

Maurizio Benaglia

Organised by



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1st International Conference on Symmetry

16-18 October 2017, Barcelona

Morning

Monday 16 October 2017	Tuesday 17 October 2017	Wednesday 18 October 2017
Check-in	S2. Physics and Symmetry Session Chairs Kimball A. Milton Iver Brevik	S3. Chemistry and Symmetry Session Chair Maurizio Benaglia
	Coffee Break & Poster Session	
	S2. Physics and Symmetry Session Chairs Kimball A. Milton Emilio Elizalde	S3. Chemistry and Symmetry Session Chair Maurizio Benaglia

Afternoon

Lunch		
Opening Ceremony Conference Chair Sergei D. Odintsov S1. Biology and Symmetry Session Chair Cino Pertoldi	S2. Physics and Symmetry Session Chairs Kimball A. Milton Carl Bender	S4. Mathematics, Computer Science and Symmetry Session Chair Sergei D. Odintsov
Coffee Break & Poster Session		
S1. Biology and Symmetry Session Chair Cino Pertoldi	S2. Physics and Symmetry Session Chairs Kimball A. Milton Klaus Kirsten	S4. Mathematics, Computer Science and Symmetry Session Chair Sergei D. Odintsov
	Conference Dinner	Final Remarks

Monday 16 October 2017: 12:00 - 13:45 Check-in / 13:45 - 18:00

Tuesday 17 October 2017: 08:30 - 12:30 / 14:00 - 18:10 / Conference Dinner: 20:30

Wednesday 18 October 2017: 08:30 - 12:30 / 14:00 - 18:00

Symposium Programme

Monday 16 October

12:00 – 13:45 Check-in

13:45 – 14:00 Opening Ceremony by Sergei D. Odintsov

Session 1 – Biology and Symmetry

Chair: Cino Pertoldi

14:00 – 14:20 **Stefan Van Dongen** “Fluctuating Asymmetry, Developmental Instability and Developmental Stress: Insights from Zebra Finches, Sticklebacks, Rabbits, Humans and Opuntia Cacti”

14:20 – 14:30 **Michael Famiano** “Selection of Amino Acid Chirality via the Stark Effect in Stellar Environments”

14:30 – 14:40 **Dilano Saldin** “Symmetry in Icosahedral Viruses: How it Exploited in the XFEL”

14:40 – 14:50 **Paul Sorba** “Symmetry and Minimum Principle at the Basis of the Genetic Code”

14:50 – 15:00 **Michael Sadovsky** “Palindromic Symmetry in Genomes and Evolution”

15:00 – 15:10 **Vladislav Biriukov** “Symmetry in the Transcriptome and Genome Sequences of Siberian Larch (*Larix sibirica* Ledeb.)”

15:10 – 15:20 **Serafima Novikova** “Symmetry in a Four-Cluster Triangle Structure of the Siberian Stone Pine (*Pinus sibirica* Du Tour) Transcriptome”

15:20 – 15:30	Dominik Schmidt “Assessing Fluctuating Asymmetry of <i>Cucumis sativus</i> Leaves for Virtual Plant Models”
15:30 – 16:00	Posters Flash Presentations (Akpojotor, G.; Balashov, T.; Cirstoiu, C.; Henrici, A.; Lévai, G.; Mahmood, I.)
16:00 – 16:30	Coffee Break & Poster Session
16:30 – 16:40	Jacob Manale “Lie Symmetry Analysis for SIS Model of Epidemiology”
16:40 – 16:50	Malte L. Petersen “Effects of Task Performance Symmetry on Human Collective Decision-Making”
16:50 – 17:00	Omid Ekrami “Fluctuating Asymmetry, Sexual Dimorphism and Attractiveness in Humans: The Development Towards a 3D Approach”
17:00 – 17:20	Karl Grammer “Human Form – An Evolutionary Psychological Approach to Beauty”
17:20 – 17:40	Michal Polak “Fluctuating Asymmetry and Sexual Selection: Integrating Cross- and within-Population Tests of Key Predictions”
17:40 – 18:00	Cino Pertoldi “Behavioural Instability; What Is Next. A Holistic Approach to Behavioural Studies”

Tuesday 17 October

Session 2 – Physics and Symmetry

Session Chair: Kimball A. Milton, Iver Brevik,
Emilio Elizalde, Carl Bender, Klaus Kirsten

08:30 – 08:50	Kimball A. Milton “Dual Symmetry: Magnetic Monopoles in Theory and Experiment”
08:50 – 09:10	Carl M. Bender “Physics in the Complex Domain”
09:10 – 09:30	Serge Reynaud “Quantum Metrology and Relativistic Symmetries”
09:30 – 09:50	Plamen Fizev “Generalization of the Noether Theorem: Global and Local Symmetries, Dynamical Functionals and Boundary Conditions”
09:50 – 10:10	Salvatore Capozziello “Noether's Symmetries in Quantum Cosmology”
10:10 – 10:30	Joan Bagaria “Symmetries in the Set-Theoretic Universe and the Higher Infinite”
10:30 – 11:00	Coffee Break & Poster Session
11:00 – 11:10	Iver Brevik “On the Symmetry of the Electromagnetic Energy-Momentum Tensor in Media”
11:10 – 11:20	Klaus Kirsten “Gluing Formula for Casimir Energies”
11:20 – 11:30	Akio Sugamoto “Generalized Heisenberg-Euler Formula and its Application to Vacuum Magnetic Birefringence Experiment”
11:30 – 11:40	Olindo Corradini “Particle Path Integrals on Maximally Symmetric Spaces and Type-A Trace Anomalies”
11:40 – 11:50	Andronikos Paliathanasis “Algebraic Solutions in Scalar Field Cosmology: Reconstruction of the Dark-Energy Equation of State and the Inflationary Potential”
11:50 – 12:00	Irina Stepanova “Application of Lie Symmetry Analysis to Heat and Mass Transfer Equations”

12:00 – 12:10	Niurka R. Quintero “Dynamical Systems with Spatiotemporal Periodicities through the Symmetries”
12:10 – 12:20	Sadataka Furui “É. Cartan’s Supersymmetry, Noncommutative Geometry and Propagation of Time in the Kaluza-Klein-Like Universe”
12:30 – 14:00	Lunch
14:00 – 14:20	Sergei D. Odintsov “Unifying the Early-Time Inflationary Era with Late-Time Dark Epoch Universe: The Case of Modified Gravity”
14:20 – 14:40	Emilio Elizalde “Zeta functions: symmetry and applications”
14:40 – 15:00	George Zoupanos “From Kaluza–Klein to Non-Commutative Gauge Theories of Gravity”
15:00 – 15:20	Luciano Rezzolla “On Symmetry Restoration in General Relativity”
15:20 – 15:30	Bruno Uchoa “Quantum Simulation of SU(4) Symmetric Spin Lattice Models”
15:30 – 15:40	Herbert Weigel “Weak Isospin Symmetry and the Vacuum Polarization Energy of Cosmic Strings”
15:40 – 16:30	Coffee Break & Poster Session
16:30 – 16:40	Uwe Guenther “PT-Symmetry and Related Geometrical Structures”
16:40 – 16:50	Astashenok Artyom “Modified Gravity and Relativistic Stars”
16:50 – 17:00	Arkadiy Popov “Wormholes Created by Vacuum Fluctuations”

17:00 – 17:10	Manuel Hohmann “Good vs. Bad Tetrads in $f(T)$ Gravity and the Role of Spacetime Symmetries”
17:10 – 17:20	Ekaterina Pozdeeva “Multifield Inflation Scenarios from MSSM”
17:20 – 17:30	Masashi Yamazaki “Relativistic Stars in dRGT Massive Gravity”
17:30 – 17:40	Alexander Balakin “Intrinsic Symmetry of the Dark Fluid Electrodynamics”
17:40 – 17:50	Dmitri Vassiliev “An Analyst's Take on Gauge Theory”
20:30	Conference Dinner

Wednesday 18 October

Session 3 – Chemistry and Symmetry

Session Chair: **Maurizio Benaglia**

- 08:30 – 08:50 **Maurizio Benaglia** “Batch and Flow Asymmetric Catalysis for the Synthesis of Chiral Active Pharmaceutical Compounds”
- 08:50 – 09:10 **Victor Borovkov** “Chirogenesis in Supramolecular Systems on the Basis of Porphyrinoids”
- 09:10 – 09:20 **Marina Balakina** “Chromophores Supramolecular Organization in Polymer Materials with Quadratic Nonlinear-Optical Activity: Symmetry Aspects”
- 09:20 – 09:30 **Nele Konrad** “Spectroscopic Study of (all-R,R)-cyclohexanohemicucurbit[8]uril and its Host-Guest Supramolecular Hexafluorophosphate Complexes”
- 09:30 – 09:50 **Jürg Hulliger** “Symmetry breaking and polarity formation in molecular crystals”
- 09:50 – 10:00 **Míriam Pérez-Trujillo** “Chiral Recognition by Dissolution Dynamic Nuclear Polarization NMR Spectroscopy”
- 10:00 – 10:10 **Bih-Yaw Jin** “Where Chemistry Meets Art: An Exploration of Nano World Through Mathematical Beading”
- 10:10 – 10:30 **Miquel Llunell** “Using the Continuous Shape and Symmetry Measures to correlate Atomic Structure and Chemical Properties”
- 10:30 – 11:00 Coffee Break & Poster Session
- 11:00 – 11:10 **Per Jensen** “The Superrotor Model for the Rovibrational Motion of CH₅⁺, an Extremely Flexible Molecule
- 11:10 – 11:20 **Natalia Laptash** “High Symmetry of Fluoro- and Oxofluoroelpasolites as a Consequence of Dynamic Orientational Disorder”

11:20 – 11:30	Pablo Ramos “Effect of Bond Tangency/Gap on the Crystallization of Athermal Polymer Packings”
11:30 – 12:30	Poster Flash Presentations (Asfar, O.; Bruzon, M.; Kgarose, M.; Petrache, H.; Quintero, N.R.; Shahzad, A.; Stepanov, G.; Sun, X.; Taranenko, E.)
12:30 – 14:00	Lunch
<p style="text-align: center;">Session 4 – Mathematics, Computer Science and Symmetry</p> <p style="text-align: center;">Session Chair: Sergei D. Odintsov</p>	
14:00 – 14:20	Bruno Volzone “Nonlinear Aggregation–Diffusion Equations: Radial Symmetry and Long Time Asymptotics”
14:20 – 14:40	Roman Cherniha “Lie and Conditional Symmetry of Nonlinear Boundary Value Problems: Definitions, Algorithms and Applications”
14:40 – 15:00	Dragan Marušić “Obvious and Hidden Symmetries of Mathematical Objects”
15:00 – 15:10	Ryad Ghanam “Symmetry Analysis of the Geodesic Equations on Lie Groups”
15:10 – 15:20	Maria Luz Gandarias “On Conservation Laws of Generalized KP and Boussinesq Equations in Two Dimensions”
15:20 – 15:30	Andronikos Paliathanasis “A Geometric View on the Symmetries of Differential Equations”
15:30 – 15:40	Chaudry Masood Khalique “Lie Group Analysis of a Coupled (2+1)-Dimensional Hyperbolic System”
15:40 – 15:50	Stephen Anco “Generalization of Noether's Conservation Law Theorem to Non-Variational Differential Equations”
15:50 – 16:30	Coffee Break & Poster Session

16:30 – 16:40	Alice Miller “GraphDraw - a Tool for the Representation of Graphs Using Inherent Symmetry”
16:40 – 16:50	Mao-Ting Chien “Construction of Symmetric Determinantal Representations of Hyperbolic Forms”
16:50 – 17:00	Maria Rosaria Posteraro “On a Class of Weighted Isoperimetric Inequalities”
17:00 – 17:10	Juliane Oliveira “Projections of Periodic Functions and Mode Interactions”
17:10 – 17:20	Remi Leandre “Bismut's Way of the Malliavin Calculus for Large Order Generator on a Lie Group”
17:20 – 17:30	Angel Garrido “Symmetry, Entropy, and Computer Science”
17:30 – 17:40	Vasyl Fedorchuk “On Classification of Symmetry Reductions for Partial Differential Equations”
17:40 – 17:50	Aamir Shahzad Secure SCADA-IoT Platform for Industrial Automation and Control: A Collaborative-Communication Designed Model”
17:50 – 18:00	Closing Remarks & Awards Ceremony

Welcome by Sergei D. Odintsov



Dear authors and attendees,

We are delighted to have you here in Barcelona to participate and share in our First International Conference on Symmetry. Thank you for coming, for reporting the results of your research work, and for joining your peers in building together the future of the field. We are proud and honored that so many of you have joined your peers in Barcelona, and we are pleased that you

have submitted such a large number of excellent contributions. This has allowed us to select the very best for an outstanding three-day conference program on Symmetry which you can all now enjoy.

In effect, Symmetry is a very broad phenomena which unifies all natural sciences in the fundamental sense. It is not surprising then that the journal Symmetry (IF=1,45), which is sponsoring this event, publishes papers from mathematics and physics to computer science and biology.

Symmetry is the ultimate goal of Physics because the final Theory of Everything is expected to be a highly symmetric theory. Symmetry plays a fundamental role in the universe history! And it is you who are creating the foundations for new discoveries related to Symmetry thanks to your research efforts and exciting results, some of which you will be sharing with us during this conference.

On behalf of the organizers of this conference, I want to welcome you warmly to Barcelona, and we would like to wish you three days of outstanding scientific presentations and discussions.

Prepare yourself to be amazed, challenged and inspired-and enjoy your stay in Barcelona!

Sergey Odintsov
Conference Chair



Symmetry (ISSN 2073-8994; CODEN: SYMMAM) is an international, open access journal covering research on symmetry phenomena wherever they occur in mathematical and scientific studies. *Symmetry* is published monthly online by MDPI. Its aim is to encourage scientists to publish their experimental and theoretical research in as much detail as possible. The journal's main subject areas include topics from physics, chemistry, biology, mathematics, computer science, symmetry and other scientific disciplines and engineering.

Among other databases, *Symmetry* by the Science Citation Index Expanded (Web of Science), MathSciNet (AMS), and Scopus.

Journal Webpage: <http://www.mdpi.com/journal/symmetry>

Impact factor: 1.457 (2016); 5-Year Impact Factor: 1.323 (2016)

The **1st International Conference on Symmetry** will be held at the Auditorium Antoni Caparros, Parc Científic de Barcelona (PCB), Barcelona (Spain) on October 16 – 18, 2017.

This exciting three-day event seeks to gather experts in the fundamental phenomenon in nature and science that is symmetry. Our First International Conference on Symmetry aims to promote cutting edge knowledge and ideas of symmetry in a variety of subjects ranging from Physics, Chemistry, Mathematics, Computer Science, to Biology. This is an opportunity to discuss important breakthroughs in the field; broaden your knowledge, meet scientists from other areas and perhaps develop new mutually beneficial collaborations.

Conference Venue

Auditorium Antoni Caparrós, Parc Científic de Barcelona (PCB)
Baldiri Reixac, 4-8, Barcelona, Spain

Registration Desk

The desk for registration, information and distribution of documents will be open from 12:00 on 16 October 2017.

Certificate of Attendance

The participants of the symposium will receive an electronic Certificate of Attendance by email once the event is concluded.

Barcelona and Catalonia

Catalonia has become one of the favourite tourist destinations of Spain, mainly because of Barcelona, a city that never sleeps and knows how to please the big majority. With a history among the oldest in Europe, Barcelona offers a mixture of inland and seaside charms that panders the interests of everybody. The variety of artistic treasures, Romanesque churches and the works of famous artists such as Dalí, Gaudí, Miró or Picasso will make of your visit to the city a remarkable experience.



Parc Güell (Source: www.viajero-turismo.com)

Barcelona is the capital and largest city of Catalonia and Spain's second largest city, with a population of over one and half million people (over five million in the whole province).

This city, bathed by the Mediterranean Sea, has become one of most cosmopolitan cities of

Europe which has transformed it into the very modern, yet incredibly old city. This beautiful city is full of what European cities are known for (outdoor markets, restaurants, shops, museums and churches) and which makes it the perfect scenario to get lost in its picturesque streets and avenues. Moreover, Barcelona's extensive and reliable Metro system will take you to more far-flung destinations. The core centre of the town, focused around the *Ciutat Vella* ("Old City"), provides days of enjoyment for those looking to experience the life of Barcelona while the beaches the city was built upon provide sun and relaxation during the long periods of agreeably warm weather. [Source: www.wikitavel.org]

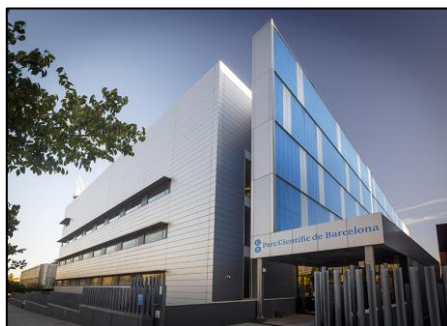


Plaza Espanya (Source: www.viajero-turismo.com)

Parc Científic de Barcelona

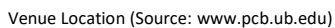
The conference will be held at the Auditorium Antoni Caparrós, in the Parc Científic de Barcelona (PCB). The PCB was created by the University of Barcelona in 1997 and it was the first Science Park in Spain and today it is an international benchmark for the promotion of innovation with more than 2,300 professionals. The Park is currently home to three research institutes and about 100 companies and other organisations.

The aim of the Park is to bring together public and private research environments, facilitating the transfer of knowledge, research and innovation in the public and private sectors via smart space, technology and relations management as well as PCB discourse. [Source: www.pcb.ub.edu]



Parc Científic de Barcelona (Source: <http://www.pcb.ub.edu>)

Address: C/ Baldiri Reixac, 4-8, Barcelona, Spain



Conference Dinner

Tuesday 17th October, 20:30



The conference dinner will be held at Agüelo013, a cutting-edge restaurant specialised in Mediterranean cuisine which, in addition to its emblematic location in the Gothic Quarter of Barcelona and its picturesque dining rooms, will make your evening at the restaurant an experience to remember.

Agüelo013 is located at *Carrer Avinyó 37*, a street at the heart of the Gothic Quarter and only a couple of minutes away from the must-see avenue *Las Ramblas*. The restaurant is easily reached from the Conference Venue either by taxi or by Metro. If you were to choose the second option, the easiest way to get there is by taking the Metro Line L3 at Palau Reial Station and drop off at Drassanes Metro Station after 9 stops.



Contact persons during the event



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Emergency Information

All emergencies in Spain: 112 (no area code needed)

Ambulance (Ambulancia) and health emergencies: 061 or 112

Fire brigade (Cuerpo de bomberos): 080 or 112

Spanish National Police (Policía nacional): 091

Abstracts

Session 1: Biology and Symmetry

Session Chair – Cino Pertoldi

Fluctuating Asymmetry, Developmental Instability and Developmental Stress: Insights from Zebra Finches, Sticklebacks, Rabbits, Humans and Opuntia Cacti

Stefan Van Dongen

Antwerp University, Antwerpen, Belgium

The use of fluctuating asymmetry as a measure of developmental instability and stress experienced during development has become one of the most controversial topics in evolutionary biology and ecology. While this controversy likely has understandably demotivated some researchers to invest more into this area of research, it also has stimulated studies in new areas, using large sample sizes and the development and application of new methods. In this presentation I will present and discuss results from a number of large studies I have been involved in, in a variety of model systems, including human and rabbit fetuses, opuntia cacti, sticklebacks and zebra finches. The focus will be on what we can expect from asymmetry measurements and how these results fit in the overall literature.

Selection of Amino Acid Chirality via the Stark Effect in Stellar Environments

Michael Famiano ¹, Toshitaka Kajino ^{2,3}, Richard Boyd ²

¹ *Western Michigan University, Kalamazoo, MI, USA*

² *National Astronomical Observatory of Japan, Mitaka, Japan*

³ *University of Tokyo, Bunkyo, Japan*

An astro-biological model is presented in which atomic nuclei bound in amino acids interact via the weak interaction in stellar environments. Amino acids are preferentially oriented in high magnetic fields of certain stellar environments via the Stark effect. The coupling of atomic nuclei with non-zero magnetic moments to the molecular orbitals via the hyperfine interaction creates additional energy splittings. It has also been found that the magnetic shielding tensor can create an asymmetry in the energy states of the molecules which is dependent on chirality, and this is exploited in this model to create a chirality-dependent asymmetry in molecular states. An enantiomeric excess is subsequently created via the selective destruction and subsequent amplification of nuclei oriented in strong fields. Possible sites are proposed in which this model may exist.

Symmetry in Icosahedral Viruses: How It Exploited in the XFEL

Fatemehsadat Jamalidinan, Daniel Agterberg, Dilano Kerzaman Saldin

Department of Physics, University of Wisconsin-Milwaukee, Milwaukee, WI, USA

We propose a new method of determining the structure of an icosahedral virus from by exploiting the point-group icosahedral symmetry in the virus particle, which Caspar and Klug (1962) said was very common in virus structures. The X-ray free electron laser produces X-rays many orders of magnitude brighter than conventional X-rays, giving rise to speculation that it will enable structure determination of individual molecules or viruses without the need to form crystals. The problem is that the particles are presented to the X-ray beam in random orientations. Nevertheless, we show that exploiting the known point-group symmetry of the particles, it is possible to solve the structural problem by using an angular correlation method in an angular momentum representation. Note that we assume symmetry only in the construction of an oversampled diffraction volume from the correlations after the symmetry is revealed by objective means. The diffraction volume is dodecahedral (which has icosahedral point group symmetry). The reconstructed real-space image obtained from an oversampled diffraction volume by an iterative phasing algorithm, is icosahedral.

References:

Caspar, D.L.D.; Klug, A. Cold Spring Harbor. *Symp. Quant. Biol.* **1962**, 27, 1–24.

Symmetry and Minimum Principle at the Basis of the Genetic Code

Paul Sorba

Laboratory of Annecy of Theoretical Physics, National Center for Scientific Research (CNRS), Paris, France

The importance of the notion of symmetry in physics is well established: could it also be the case for the genetic code? In this spirit, a model for the Genetic Code based on continuous symmetries and entitled the “Crystal Basis Model” was proposed a few years ago and applied to different problems, such as the elaboration and verification of sum rules for codon usage probabilities, relations between physico-chemical properties of amino-acids and some predictions [1–3]. Defining in this context a “bio-spin” structure for the nucleotids and codons, the interaction between a couple of codon–anticodon can simply be represented by a (bio) spin–spin potential. Then, imposing the minimum energy principle, an analysis of the evolution of the genetic code can be performed with good agreement with the generally accepted scheme. A more precise study of this interaction model provides information on codon bias, consistent with data [4–6].

References:

1. Frappat, L.; Sciarrino, A.; Sorba, P. Crystalizing the Genetic Code. *J.Biol.Phys.* **2001**, *27*, 1–34.
2. Frappat, L.; Sciarrino, A.; Sorba, P. Prediction of Physical-Chemical Properties of Amino Acids from Genetic Code. *J.Biol.Phys.* **2002**, *28*, 17–26.
3. Frappat, L.; Sciarrino, A.; Sorba, P. Sum rules for codon usage probabilities. *Phys. Lett.* **2003**, A311, 264–269.
4. Sciarrino, A.; Sorba, P. A minimum principle in codon-anticodon interaction. *BioSystems.* **2012**, *107*, 113–117.
5. Sciarrino, A.; Sorba, P. Codon-anticodon interaction and the genetic code evolution. *BioSystems.* **2013**, *111*, 175–180.
6. Sciarrino, A.; Sorba, P. Codon bias from minimization of codon-anticodon interaction. *BioSystems.* **2016**, *141*, 20–30.

Palindromic Symmetry in Genomes and Evolution

Michael Sadovsky ¹, Yaroslav Grebnev ²

¹ *Institute of Computational Modelling of SB RAS, Krasnoyarsk, Russia*

² *Institute of Fundamental Biology and Biotechnology, Siberian Federal University, Krasnoyarsk, Russia*

Any genome is a symbol sequence from a four-letter alphabet. A lot can be retrieved from the studies of frequency distribution in ensembles of considerably short strings, of a given length. A palindrome is two strings that read equally in opposite directions; a complementary palindrome is two strings that read equally in opposite directions with respect to Chargaff's substitution rule ($A \leftrightarrow T$ and $C \leftrightarrow G$). The symmetry observed over a genome manifests in a proximal equivalence of the strings comprising a complementary palindrome; it should be stressed that the frequencies are counted over a single strand. Thus, it seems that a duality exists between the symmetry and the double helix structure. The frequency equality is not exact, but shows some deviations. We studied a number of genomes of various taxa to determine the deviation figures in order to learn the relation between the deviation figure, and taxonomy of a genome bearer. The deviation figures have been studied for the strings that range from 1 to 8 in length. Also, a theoretical estimation of the deviation figures has been obtained, for various models of a genetic sequence. A dependence of deviation figures from taxonomy has been observed for high taxa ranks, only. Besides, an inhomogeneity of a genome in terms of the figures has been studied for a number of organisms. A new inner structuredness manifesting in divergence of the deviation figures observed for various genome regions was found in all the genomes.

Symmetry in the Transcriptome and Genome Sequences of Siberian Larch (*Larix sibirica* Ledeb.)

Vladislav V. Biriukov ¹, Michael G. Sadovsky ², Yuliya A. Putintseva ¹, Natalia V. Oreshkova ^{1,3}, Konstantin V. Krutovsky ^{1,4,5,6}

¹ Laboratory of Forest Genomics, Genome Research and Education Center, Siberian Federal University, Krasnoyarsk, Russia

² Institute of Computational Modelling, Federal Research Center "Krasnoyarsk Science Center" of the Siberian Branch of the Russian Academy of Sciences, Novosibirsk, Russia

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⁴ Department of Forest Genetics and Forest Tree Breeding, Georg-August University of Göttingen, Göttingen, Germany

⁵ Laboratory of Population Genetics, N. I. Vavilov Institute of General Genetics, Russian Academy of Sciences, Moscow, Russia

⁶ Department of Ecosystem Science and Management, Texas A&M University, 2138 TAMU, College Station, TX, USA

We studied the structuredness and order in draft assemblies of the Siberian larch (*Larix sibirica* Ledeb.) transcriptome and genome. Assembled contigs were converted into the triplet frequency dictionaries followed by their cluster analysis. The transformation maps the contigs into a metric space. We used *K*-means clusterization to analyze the transcriptome and genome structures, which were visualized with the elastic map technique. The observed clusters demonstrated several interesting symmetries, also including those in the statistical and combinatorial properties. For instance, clustering in two classes yields stable classification with a good separability of clusters. We have checked the pattern of the second Chargaff's parity rule implementation for pairs of palindromic triplets within the first and the second classes and between them. It was found that the transcriptome sequences had significantly less discrepancy between the classes compared to genome sequences. Probably, it was due to the presence of contigs in the transcriptome assembly representing RNA sequences transcribed from opposite strands. Unlike the transcriptome, genome contigs demonstrated an inverse pattern of discrepancies regarding the second Chargaff's parity rule. The hypothesis was confirmed by BLAST. In addition, an unexpected octahedral structure exhibiting rotational symmetry was discovered in triplet frequency dictionary ensembles.

Symmetry in a Four-Cluster Triangle Structure of the Siberian Stone Pine (*Pinus sibirica* Du Tour) Transcriptome

Serafima V. Novikova ¹, Michael G. Sadovsky ², Yulia A. Putintseva ¹, Natalia V. Oreshkova ^{1,3}, Konstantin V. Krutovsky ^{1,4,5,6}

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² Institute of Computational Modelling, Federal Research Center “Krasnoyarsk Science Center” of the Siberian Branch of the Russian Academy of Sciences, Novosibirsk, Russia

³ Laboratory of Forest Genetics and Selection, V.N. Sukachev Institute of Forest, Federal Research Center “Krasnoyarsk Science Center” of the Siberian Branch of the Russian Academy of Sciences, Krasnoyarsk, Russia

⁴ Department of Forest Genetics and Forest Tree Breeding, Georg-August University of Göttingen, Göttingen, Germany

⁵ Laboratory of Population Genetics, N. I. Vavilov Institute of General Genetics, Russian Academy of Sciences, Moscow, Russia

⁶ Department of Ecosystem Science and Management, Texas A&M University, 2138 TAMU, College Station, TX, USA

The RNA isolated from three different tissues of Siberian stone pine—cambium, needles and buds—were sequenced and assembled for each tissue separately. The transcriptomes were converted into the triplet frequency dictionaries (FD) of two types. The first type FD allows to detect the strand specificity of clusters via the Chargaff’s second parity rule. The clusters were identified using *K*-means applied to the FD of contigs. We observed a four-cluster triangle structure in the distribution of the FDs. The observed symmetry of the clusters was apparently based on the strand specificity of contigs.

The second FD type was developed separately only for well annotated and sufficiently long contigs for each transcriptome. Each sequence has been tiled using a 300 bp long moving window with a 8 bp step and converted into a triplet FD. Then, each FD has been labelled by phase index. The fragments falling out of a coding region were labelled by 0. Otherwise, they were labelled according to the reading frame shift from 1 to 3, respectively. All the FDs were clustered by *K*-means, yielding a four-cluster pattern, where the clusters included the FDs with the same phase index. A highly symmetric four-cluster triangle pattern was observed.

Assessing Fluctuating Asymmetry of *Cucumis sativus* Leaves for Virtual Plant Models

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Fluctuating asymmetry in plant leaves is a widely used measure in geometric morphometrics. For example, starting from a Procrustes superimposition of a prototype leaf, measurements can be fitted before performing statistical analyses of symmetry. The goal of this study was an adaptation of this concept to improve prototype leaf shapes for virtual plant models based on analysis of fluctuating asymmetry between measurements and model. Several hundred cucumber leaves were digitized in situ with a magnetic field digitizer, where each leaf is represented by 17 unique landmarks. Furthermore, destructive leaf area measurements were performed afterwards. Based on these data, leaves were reconstructed from area and orientation measurements using a simplified shape definition of a virtual plant model. To improve this prototype shape, we conducted point-wise comparisons of fluctuating asymmetry between measurements and model. Robust Bayesian comparison of groups was used to assess statistical differences between leaf halves. Results indicate almost no directional asymmetry in leaves comparing different distances from the prototype, while detecting systematic deviations shared by both halves. This information on leaf symmetry was successfully included in an improved leaf prototype. Further studies will focus on the influence of stress factors on cucumber leaf symmetry.

Lie Symmetry Analysis for the SIS Model of Epidemiology

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A system of nonlinear ordinary differential equations arising from the SIS model of epidemiology is transformed into a system of one equation of second order. This is a simple model proposed in 1927 by Kermack and Mckendick. The modified symmetry method is applied and differential invariants are used to obtain some exact solutions of the SIS model.

Effects of Task Performance Symmetry on Human Collective Decision-Making

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In human joint decision-making, a prevalent question is whether the two persons could have solved the tasks equally well on their own, or possibly better as individual task-decision-makers? When allowed to communicate and hence combine perceived sensory information among individuals in a group, previous studies have indicated that symmetry in task performance between subjects promotes a synergetic performance effect. In other words, two heads are better than one when there is equality or symmetry in perceptual sensitivity and task performance. However, when task performance is asymmetrical between individuals, the collective performance is actually worse than the better performing individual. Similar findings exist with language symmetry: context-specific alignment can lead to collective benefit but, e.g., indiscriminate repetitions of the interaction partner's words can worsen the collective performance. This study deals with the comparison of results from different sensory modalities and hence addresses whether or not this effect seems domain specific or presents a robust general pattern across sensory modalities. Two analyses (Frequentist and Bayesian) are employed since previous studies utilize the frequentist approach and hence allow us to make a comparison. The Bayesian analysis, however, allows us to explicitly specify all assumptions, carry the uncertainty all the way through the model, and directly compare the predictive power of the proposed effects.

Fluctuating Asymmetry, Sexual Dimorphism and Attractiveness in Humans: The Development towards a 3D Approach

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Perfect bilateral symmetry is the optimal outcome of the development of bilateral traits in the absence of developmental perturbations. Any random perturbation in this perfect symmetrical state, called Fluctuating Asymmetry (FA), is an indicator of Developmental Instability (DI). Fluctuating asymmetry has been proposed to reflect an individual's fitness in a good genes context in different species, including humans. From an evolutionary perspective, where selection for good genes plays a major role in sexual selection, it is hypothesized that more symmetric people should appear more attractive to their potential mates. This hypothesis has been studied mostly using 2D images and a limited number of landmarks to assess the asymmetry of the subjects.

We develop an analysis protocol to use high density 3D scans of human faces and bodies to analyze the level of FA and its correlation with attractiveness and fitness-proxies. A symmetric high density anthropometric mask is mapped on all faces using a non-rigid registration algorithm. A set of 20 manually indicated landmarks are used to validate the precision of the algorithm. In this presentation, the algorithm pipeline as well as the validation results will be presented and future steps and the possible applications will be discussed.

Human Form—An Evolutionary Psychological Approach to Beauty

Karl Grammer

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Humans tend to judge and sort parts of their social and non-social environment permanently into a few basic categories: those parts they like and those parts they do not. Indeed, we have developed aesthetic preferences for those things and people we are exposed to. Furthermore, needless to say, these preferences shape our behavioural choices—our tendency to seek out or avoid what the world has to offer to us. Humans and other animals have evolved preferences for food and habitats, for naturally occurring sensations such as smells and sounds, as well as for the broad array of culturally created artefacts.

Humans have also evolved aesthetic preferences for their sexual and social companions. In this talk, I will review the current approaches in attractiveness research, I will deal with the obsession about beauty, and review the biological constraints, which create the bases for beauty traits as honest mating signals. If evolutionary approaches to beauty are correct, beauty signals should have a direct relation to health, and reproductive success [1].

The pillars of beauty identified up to now are averageness, symmetry, and sex-hormone markers, which find their expression in form, skin texture, body motion, body odour, voices and hair complexion. One of the major players is symmetry and I will discuss several methods for the measurement of symmetry, the role of different types of symmetry and its relation to beauty perception. In fact, a preference for symmetry in mate selection is a general trait found in most bilateral animals and even plants. We suggest that the content of these signals is redundant, and points in the same direction [2]. For instance, how can it happen that people with symmetrical bodies have more attractive voices.

On the side of the perceiver, I will explore which brain structures are responsible for beauty perception and propose a perceptive model which is based on biologically based construction rules for “what is beautiful” and not on the content of the signals themselves. These construction rules can be modified by several constraints such as female hormonal cycle, socioeconomic status or self-perception—which makes beauty perception a plastic concept which is able to adapt to a range of socioeconomic situations and environments [3].

In the final part, I will present evidence on how beauty traits develop and consider the evidence for their relation to genetic factors such as genetic heterozygosity and developmental factors such as prenatal hormonal environment.

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Fluctuating Asymmetry and Sexual Selection: Integrating Cross- and Within-Population Tests of Key Predictions

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The relationship between morphological symmetry and mating success in animals varies dramatically across species and populations. The reasons for this heterogeneity in effect size are poorly understood, which has led to intense debate among evolutionary biologists. I will evaluate the general hypothesis that differences in the level of developmental instability (DI) across populations accounts for heterogeneity in the effect of symmetry on sexual selection. According to this hypothesis, most populations have levels of DI insufficient to propel adaptive processes such as mate selection; only when DI levels surpass a critical threshold will selection operate and be detectable. I will test this hypothesis using results of our work with *Drosophila bipectinata* Duda (Diptera: Drosophilidae), focusing on fluctuating asymmetry (FA) and size of the male sex comb, a model secondary sexual trait for animal studies. The following key predictions will be tested: (1) Intensity of sexual selection depends on the level of DI in the population. Data from nine distinct populations sampled throughout Australasia and the South Pacific will be evaluated for this test; (2) the level of DI in a population, in turn, is the result of the particular history of directional selection for trait size experienced by that population. This prediction will be evaluated using comparative data as well as the results of artificial selection for increasing trait size under laboratory conditions. This study will provide a framework for understanding the dramatic variation in effect size across FA-sexual selection studies.

Behavioural Instability; What Is Next. A Holistic Approach to Behavioural Studies

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Phenotypic variability and fluctuating asymmetry are the most often used indices for the estimation of developmental instability of an individual. These indices are often measured on morphological traits, which supposedly are affected during their development by intrinsic (genetic) and extrinsic (environmental) factors. Developmental instability is therefore suggested as a useful tool in environmental monitoring. However, the relatively large time windows during which a trait develops increases the possible confounding effect of environmental variability on such development. The expected relationship between the intensity of an environmental insult and the developmental instability of a trait can be confused by the random noise added by the environmental variability. The need for a “more immediate and reliable” signal of environmental disturbance could therefore be addressed by investigating the alteration of the behaviour of an individual. The behaviour is an immediate reaction to a given stressor and therefore it should reveal any association between the stressor and a behavioural alteration more directly. Several toxicological and behavioural ecology studies are now accurately quantifying the behaviour by measuring, for example, the speed and the acceleration of an individual. Subsequently, these parameters and their changes can be related to changes of the environmental conditions. We propose in this investigation to add additional parameters for the quantification of behavioural traits using modified indices which are traditionally used to investigate developmental instability. We focus on indices in which the scaling effect of the variance with the mean and deviation from the normal distribution (skewness and kurtosis) of the behavioural trait are taken into account. Additionally, sequence analysis and autocorrelation of the behavioural traits will also be considered as potential indicators of environmental disturbance. An experimental approach in which changes in behavioural traits are associated with environmental changes will be presented as an example of the application of these modified indices. The concept of behavioural instability will be discussed as an alternative and/or complementary tool for the analysis of behavioural data.

Abstracts

Session 2: Physics and Symmetry

Session Chair – Kimball A. Milton

Dual Symmetry: Magnetic Monopoles in Theory and Experiment

Kimball Milton

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The greater symmetry imparted to the Maxwell–Heaviside equations by the existence of magnetic charge was noted in the 19th Century, and the peculiar properties of magnetic charges were explored by Poincare and Thomson; the heuristic value of magnetic charge had already been noted by Faraday. However, it was not until Dirac showed that magnetic charge was consistent with quantum mechanics in 1931 that the modern concept of magnetic charge was born. Dirac showed that a single magnetic charge in the universe would quantize all electric charges, in that the product of any electric charge e and any magnetic charge g must satisfy $eg = n h c/4 \pi$. If a magnetic monopole exists, a Dirac “string” is associated with it, because the vector potential cannot be a single-valued regular function. The string is invisible; changing the orientation of the string is a singular gauge transformation. The quantization condition and the existence of the string renders perturbation theory untenable.

Since the time of Dirac, there have been many developments in the theory, and numerous dedicated searches made for magnetic monopoles both terrestrially and cosmically. Most unified gauge theories predict the existence of monopoles resulting from symmetry breaking; the mass of such monopoles is set by the symmetry-breaking scale. This talk will review some of the theoretical issues involved in the subject, and the status of the latest experiments, which have, to date, yielded no evidence for magnetic charge. We will also discuss recent “discoveries” of analogues to magnetic monopoles, and discuss the significance of these.

Physics in the Complex Domain

Carl M. Bender

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The theory of complex variables is extremely useful because it helps to explain the mathematical behavior of functions of a real variable. Complex variable theory also provides insight into the nature of physical theories. For example, it provides a simple and beautiful picture of quantization and it explains the underlying reason for the divergence of perturbation theory. By using complex-variable methods, one can generalize conventional Hermitian quantum theories into the complex domain. The result is a new class of parity-time-symmetric (PT-symmetric) theories whose remarkable physical properties have been studied and verified in many recent laboratory experiments.

Quantum Metrology and Relativistic Symmetries

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Modern metrology is based on quantum and relativistic physics. The second is defined as a fixed integer number of periods of atomic caesium clocks while the meter is derived from the exact value fixed for the speed of light in vacuum c . Clock synchronization, distance measurement (ranging) or localization in space-time (GNSS localization) are built on the remote distribution of electromagnetic field phases. In 2018, the Planck constant h and elementary charge e should be defined to have exact values, replacing the old definitions of the kilogram and Ampere units.

However, the quantum status of time, space and mass observables and its compatibility with relativistic symmetries remain open questions. We address this problem in a quantum algebraic approach where observable positions in space and time are defined so that they obey relativistic and quantum requirements. A mass observable is defined which is no longer a constant as expected from its dimension with respect to dilatation.

The commutators of quantum positions involve spin, and frame transformations to accelerated frames differ from their classical counterparts. Relativistic symmetries nevertheless allow one to extend the covariance rules of general relativity to the quantum algebraic framework. It leads to a quantum version of the Einstein equivalence principle identified to the transformation of the mass observable.

Generalization of the Noether Theorem: Global and Local Symmetries, Dynamical Functionals and Boundary Conditions

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We consider the most general form of the Noether theorem which is suitable for the treatment of global symmetries, described by symmetry-groups, and local symmetries, described by symmetry-algebras, which may not be integrable to symmetry groups. The principle new notion is specific dynamical functionals which solve the problem by replacing the standard action functionals. We also discuss the compatibility of the boundary conditions and the corresponding variational principles. Many illustrative examples are shown.

Noether's Symmetries in Quantum Cosmology

Salvatore Capozziello

University of Naples "Federico II", Napoli, Italy

We discuss the Hamiltonian dynamics for cosmologies coming from theories of gravity. In particular, minisuperspace models are taken into account searching for Noether symmetries. The existence of conserved quantities gives selection rules to recover classical behaviors in cosmic evolution according to the so-called Hartle criterion, that allows to select correlated regions in the configuration space of dynamical variables. We show that such a statement works for general classes of Theories of Gravity and is conformally preserved. Furthermore, the presence of Noether symmetries allows a straightforward classification of singularities that represent the points where the symmetry is broken. Examples for nonminimally coupled and higher-order models are discussed.

Symmetries in the Set-Theoretic Universe and the Higher Infinite

Joan Bagaria

ICREA & University of Barcelona, Barcelona, Spain

The set-theoretic universe, as described by the standard Zermelo-Fraenkel axioms of set theory plus the Axiom of Choice (ZFC), provides the standard ontology for mathematics. However, the ZFC axioms are insufficient for answering many fundamental mathematical questions involving infinite sets, such as the Continuum Hypothesis, Lebesgue's measure extension problem, regularity properties for projective sets of real numbers, etc. We will argue that additional axioms of set theory asserting the existence of very large infinite cardinal numbers, known as large cardinal axioms, may be regarded as imposing strong symmetry conditions on the set-theoretic universe, which yield a solution to many of the ZFC-independent questions.

On the Symmetry of the Electromagnetic Energy-Momentum Tensor in Media

Iver Brevik

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The electromagnetic energy-momentum tensor in media has been under discussion for more than 100 years. The interest in this topic has become quite large in recent years, most likely related to the advent of very accurate measurement techniques in optics. The purpose of this contribution is two-fold: (1) to demonstrate by means of a mapping procedure how the electromagnetic field in a medium can be mapped into a corresponding field in vacuum, showing how naturally the Minkowski energy-momentum tensor fits into the canonical formalism, and (2) to give a critical analysis of some recent experiments in radiation optics. In several of the experiments, it turns out that it is the surface force (common for the Minkowski and Abraham tensors) that is measured, instead of the electromagnetic momentum itself. The talk is based upon the recent paper of I. Brevik published in *Annals of Physics*, **2017**, 377, 10.

Gluing Formula for Casimir Energies

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Let M_1 and M_2 be two Riemannian manifolds each of which have the boundary N . Consider the Laplacian on M_1 and M_2 augmented with Dirichlet boundary conditions on N . A natural question to ask is if there is any relation between spectral properties of the Laplacian on M_1 , M_2 , and the Laplacian on the manifold M (without boundary) obtained by gluing together M_1 and M_2 . A partial answer is given by the Burghelea-Friedlander-Kappeler-gluing formula for zeta-determinants. This formula contains an (in general) unknown polynomial which is completely determined by some data on a collar neighborhood of the hypersurface N . In this talk I present results for the polynomial in terms of suitable geometric tensors on N . Choosing M_1 , M_2 and M suitably, a gluing formula for Casimir energies results.

Generalized Heisenberg–Euler Formula and Its Application to Vacuum Magnetic Birefringence Experiment

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The Heisenberg–Euler formula, describing the non-linear effective action of a photon, is generalized to include parity violating effects. Using the formula, how to probe the dark sector via the magnetic birefringence experiments is studied, in which a new scheme has emerged. The scheme uses a ring Fabry–Pérot resonator which can measure the parity-violating effects directly without QED background. As an example, the sensitivity of the measurements (ellipticity and polarization rotation) is given, in the presence of a dark sector neutrino, as a function of a mixing parameter between visible and dark sectors and the mass of the dark sector neutrino.

Particle Path Integrals on Maximally Symmetric Spaces and Type-A Trace Anomalies

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Particle path integrals in curved spaces can be employed to compute trace anomalies in quantum field theories, and more generally to study properties of quantum fields coupled to gravity. Their construction in arbitrary coordinates is well understood, and known to require the use of a regularization scheme. In the present talk, we elaborate on an old proposal that focuses on the construction of the path integral by using Riemann normal coordinates. The main method's conjecture is that curvature effects are taken care of by a scalar effective potential, so that the particle Lagrangian is reduced to that of a linear sigma model interacting with the effective potential. We show the explicit validity of the simplified path integral on maximally symmetric spaces, and test it to compute heat kernel coefficients and type-A trace anomalies for a scalar field in arbitrary dimensions up to $d = 12$. The results agree with those expected, which are reproduced with great efficiency and extended to higher orders. Finally, we point out that this simplified path integral might be of further use in worldline applications, though its application on spaces of arbitrary geometry remains unclear.

Algebraic Solutions in Scalar Field Cosmology: Reconstruction of the Dark-Energy Equation of State and the Inflationary Potential

Andronikos Paliathanasis

Austral University of Chile, Valdivia, Chile

An algebraic solution for arbitrary potential is presented in the context of scalar field cosmological models. That result is used to generate new solutions of the scalar field equations in homogeneous and isotropic universes. A series of generalizations of the Chaplygin gas and bulk viscous cosmological solutions for inflationary universes are found. Finally, we show how the Hubble slow-roll parameters can be calculated using the solution algorithm and we compare these inflationary solutions with the observational data provided by the Planck 2015 collaboration to constraint and rule out some of these models.

Application of Lie Symmetry Analysis to Heat and Mass Transfer Equations

Irina Stepanova

Institute of Computational Modelling of SB RAS, Krasnoyarsk, Russia

This talk is devoted to the study of equations describing the thermal diffusion process in a binary mixture via the Lie symmetry approach. Thermal diffusion is the component separation in non-uniformly heated fluid. The mathematical model of the process is described by Navier–Stokes equations and mass and heat transport equations.

The group classification problem for thermal diffusion equations is solved in correspondence with five arbitrary functions concerning the physical properties of the mixture. Some invariant solutions of the governing equations are constructed and applied to describe the thermal diffusion convection in the simple physical applications.

Special attention is paid to the thermal diffusion equations without convection. We take into account the thermal diffusion conductivity as well as simple thermal diffusion. The symmetries of these equations are found based on the forms of the transport coefficients. Some theorems concerning the general symmetry properties of such equations are proven.

This work is supported by the Russian President Grant (project MK-4519.2016.1).

Dynamical Systems with Spatiotemporal Periodicities through the Symmetries

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Dynamical systems often contain oscillatory forces or depend on periodic potentials. Time or space periodicity is reflected in the properties of these systems through a dependence on the parameters of their periodic terms [1,2]. In this talk, it is shown that simple symmetry considerations determine how their properties depend functionally on the amplitudes and the phases of the periodic terms, regardless of whether they are classical or quantum, stochastic or deterministic, dissipative or nondissipative [3]. This formalism is applied to find the functional dependence of the expectation value of the momentum of a Bose–Einstein condensate, described by the Gross–Pitaevskii equation [4,5], when it is exposed to a bi-harmonic potential whose amplitude is periodically modulated in time. It is shown that, by using this formalism, a small set of measurements is enough to obtain the functional form for a wide range of parameters.

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É. Cartan's Supersymmetry, Noncommutative Geometry and Propagation of Time in the Kaluza-Klein-Like Universe

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É. Cartan has shown that in a space E_{2V} or E_{2V+1} in which the fundamental form of vector fields $F = x^1x^{1'} + x^2x^{2'} + \dots + x^Vx^{V'}$ is defined, semi-spinors φ, ψ and vectors or bivectors that satisfy specific symmetry can be introduced. When $v = 4$, he showed that there exists a group G which leaves invariant the trilinear form $F = \varphi^T C X \psi$, where $X = (x^1, x^2, x^3, x^4, x^{1'}, x^{2'}, x^{3'}, x^{4'})$ and three quadratic forms $F = x^1x^{1'} + x^2x^{2'} + x^3x^{3'} + x^4x^{4'}$, $\phi = \Phi^T C \Phi$ and $\psi = \varphi^T C \varphi$. The transformation group G of vectors and semi-spinors consists of five types $G_{23}, G_{12}, G_{13}, G_{123}$ and G_{132} . When one adopts non-commutative geometry like Connes, one can pull back at each bundle point on the S^3 model, two fibre points corresponding to $x^4 \in U(1)$ and $x^{4'} \in U(1)'$. We allow x^4 and $x^{4'}$ to run in different directions of time.

The transformations $G_{23}, G_{12}, G_{13}, G_{123}$ and G_{132} contain the triality symmetry of octonions which can appear as the colour degrees of freedom of quark gluon systems. The transformation properties of vectors and semi-spinors which have the transformation property similar to G_2 symmetry could be the origin of different properties of baryonic systems, from those of leptonic systems which are defined by the quaternion symmetry of the Dirac equations. A new view of Kaluza–Klein-like universe, a definition of state-dependent time flow based on non-commutative geometry which contains that of Connes and Rovelli, and applications to the theory to time-reversal symmetry violating physical processes will be discussed.

Unifying the Early-Time Inflationary Era with Late-Time Dark Epoch Universe: The Case of Modified Gravity

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We discuss various theories of modified gravity which aim to describe the whole evolution of the universe, from early-time inflation via radiation/matter dominance and finally to the dark energy era. Such unified evolution may be described in frames of the same modified gravity. Special attention is paid to $F(R)$ gravity where R is scalar curvature and modified Gauss–Bonnet gravity. The modified gravity solves the problem of universe acceleration without the need to introduce inflation or unknown dark fluid. The explicit models of such $F(R)$ gravity are presented where quantum gravity effects may also be taken into account. The possible generalizations of modified gravity to non-local gravity, string-inspired gravity, and teleparallel gravity are briefly discussed. A number of applications such as the qualitative change of mass-radius relation in neutron stars or the anti-evaporation effect in multiple-horizon black holes are mentioned.

Zeta Functions: Symmetry and Applications

Emilio Elizalde

National Higher Research Council of Spain, Madrid, Spain

A short summary of some symmetry properties of the zeta function and of different zeta functions corresponding to pseudodifferential operators will be given. After that, some applications of zeta function regularization in quantum field theory and cosmology will be discussed, together with some associated problems.

From Kaluza–Klein to Non-Commutative Gauge Theories of Gravity

George Zoupanos

National Technical University of Athens, Athens, Greece

Firstly, a short reminder of the Kaluza–Klein programme and a review of the Coset Space Dimensional Reduction of higher dimensional gauge theories will be given. Then, the “fuzzy sphere” will be presented, as a representative example of a non-commutative coset as well as the construction of gauge theories on such spaces.

Eventually, examples will be presented of (a) a higher dimensional Unified Theory with fuzzy coset spaces as extra dimensions, (b) gravity as a gauge theory on non-commutative spaces.

On Symmetry Restoration in General Relativity

Luciano Rezzolla

Institute for Theoretical Physics, Frankfurt, Germany

Einstein's theory of general relativity is often regarded as the best theory of gravity that we know. Yet, this theory often manifests itself under conditions where no symmetry is present and nonlinear dynamics dominates. I will discuss how these conditions are systematically accompanied by the restoration of some degree of symmetry. Hence, despite gravity appearing often under conditions devoid of symmetry, asymptotic solutions tend to restore symmetry.

Quantum Simulation of SU(4) Symmetric Spin Lattice Models

Bruno Uchoa

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Quantum spin-orbital liquids are strongly correlated states that emerge from quantum frustration between spin and orbital degrees of freedom. Those states are highly entangled, have non-local excitations but do not break any symmetries. A promising route towards observing those elusive states is the creation of artificial Mott insulators, where antiferromagnetic correlations between spins and orbitals can be designed. I will show that Coulomb impurity lattices on the surface of gapped honeycomb substrates, such as graphene on SiC, can be used to simulate SU(4) symmetric spin-orbital lattice models in the Mott regime. The antiferromagnetic correlations follow from super-exchange interactions between Coulomb impurity bound states at quarter filling, with spin and valley degeneracies. I propose that quantum spin-orbital liquids can be engineered in artificially designed solid-state systems at vastly higher temperatures than achievable in optical lattices with cold atoms.

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Weak Isospin Symmetry and the Vacuum Polarization Energy of Cosmic Strings

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The vacuum polarization energy is the leading quantum correction to the energy of a localized field configuration. Spectral methods are an effective means to calculate vacuum polarization energies. When computing these energies for cosmic strings in models similar to the standard model of particle physics, regularization and renormalization requires operations that individually are not manifestly consistent with the isospin symmetry of the model. Formally, i.e., before regularization and renormalization, the vacuum polarization energy is defined via the single particle energies of the quantum fluctuations that interact with a background potential which is generated by the cosmic string. Fortunately, there exists a particular global isospin transformation of the string configuration that leaves the single particle energies invariant. By numerical simulations, it is thus possible to verify that the renormalized vacuum polarization energy computed by spectral methods indeed preserves isospin symmetry. The particular construction even confirms that the spectral methods approach is consistent with local isospin symmetry. These findings strongly support the use of spectral methods to compute vacuum polarization energies. It is then shown that the quantum corrections lead to stabilization of a cosmic string when the parameters of the model are slightly changed from their standard model values.

PT-Symmetry and Related Geometrical Structures

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In non-relativistic quantum mechanics, the dynamics of closed quantum systems is described by Hamiltonians which are self-adjoint in appropriately chosen Hilbert spaces. For PT-symmetric quantum systems, the Hamiltonians are, in general, no longer self-adjoint in standard Hilbert spaces, rather they are selfadjoint in Krein spaces—Hilbert spaces endowed with indefinite metric structures. Moreover, the spectra of PT-symmetric Hamiltonians are symmetric with regard to the real axis in the spectral plane. Apart from Hamiltonians with purely real spectra, this includes also Hamiltonians whose spectra may contain sectors of pairwise complex-conjugate eigenvalues. Considering families of parameter-dependent Hamiltonians, one can arrange parameter-induced passages from sectors of purely real spectra to sectors of complex-conjugate spectral branches. Corresponding passages can be regarded as PT-phase transitions from sectors of exact PT-symmetry to sectors of spontaneously broken PT-symmetry. Approaching a PT-phase transition point, the eigenvectors of the Hamiltonian tend toward their isotropic limit—an, in general, infinite-dimensional (Krein-space) generalization of the light-cone limit in Minkowski space. At a phase transition, the Hamiltonian is no longer diagonalizable, but similar to an arrangement of nontrivial Jordan-blocks. The interplay of these structures is briefly reviewed with special emphasis on the related Lie-algebraic and Lie-group aspects. With the help of Cartan-decompositions, associated hyperbolic structures and Lie-triple-systems are discussed for finite-dimensional setups as well as for their infinite-dimensional generalizations (Hilbert–Schmidt (HS) Lie groups, HS Lie algebras, HS Grassmannians). The interconnection of Krein-space structures and PT-phase transitions is demonstrated on two exactly solvable models: PT-symmetric Bose-Hubbard models and PT-symmetric plaquette arrangements.

Modified Gravity and Relativistic Stars

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We construct nonperturbative models of compact stars in $f(R) = R + \alpha R^2$ - gravity and scalar-tensor gravity. For $\alpha > 0$ the shooting method of solution gives that there is unique value of curvature at the center of star at which solution has required Schwarzschild asymptotic. For distant observer the gravitational mass of star increases negligibly for realistic values of α with increasing α . One can say that increasing of mass occurs by “gravitational sphere” outside the star with some “effective mass”. For $\alpha < 0$ we have no rigid condition on R at center of star but there are no realistic solutions. The contribution to mass from gravitational field grows infinitely with distance.

Wormholes Created by Vacuum Fluctuations

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Possible vacuum fluctuations of quantized fields can create wormholes. The description of such effects is possible within the framework of the semiclassical theory of gravitation. The main difficulty of such a theory is that the vacuum polarization effects are determined by the topological and geometrical properties of spacetime as a whole or by the choice of quantum state in which the expectation values are taken. Only some spacetimes with high degrees of symmetry for the conformally invariant field equations of the theory of semiclassical gravity can be solved exactly. Let us stress that the single parameter in the problem is the Planck length l_{PL} . This implies that the characteristic scale of the spacetime curvature can differ from l_{PL} only if there is a large parameter. As an example of such a parameter, one can consider the non-zero temperature of quantum state for the quantized field. It is known that the high-temperature limit $\langle T_{\mu\nu} \rangle$ for such a thermal state is proportional to the fourth power of the temperature. Here, the vacuum polarization effect of a quantized scalar field in a thermal state at an arbitrary temperature is considered. The scalar field is assumed to be both massive and massless, with an arbitrary coupling ξ to the scalar curvature, and in a thermal state at an arbitrary temperature. The gravitational background is assumed to be static spherically symmetric and slowly varying.

Good vs. Bad Tetrads in $f(T)$ Gravity and the Role of Spacetime Symmetries

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It is well known that the field equations of $f(T)$ gravity break local Lorentz invariance if one a priori assumes a vanishing spin connection, except in the teleparallel equivalent of general relativity (TEGR) case $f(T) = T + \Lambda$. One consequence is the existence of “bad” tetrads, i.e., tetrads which force a constraint on the field equations, which can be satisfied only in the TEGR case, hence prohibiting any modification of the gravitational dynamics. In order to overcome this difficulty, one may either restrict oneself to “good” tetrads, from which no such constraint arises, or introduce a suitable spin connection, which cancels the constraint. However, there is no simple procedure or general formula for these good tetrads or suitable spin connections, and only particular examples have been constructed. I will show how spacetime symmetries act on good and bad tetrads, and can be used to distinguish them, hence giving a simpler criterion for good tetrads. I will also show how a sufficiently high amount of symmetry can be used to determine either the good tetrads or the required spin connection.

Multifield Inflation Scenarios from MSSM

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We consider the possible application of the two-Higgs-doublet potential of the Minimal Supersymmetric Standard Model (MSSM) to construct inflation scenarios. We introduce a non-minimal coupling to gravity that includes five scalar fields related with two doublets. We construct inflationary scenarios that are compatible with observational data using specially selected model parameters.

Relativistic Stars in dRGT Massive Gravity

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The de Rham–Gabadadze–Tolley (dRGT) massive gravity describes a massive spin-2 particle. The theory is one of modified gravities, where cosmological behaviors change from those in general relativity. In order for the massive gravity theory to provide solar system observations, in short-range scale, the theory needs to show similar behaviors to those in general relativity. The behaviors can be obtained by the Vainshtein mechanism, where the non-linear kinetic terms in the dRGT massive gravity allow an extra degree of freedom in the theory. Although the mechanism has only been verified in a vacuum in static and spherically symmetric configurations, such as a point-like particle, it is not apparent whether the Vainshtein mechanism could work if matter exists in non-static or non-spherical configurations.

In the environment of relativistic stars, the gravity is strong and the density of the matter is high, which could lead to non-trivial behaviors in the Vainshtein mechanism. In our research, we construct solutions describing static and spherical relativistic stars in the minimal model of the theory. A new equation, derived from consistency conditions, determines the behavior of the extra degree of freedom. By numerical calculation, we show that the maximal mass in massive gravity is smaller than that in general relativity for several equations of state. The results could be consistent with previous studies on the energy scales in which non-linear kinetic terms appear. Moreover, we report the studies of relativistic stars in the non-minimal model of the theory.

Intrinsic Symmetry of the Dark Fluid Electrodynamics

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Cosmic Dark Fluid is considered as a non-stationary medium, in which electromagnetic waves propagate, and magneto-electric field structures emerge and evolve. The Dark Fluid is assumed to be formed by a duet of Dark Matter (a pseudoscalar axionic constituent) and Dark Energy (a scalar element). The purpose of the talk is two-fold: on the one hand, we distinguish electrodynamic effects induced by these two constituents of the Dark Fluid; on the other hand, we try to find a specific internal symmetry between them. A medium-type representation of the Dark Fluid allows us to involve into analysis the concepts and mathematical formalism elaborated in the framework of classical covariant electrodynamics of continua, and to distinguish dark analogs of well-known medium-effects, such as optical activity, pyro-electricity, piezo-magnetism, electro- and magneto-striction and dynamo-optical activity. We discuss ten models, which describe electrodynamic effects induced by the Dark Matter and/or Dark Energy. The discussion of the structure of these models is accompanied by examples of exact solutions to the master equations, correspondingly extended; applications are considered for cosmology and space-times with spherical and pp-wave symmetries.

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An Analyst's Take on Gauge Theory

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We work with a pair of complex-valued scalar fields over a 4-manifold. Our object of study is a first-order Hermitian sesquilinear form, i.e., an integral over the manifold whose integrand is a linear combination of terms “product of gradient of scalar field and scalar field” and “product of two scalar fields”, with complex conjugation in the appropriate places.

We call two sesquilinear forms equivalent if one is obtained from the other by some x -dependent $GL(2, \mathbb{C})$ transformation, i.e., by a change of basis in the infinite-dimensional vector space of pairs of complex-valued scalar fields. Our aim is to provide an explicit description of equivalence classes of sesquilinear forms. We achieve this aim, and in doing this we show that our sesquilinear forms implicitly contain geometric constructs such as Lorentzian metric, connection coefficients and electromagnetic covector potential.

The talk is based on DOI:10.1088/1751-8113/48/16/165203 and arXiv: 1611.08297 (to appear in JMP).

Abstracts

Session 3: Chemistry and Symmetry

Session Chair – Maurizio Benaglia

Batch and Flow Asymmetric Catalysis for the Synthesis of Chiral/Active Pharmaceutical Compounds

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Continuous-flow systems have emerged as a powerful technology for performing chemical transformations and have recently attracted attention also for the preparation of chiral APIs (active pharmaceutical ingredients). Recently developed technology-assisted stereoselective reactions will be discussed, including reactions of nitroacrylates under MW irradiation and organocatalyzed reactions in alternative reaction media (Deep Eutectic Solvents). Some stereoselective transformations have been performed in chiral organocatalytic reactors (packed-bed and monolithic) under continuous flow conditions. Recent developments will be presented, also highlighting the possibility to perform organocatalytic reactions in (micro)-mesoreactors and to synthesize in flow-mode chiral intermediates of pharmaceutical interest. Preliminary results of stereoselective catalytic reactions in 3D-printed reactors will also be briefly highlighted.

Chirogenesis in Supramolecular Systems on the Basis of Porphyrinoids

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Chirogenesis is a phenomenon of symmetry breaking in achiral multi- or unimolecular host systems by chiral guests (and vice versa), and is achieved by the rational application of specific non-covalent interactions via a chirality information transfer mechanism. With supramolecular interactions being responsible for these chiral transformations, they come under the heading of supramolecular chirogenesis, which is a fundamentally novel interdisciplinary field of research—a smart combination of supramolecular/nano chemistry and chiral science.

Recently, a novel and very efficient supramolecular chirogenic system based upon an achiral ethane-bridged bis(metallo- or free base octaethylporphyrin) was developed and well-investigated. Upon interaction with the corresponding chiral guests, ligand-induced structural deformations are produced in this achiral host, resulting in an asymmetric orientation of the two porphyrin subunits and subsequent pronounced and easily detectable spectral changes monitored by various spectroscopies. Particularly, through-space exciton coupling between the porphyrin electronic transitions generates bisignate Cotton effects in the circular dichroism (CD) spectra. Significantly, the sign of the observed CD couplet is unequivocally correlated with the substituents' bulkiness around the stereogenic center. In turn, this results in the absolute configuration assignment of the chiral ligand used, hence allowing us to develop an absolute configuration sensor for enantiopure amines, alcohols, and acids. This system possesses a high degree of chiroptical activity and sensitivity to various internal and external controlling factors such as the structure of guest molecules, stoichiometry, number of binding sites, solvent, temperature, and phase transition.

Further developments and prospects toward new supramolecular chirogenic systems on the basis of heterometallic bis- and multi-porphyrin structures will be discussed.

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Chromophores Supramolecular Organization in Polymer Materials with Quadratic Nonlinear-Optical Activity: Symmetry Aspects

Marina Balakina, Olga Fominykh, Timur Burganov, Anastasiya Sharipova, Sergey Katsyuba

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Organic dipole chromophores incorporated into polymer matrix serve as molecular sources of its nonlinear-optical (NLO) activity. To exhibit quadratic NLO response polymer material should be noncentrosymmetrical, what is achieved by the chromophores orientation in the applied electric field. Atomistic modelling of oligomers with covalently bound chromophores revealed the formation of stacked structures formed by chromophores with codirected dipole moments, in which from two to four chromophores participate. The chromophores in the stacks are shown to be mutually shifted, the shift value determining the NLO characteristics of such structures. Another way of supramolecular organization of chromophore groups in the material is realized via Hydrogen bonds with the formation of the so-called J-dimers composed of chromophores, which results in the considerable growth of NLO characteristics of the material. Thus the formation of supramolecular aggregates could contribute to optimization of the optical nonlinearity of the material.

Vibrational spectroscopy provides the tool to monitor the presence of such aggregates. The comparison of experimental and quantum-chemically calculated spectra permits revealing separate chromophores, H-dimers with different structures and J-dimers in the material, and provides guidelines for the design of chromophores effective for the realization of materials with high quadratic NLO activity.

Spectroscopic Study of (*all-R,R*)-cyclohexanohemicucurbit[8]uril and Its Host–Guest Supramolecular Hexafluorophosphate Complexes

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(*all-R,R*)-Cyclohexanohemicucurbit[8]uril (cycHC[8]) is a chiral macrocycle binding anions [1] with 1:1 stoichiometry in protic solvents with the association constant of $K_a = 3 \times 10^4 \text{ M}^{-1}$ in the case of the PF_6 anion. Spectroscopic properties of cycHC[8] have been analysed by ultraviolet and circular dichroism spectroscopy exhibiting the corresponding electronic absorption. Host–guest complexation of cycHC[8] with the hexafluorophosphate anion containing chromophores was studied in different solvents. It was found that using ultraviolet, fluorescence and circular dichroism spectroscopies, it is possible to follow the supramolecular interaction between cycHC[8] and chromophore containing the hexafluorophosphate anion in methanol through the spectral changes of its cationic moiety. Furthermore, it was shown with circular dichroism that the cycHC[8] host uptakes the achiral hexafluorophosphate anion into its cavity, whilst the remaining chromophoric cation binds the cycHC[8]–anion complex via the corresponding electrostatic interactions. In the case of the chiral chromophoric guest, the effect of chiral discrimination is observed. The scope of chiral cations for enantio selectivity and achiral cations for chirality induction will be discussed.

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Symmetry Breaking and Polarity Formation in Molecular Crystals

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Dipolar molecules restricted to one single degree of freedom (180° orientation disorder) can produce growth induced polar order in particular sectors of molecular crystals. The phenomenon can theoretically be described by an Ising model with a free boundary surface perpendicular to the growth direction. In fact, the model Hamiltonian contains a linear coupling of the spin variable of surface molecules and the elementary microscopic two-body energy. Such coupling is formally equivalent to an effective electrical field acting on those spin, breaking in this way the intrinsic spin flip symmetry [1]. This description applies to nm sized seed crystals as well as to crystals growing to the macroscopic size. In the first case, the system at equilibrium consists of a bi-polar state of general ∞/∞ m symmetry. In the case of growth, a polar seed undergoes a reversal transition which transforms the mono-domain state also into a bi-polar one [2].

Phenomena to be reported represent a general behavior of condensed molecular matter formed by asymmetrical but not necessarily chiral building blocks, which split into a bi-polar state featuring zero net polarity. This is in agreement with a general statistical mechanical statement saying that a system in a stationary state does not show an electrical dipole moment [3].

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Chiral Recognition by Dissolution Dynamic Nuclear Polarization NMR Spectroscopy

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The recognition of enantiomeric molecules by chemical analytical techniques is still a challenge. A method based on d-DNP (dissolution dynamic nuclear polarization) NMR spectroscopy to study chiral recognition was described for the first time [1]. DNP allows NMR sensitivity to be boosted by several orders of magnitude, overcoming one of the main limitations of NMR spectroscopy [2]. A method integrating d-DNP and ¹³C NMR-aided enantiodifferentiation using chiral solvating agents (CSA) was developed, in which only the chiral analyte was hyperpolarized and selectively observed by NMR. The described method enhances the sensitivity of the conventional NMR-based procedure [3] and lightens the common problem of signal overlapping between analyte and CSA. As proof of concept, racemic metabolite ¹³C-labeled DL-methionine was enantiodifferentiated by a single-scan ¹³C NMR experiment. This method entails a step forward in the chiral recognition of small molecules by NMR spectroscopy; it opens new possibilities in situations where the sensitivity is limited, for example, when low analyte concentration is available or when measurement of an insensitive nucleus is required. The advantages and current limitations of the method, as well as future perspectives, are discussed.

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Where Chemistry Meets Art: An Exploration of Nano World through Mathematical Beading

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Polyhedra excite the imagination not only of mathematicians, engineers, architects, and artists, but also of biologists and chemists. "Molecular modelling is a constitutive, yet overlooked, element of the practice of chemistry."¹ A case in point is C₆₀ or Buckyball, where paper models played a pivotal role in elucidating the truncated icosahedral shape of C₆₀, for which Kroto, Curl, and Smalley were awarded the 1996 Nobel Prize in Chemistry. Unfortunately, some molecular structures, including fullerenes, are inaccessible with standard molecular modeling kits due, in part, to the large number of atoms involved. In this poster, a simple method to construct molecular models for arbitrary fullerenes, nanotori, high-genus fullerenes, helically coiled carbon nanotubes, carbon torus knots, and carbon schwarzites using beads is described. 2–4 in a short amount of time, students of all ages can create a fullerene museum on their desk. Bead models of C₆₀ and C₇₀ constructed from 90 and 105 beads and single nylon fishing threads are shown in the following figure, respectively. In an over-simplified view, bead models of fullerenes represent the electron-pair domain model for trivalent systems where each bead represents the electron density of a carbon-carbon bond in the fullerene. Owing to the similarity between microscopic valence shell electron pair repulsion and macroscopic mechanical hard-sphere interactions in the trivalent beaded models, the shape of a bead model is similar to the true molecular structure of the corresponding fullerene. In addition to trivalent graphitic structures, other successful applications of mathematical beading to molecular physical modeling include valence sphere models of simple organic molecules, extended metal atom chains, polyhedral models of inorganic structures, Mackay's polyhedra, diamond, lonsdaleite, and various tetravalent zeolites.

Using the Continuous Shape and Symmetry Measures to Correlate Atomic Structure and Chemical Properties

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In the field of structural chemistry, many geometrical and structural measures of molecules, clusters or crystals have been largely used to correlate them with physical or chemical properties. The main advantage of these correlations is the fact that no information about the electronic structure should be known, since just topological measures are considered. Considering shape or symmetry as a continuous real value property of a given topological structure instead of a binary property, many different shape and symmetry measures have been proposed. In this talk the Continuous Shape Measures (CShM) and the Continuous Symmetry Measures (CSM) and some of their applications in structural chemistry will be introduced. Although its apparent simplicity, the structural analysis of the atomic positions by means of these shape or symmetry measures have demonstrated to be a useful tool for the structure-property correlation analysis.

The Superrotor Model for the Rovibrational Motion of CH_5^+ , an Extremely Flexible Molecule

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We discuss here the low-energy rotation-vibration problem in CH_5^+ , an extremely flexible molecule lacking a well-defined structure. Using $\text{SO}(5)$ symmetry we determine zeroth order energies, and complete nuclear permutation S_5 symmetries, using a five-dimensional model involving rotation and two vibrations (which one might imagine as internal rotations of a 2-proton-moiety relative to a 3-proton-moiety). These two vibrations are presumed to be unhindered by the molecular potential function and their analytical form is not determined. The other ten vibrational degrees of freedom are presumed to be “rigid” (or averaged over). The general energy expression for this “rigid superrotor” is relatively simple and contains one parameter only, the rotational constant B , together with two non-negative integers defining the irreducible representations of $\text{SO}(5)$. The superrotor predictions agree favourably with the available experimental data.

High Symmetry of Fluoro- and Oxofluoroelpasolites as a Consequence of Dynamic Orientational Disorder

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There is a large family of A_2BMX_6 compounds (A, B = monovalent cations or ammonium; M = metal; X = O, F) with an elpasolite structure derived from a perovskite superstructure with doubled cell parameter. Named after the mineral K_2NaAlF_6 , elpasolite compounds are cubic face-centered with $Fm\bar{3}m$ space group ($Z = 4$). We found new crystallographic features of this structure associated with the disordering of both anionic and cationic positions, especially in the case of ammonium fluoro- and oxofluorometallates. The disorder in these compounds has a dynamic nature. Upon cooling, they undergo phase transitions of the order–disorder type with a rather large value of entropy change. It is virtually impossible to differentiate oxygen and fluorine atoms by X-ray diffraction in disordered structures. We found that it became possible in the case of dynamically disordered oxide fluoride polyhedra. During such dynamics, the central atom is shifted towards the edge, face, or apex of the octahedron, giving its disordering on the cuboctahedron, cube, or octahedron, respectively. Such a displacement enables one to identify the O and F atoms owing to the inherent differences between M–O and M–F bondings and determine the real polyhedral geometry.

Effect of Bond Tangency/Gap on the Crystallization of Athermal Polymer Packings

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We present results from extensive Monte Carlo simulations on dense and nearly-jammed packings of chains of hard spheres of uniform size [1]. Local environment and similarity to specific crystal structures are gauged through the crystallographic element norm (CCE) metric [2]. We study the role of bond constraints on the packing behavior and structural characteristics of polymer assemblies: by increasing the bond tolerance (bond gaps), we observe accelerated crystal nucleation and growth which in turn lead to a wealth of ordered morphologies [3]. In their majority, crystals structures with bond gaps are significantly different from the random hexagonal close packing which prevails in the strict tangent limit [4–6]. In general, bond tangency shifts the occurrence of the phase transition to higher packing densities compared to monomers [7] and to chains with bond gaps. Based on these findings, by using simple geometric arguments, we explain the role of rigid and flexible constraints in the packing behavior (crystal nucleation and growth) of general atomic and particulate systems.

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Abstracts

Session 4: Mathematics, Computer Science and Symmetry

Session Chair – Sergei D. Odintsov

Nonlinear Aggregation–Diffusion Equations: Radial Symmetry and Long Time Asymptotics

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One of the archetypical aggregation–diffusion models is the so-called classical parabolic–elliptic Patlak–Keller–Segel (PKS) model. This model was classically introduced as the simplest description for chemotactic bacteria movement in which the tendency of linear diffusion to spread fights the attraction due to the logarithmic kernel interaction in two dimensions. For this model, there is a well-defined critical mass. In fact, here, a clear dichotomy arises: if the total mass of the system is less than the critical mass, then the long time asymptotics are described by a self-similar solution, while for a mass larger than the critical one, there is finite time blow-up. In this talk, we will show some recent results concerning the symmetry of the stationary states for a variant of the PKS model with a nonlinear diffusion. In particular, in the bidimensional case ($d = 2$), we will show that there exists a unique stationary state for the model and it coincides, according to one of the main results in the joint works with J.A. Carrillo, D. Castorina, S. Hittmeir and Y. Yao, with the global minimizer of the free energy functional associated to the model. Just in the case $d = 2$, we will also show how such steady state coincides with the asymptotic profile of the model. Finally, we will also discuss some recent results concerning a modification of the previous model, when the aggregation kernel is more singular than the Newtonian one (e.g., the Riesz kernel). In particular, all stationary states of the model are shown to be radially symmetric decreasing and global minimizers of the associated free energy are compactly supported, uniformly bounded, Hölder regular, and smooth inside their support. These last results are objects of a joint work with J.A. Carrillo, F. Hoffmann and E. Mainini.

Lie and Conditional Symmetry of Nonlinear Boundary Value Problems: Definitions, Algorithms and Applications

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Nowadays Lie and conditional symmetries are widely applied to study nonlinear partial differential equations (including multidimensional PDEs), notably for their reductions to ordinary differential equations and constructing exact solutions. There are a huge number of papers and many excellent books devoted to such applications. Over recent decades, other symmetry methods, which are based on the classical Lie method, were also derived and applied for solving nonlinear PDEs. On the other hand, one may note that the symmetry-based methods were not widely used for solving boundary-value problems (BVPs).

In our recent papers [1,2], a new definition of Lie and conditional invariance of BVPs with a wide range of boundary conditions (including those at infinity and moving surfaces) was formulated and an algorithm for finding such symmetries for the given class of BVPs was worked out. The definition and algorithm were applied to some classes of nonlinear (including multidimensional) BVPs arising in physical and biological applications in order to show their efficiency. As a result, Lie and conditional symmetries for these BVPs were completely described, reductions to BVPs of lower dimensionality were constructed and examples of exact solutions with physical/biological meaning were found. The talk is based on the results obtained in [3] and some unpublished results.

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Obvious and Hidden Symmetries of Mathematical Objects

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One of the core concepts essential to understanding natural phenomena and the dynamics of social systems is the concept of “relation”. Social and interconnection networks, traffic systems, chemical structures, etc. can be expressed as relational structures. Furthermore, scientists rely on relational structures with high levels of symmetry because of their optimal behavior and high performance. A mathematical model capturing the essence of this situation is a graph exhibiting a high level of symmetry. The underlying mathematical discipline is algebraic graph theory involving a wide range of methods from combinatorics, algebra, algorithms, geometry, topology, etc. While some symmetries are obvious, certain additional symmetries remain hidden or difficult to grasp. Knowing the full (or as near as possible) set of symmetries of an object is important because it provides the most complete description of that object’s structure.

This brings us to the crucial question: given a graph or more general a discrete mathematical object, are there any symmetries beyond the obvious ones, and, if yes, how can one determine the full set? In this talk I will present some recent developments with regards to this question together with some applications within mathematics as well as other scientific disciplines.

Symmetry Analysis of the Geodesic Equations on Lie Groups

Ryad Ghanam

Virginia Commonwealth University in Qatar, Ar-Rayyan, Qatar

We consider the geodesic equation of the canonical connection on Lie groups. We analyze the symmetry Lie algebra of the geodesics in dimensions two and three.

On Conservation Laws of Generalized KP and Boussinesq Equations in Two Dimensions

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Nonlinear generalizations of integrable equations in one-dimension, such as the KdV and Boussinesq equations with p -power nonlinearities, arise in many physical applications and are interesting in analysis due to their critical behaviour. In this talk, we study analogous nonlinear generalizations of the integrable KP equation and the 2D Boussinesq equation. We give a complete classification of low-order conservation laws and Lie symmetries for these two-dimensional equations with p -power nonlinearities. We also consider exact solutions obtained by symmetry reduction.

A Geometric View on the Symmetries of Differential Equations

Andronikos Paliathanasis

Austral University of Chile, Valdivia, Chile

We study the Lie and Noether point symmetries of a class of systems of second-order differential equations with n independent and m dependent variables ($n \times m$ systems). We solve the symmetry conditions in a geometric way and determine the general form of the symmetry vector and of the Noetherian conservation laws. We find geometric criteria for the existence and the derivation of the symmetries. Specifically we prove that the point symmetries are generated by the collineations of two (pseudo)metrics, which are defined in the spaces of independent and dependent variables. Applications in systems of physical interests are presented.

Lie Group Analysis of a Coupled (2 + 1)-Dimensional Hyperbolic System

Chaudry Khalique

North-West University, Kirkland, WA, USA

In this talk we perform Lie symmetry analysis and Noether symmetry classification of a coupled (2 + 1)-dimensional hyperbolic system. Moreover, conservation laws for several cases which admit Noether point symmetries are established for the underlying system.

Generalization of Noether's Conservation Law Theorem to Non-Variational Differential Equations

Stephen Anco

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Noether's theorem provides a systematic method to obtain conservation laws (conserved integrals) for differential equations but it requires an equation to have a variational (Lagrangian) formulation. In a series of publications, a generalization of Noether's theorem has been developed using the concept of adjoint-symmetries. This generalization applies to all differential equations, without requiring that a variational formulation exists, and is algorithmic in the same sense as Lie's method for finding symmetries of differential equations. The main steps in the generalization will be outlined and examples of finding conservation laws for non-variational differential equations will be illustrated.

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GraphDraw—A Tool for the Representation of Graphs Using Inherent Symmetry

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When drawing small graphs (with up to five or six vertices) we can use their underlying symmetry to represent them in a clear and natural way. For example, to draw a graph G with vertex set $V = \{0,1,2,3\}$ and edge set $E = \{(0,1), (1,2), (2,3), (3,0)\}$ it would be natural to use a square, or if $V = \{0,1,2,3,4\}$ and $E = \{(0,2), (0,3), (1,3), (1,4), (2,4)\}$ we might use a star to represent G . Even if the vertex labels were permuted, it would not be difficult to uncover the underlying shape. As the number of vertices increases, it becomes impossible to manually choose a suitable and informative representation, i.e., to choose where on the plane to place each of the vertices in order to produce a clear graph, rather than just a confusing mess. Existing graph drawing applications (like yEd) require the user to decide where to place the vertices.

In this paper, we present a tool—GraphDraw—which uses the underlying automorphism group of a graph ($A(G)$) to create graphs from an initial index array representation of G . Cycles in the generators of $A(G)$ are used to place the vertices in such a way as to exploit the underlying symmetry in the drawing, thus producing a clearer and more intuitive representation. Parameter selection allows the user to choose from a range of representations and to optimise the graphs in terms of edge crossings or total edge length. We give a description of the tool and present a suite of example graphs, illustrating the effect of different parameter selections.

Construction of Symmetric Determinantal Representations of Hyperbolic Forms

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Let A be an n -by- n matrix. The determinantal ternary form associated to A , defined by $F(t,x,y;A) = \det(tI + xH + yK)$, is hyperbolic with respect to $(1,0,0)$, where $H = (A + A^*)/2$ and $K = (A - A^*)/(2i)$. Kippenhahn (1951) characterized the numerical range of a matrix A as the convex hull of the real affine part of the dual curve of the curve $F(t,x,y;A) = 0$. The Fiedler–Lax conjecture has recently been proved by Helton and Vinnikov (2007) which confirms that every hyperbolic ternary form admits a symmetric determinantal representation. In other words, for any real hyperbolic ternary form $F(t,x,y)$, there exist real symmetric matrices H and K such that $F(t,x,y) = F(t,x,y;H + iK)$. We construct real symmetric matrices for the determinantal representations of some hyperbolic ternary forms and the orbits of a point mass under central forces.

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On a Class of Weighted Isoperimetric Inequalities

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We study a class of isoperimetric problems on \mathbb{R}^N with respect to weights that are powers of the distance to the origin. We consider different weights in the volume and in the perimeter. We investigate cases in which, among all smooth sets Ω in \mathbb{R}^N with fixed weighted measure, the ball centered at the origin has minimum weighted perimeter. The results also imply a weighted Pólya–Szegő principle. In turn, we establish radially of optimizers in some Caffarelli–Kohn–Nirenberg inequalities, and we obtain sharp bounds for eigenvalues of some nonlinear problems.

Projections of Periodic Functions and Mode Interactions

Juliane Fonseca Oliveira

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This work is related to the study of pattern formation in symmetric physical systems. Our purpose is to discuss a possible model, namely the projection model, to explain the appearance and evolution of regular patterns in symmetric systems of equations. Results found in Crystallography and Equivariant Bifurcation Theory are used extensively in our work. In particular, we provide a formalism of how the model of projection can be used and interpreted to understand experiments of reaction-diffusion systems. In order to do it, we study solutions of bifurcation problems with periodic boundary conditions, with periods in an $n + 1$ -dimensional lattice and their projection into n -dimensional space through integration of the last variable. We show that generically the projection of a single mode solution is a mode interaction. This can be applied to the study of black-eye patterns.

Bismut's Way of the Malliavin Calculus for Large Order Generator on a Lie Group

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We give an adaptation of the Malliavin Calculus of Bismut type in order to show that an operator of big order on a compact connected Lie group is such that the associated semi-group has a heat-kernel. By mixing Wentzel-Freidlin estimates which were established by us for non-markovian semi-groups and the Malliavin Calculus, we deduce logarithmic estimates of the heat-kernel in small time. We use deeply the symmetry of the group in the proof of the theorem.

Symmetry, Entropy, and Computer Science

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We analyze Symmetry, Entropy, and therefore, Uncertainty Measures, to obtain new ways to model adequate conditions, constructed from vague pieces of information. Over time, it was adapted by Shannon, thus creating the Information Theory. However, the Hungarian mathematician Rényi shows that there exist different and valid entropy measures, according to the need of applications. So, it will be very necessary to clarify the different types of measures, and their mutual relationships.

The contributions of Kolmogorov to this mathematical theory provide great advances to the Shannon formulations, proposing a new complexity theory, now translated to Computation. According to such theory, the complexity of a message is given by the size of the program necessary to make possible the reception of such a message. From these ideas, he analyzes the entropy of literary texts. Such entropy appears as a function of the semantic capacity of the texts, depending on factors as their extension and also the flexibility of the corresponding language.

Wiener, founder of Cybernetics, also proposed a similar vision of such a problem in 1948. However, the approach used by Shannon differs from that of Wiener in the nature of the transmitted signal and in the type of decision made at the receiver. In the Shannon model, messages are firstly encoded, and then transmitted, whereas in the Wiener model the signal is communicated directly through the channel without it needing to be encoded.

On Classification of Symmetry Reductions for Partial Differential Equations

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Symmetry reduction is one of the most powerful tools for investigation of partial differential equations. In particular, for this purpose, we can use a classical Lie method. To try to explain some of the differences in the properties of the reduced equations, we suggest to investigate the relationship between the structural properties of nonconjugate subalgebras of the Lie algebras of the symmetry groups of the equations under consideration and the properties of the reduced equations corresponding to them. In our talk, we plan to present some of the results concerning the relationship between the structural properties of low-dimensional ($\dim L \leq 3$) nonconjugate subalgebras of the Lie algebra of the generalized Poincaré group $P(1,4)$ and the types of symmetry reduction for some $P(1,4)$ -invariant equations in the space $M(1,3) \times R(u)$.

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Secure SCADA-IoT Platform for Industrial Automation and Control: A Collaborative-Communication Designed Model

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This paper discusses the new auspicious trends of internet of things (IoT) and its advanced developments in various sectors of today's IT arena, including for industrial sectors. Each object acts as a communication node (or entity) that is able to communicate with other nodes, and corresponding information could be accessed and controlled, via several of today's commonly used electronic devices such as laptops and cellular devices, etc., through an IoT-designed platform. Moreover, in industrial automation sectors, the employment of IoT is very advantageous, in terms of remote communication support; low-cost operations and maintenance; and autonomous collaborations among remote networked field devices, etc. The facility of autonomous collaborations provisioned by IoT, in the context of a supervisory control and data acquisition (SCADA) system as part of an industrial control system, somehow exists in a distributed network protocol (DNP3) during automation and controls. Therefore, the current study takes the step to model a new IoT framework for a SCADA system, which will be efficient at facilitating industrial automation through the collaborative DNP3-Modbus acquisitions and automation, called the SCADA-IoT system. An IoT gateway is employed and configured that supports for both SCADA protocols, such as DNP3 and Modbus and is efficient at communicating, from networked field devices, with inter-processing from both. In the overall SCADA-IoT design, the transmission is carried from an enormous amount of sensors and/or field devices, employing proprietary and non-proprietary protocols; further, sent information is analyzed via big data, stored in a cloud center, monitored and controlled over a SCADA-IoT supportive platform. At the same time, information security (IS) is a big associated challenge and one of the main contributions of this study. Thus, this study also analyzed the potential security mechanisms for securing SCADA-IoT and found cryptography to be a noteworthy security solution, based on the proposed system requirements and its communication demands.

This work was supported by Institute for Information & communications Technology Promotion (IITP) grant funded by the Korea government (MSIT) (No. 2017-0-00756, Development of interoperability and management technology of IoT system with heterogeneous ID mechanism).

Abstracts

Poster Exhibition

1 Dynamic Feedback Balancing Algorithm for Data Management of an Integrated Sensing Network

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With the development of an integrated sensing network (ISN) which supports generalized mobility and will allow consistent and ubiquitous provision of sensed data services to any object, anywhere and at any time, it is necessary to implement data management with high efficiency for data accessing and processing so that it can improve the quality of data service. In this paper, the dynamic feedback balancing algorithm for static initialization and dynamic data allocation is proposed, which realizes real-time data monitoring, query and real-time or stationary synchronization in an ISN. In order to implement data balance, we make sure of the data service levels and distinguish between heavy nodes and light nodes with the dynamic information reported by each node in an ISN, then transfer the data from heavy nodes to light nodes. Comparing with the consistent hash algorithm, the quality of data service provided by the proposed algorithm is improved significantly.

2 4-Hydroxyproline Containing Podands: New Chiral Catalysts of the Asymmetric Biginelli Reaction

Yulia Titova, Irina Ovchinnikova, Olga Fedorova, Gennady Rusinov, Valery Charushin

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4-Aryl substituted dihydropyrimidines (DHPMs), the products of the multicomponent Biginelli reaction, are well known as cardiotropic, hypotensive, antitumor, anti-inflammatory, antifungal and antiviral agents. Considerable attention is paid to their asymmetric synthesis due to the fact that the pharmacological activity of enantiomers of chiral DHPMs can vary considerably.

Previously, we showed the prospects of using proline derivatives as chiral catalysts in the asymmetric Biginelli reaction [1,2].

Herein, we report the synthesis of new C₂-symmetric chiral catalysts based on acyclic analogs of crown-ether (podands) and 4-hydroxyproline.

The combination of the S-shaped conformation of the polyester chain with the optically active centers of the proline fragment in C₂-symmetric organocatalysts made it possible to obtain the product of the Biginelli reaction with 68–72% ee.

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3 An Analysis of the Localized Airy–Laguerre–Gaussian Wave Packets Using Modified One-Parameter Point Symmetries

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In their treatment of the Airy–Laguerre–Gaussian equation, Zhong, Belic and Zhang constructed an alternative solution for the azimuthal case; for the Airy case, they constructed finite pulses. The third case led to the Gaussian, considered to be un-integrable by some. To circumvent the need to construct solutions, which is susceptible to errors, as opposed to quadrature, we introduce the notion of modified one-parameter point symmetries. From this, we demonstrate that there is an error in the traditional solution for linear differential equations, such as the azimuthal equation, as Zhong, Belic and Zhang suspected, and provide the exact result. A finite solution for the Airy equation follows from the inverted monomials of its determining equation. Finally, we integrate the Gaussian integral. As an application, we propose how the analysis can be extended to Newtonian gravitation, and a technology for tapping space energy.

4 Combinatoric Properties of Restriction Sites

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Endonucleases from the restriction–modification complex are known to recognise specific sites with tremendous precision. The symmetry of the site is said to allow an enzyme to recognise the pattern despite the strand. However, there are many exceptions towards non-symmetrical restriction sites, and even enzymes that are not strictly specific to only one site.

We study four- and six-nucleotide palindromes that also happened to function as restriction sites. The study revealed that not all positions in the palindrome are equally important for the enzyme while recognition—symmetry of a palindrome—is strict only in the middle of the site, whereas at the periphery it may end in a non-palindromic sequence.

Based on the duplets ‘strength’ method and editing distance algorithms, these restriction sites were compared pairwise and clusters of resembling sites were found. Due to different costs for reverse substitutions, it was possible to assume which sequence out of two was more likely the original since its conversion in another sequence costed less. The idea is to track down evolutionary modified restriction sites to those original sequences. Therefore, a phylogenetic tree was constructed using respective restrictases and their clusters obtained from the tree were used for primary pairwise comparison.

5 Enhanced and Optimal Development Contributed in Finding Unknown Sources of Interference in Wireless Communication

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Radio frequency interference has been considered a major common issue in wireless communication systems; among several other potential major issues, the emergence and massive development of Internet of things (IoT) is also considered a crucial issue as each device connected wirelessly causes enough of an increment to have destructive effects on radio-frequency interference (RFI). Thus, the identification of RFI signals and the measurement of the position from which they originated is a major challenge of today; for that reason, several inclusive deployments have been made in the literature of RFI geolocation to find the origin of RFI. Further, in this study, a standard optimal approach is defined, considering the destructive effects of RFI in wireless communication, and implemented to find the origin of RFI, i.e., the RFI location. For measurement purposes, the promising location-finding paradigms, such as the time difference of arrival and the frequency difference of arrival, are efficiently applied, computed and cross-correlated, and further optimized in searching for the actuated position of unknown interference. The measurements conducted in this study are evaluated which resulted in the relative best performance and high accuracy, to find the actual location of the interference.

This work was supported by Institute for Information & communications Technology Promotion (IITP) grant funded by the Korea government (MSIT) (No. 2017-0-00756, Development of interoperability and management technology of IoT system with heterogeneous ID mechanism).

6 Functionals of Harmonics Functions

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Let C_T^S , with $T > 0$, be the set of continuous, T -periodic functions $\mathbf{f}: \mathbb{R} \rightarrow \mathbb{R}^s$, and let $\Gamma: C_T^S \rightarrow \mathbb{R}$ be a real functional on C_T^S . If Γ is n times Fréchet differentiable on C_T^S , then it has an n -th order Taylor expansion around $\mathbf{0}$ (see e.g., [1]). Such a Taylor expansion can be obtained as the n -th order truncation of the series

$$\begin{aligned} \Gamma[\mathbf{f}] = & \sum_{n_1=0}^{\infty} \dots \sum_{n_s=0}^{\infty} \langle c_{\mathbf{n}}(t_{11}, \dots, t_{1_{n_1}}, \dots, t_{s1}, \dots, t_{s_{n_s}}) \\ & \times f_1(t_{11}) \dots f_1(t_{1_{n_1}}) \dots f_s(t_{s1}) \dots f_s(t_{s_{n_s}}) \rangle \end{aligned} \quad (1)$$

where $\mathbf{n} = (n_1, \dots, n_s)$ and we have introduced the notation

$$\langle \Omega(t_1, \dots, t_r) \rangle = \frac{1}{T^r} \int_0^T dt_1 \dots \int_0^T dt_r \Omega(t_1, \dots, t_r) \quad (2)$$

The kernels $c_{n_1, \dots, n_s}(t_{11}, \dots, t_{s_{n_s}})$ are all real, T -periodic, and symmetric in all their arguments.

In this contribution we will prove the following theorem.

Theorem 1. Let Γ be a functional with Taylor series (1), and take

$$\mathbf{f}(t) = \dot{q}_1 \cos(q_1 \omega t + \phi_1), \dots, \dot{q}_s \cos(q_s \omega t + \phi_s), \quad (3)$$

where $\mathbf{q} \equiv (q_1, \dots, q_s) \in \mathbb{R}^s$ is such that $\gcd(q_1, \dots, q_s) = 1$ and $\omega = 2\pi/T$. Then,

$$\Gamma[\mathbf{f}] = C_0(\varepsilon) + \sum_{\mathbf{x} \in S_+} \varepsilon_1^{|\mathbf{x}_1|} \dots \varepsilon_s^{|\mathbf{x}_s|} C_{\mathbf{x}}(\varepsilon) \cos(\mathbf{x} \cdot \boldsymbol{\phi} + \theta_{\mathbf{x}}(\varepsilon)) \quad (4)$$

where, $\boldsymbol{\phi} \equiv (\phi_1, \dots, \phi_s)$, $\boldsymbol{\varepsilon} \equiv (\varepsilon_1, \dots, \varepsilon_s)$, and functions $C_{\mathbf{x}}(\varepsilon)$ and $\theta_{\mathbf{x}}(\varepsilon)$ do not depend on $\boldsymbol{\phi}$ and are even in each ε_i , $i = 1, \dots, s$, for every $\mathbf{x} \in S_+$. $\mathbf{x} \in S_+$ is the set of vectors \mathbf{x} whose leftmost nonzero component is positive.

In the special case when Γ is invariant under time-shift, i.e., $\Gamma[\mathbf{f}(t + \tau)] = \Gamma[\mathbf{f}(t)]$ for all $0 < \tau < T$, we recover the results in [2]

$$\Gamma[\mathbf{f}] = C_0(\varepsilon) + \sum_{\mathbf{x} \in D_+} \varepsilon_1^{|\mathbf{x}_1|} \dots \varepsilon_s^{|\mathbf{x}_s|} C_{\mathbf{x}}(\varepsilon) \cos(\mathbf{x} \cdot \phi + \theta_{\mathbf{x}}(\varepsilon)) \quad (5)$$

where D_+ denote the set of nonzero solutions of the Diophantine equation $\mathbf{q} \cdot \mathbf{x} = q_1 x_1 + \dots + q_s x_s = 0$, whose leftmost nonzero component is positive.

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7 Generalized Circulant Matrices

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Circulant matrices have applications in signal processing, numerical calculations of Fourier transforms, as well as encryption methods. By using a coset group construction of algebras [1], we find a class of generalized circulant matrices with interesting and possibly useful properties for numerical analysis that can expand the use of simple circulants. We show the construction of generalized circulants and discuss their properties and possible applications.

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8 Improving space based snowfall rate retrievals with refined considerations of snow microstructure

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Launched in 2014 as a joint mission by the Japanese Aerospace Exploration Agency (JAXA) and the National Aeronautics and Space Administration (NASA), a key goal of the Global Precipitation Mission (GPM) is to quantify when, where, and how much it rains or snows around the world. In contrast to rainfall measurements, whereby scattering theory works considerably better with the assumption of spherically symmetric hydrometeors, snowfall retrievals are complicated by the microstructure of the snowflakes. Though symmetric in many cases, snowflakes also possess complex shapes which makes microwave scattering and related snowfall rate retrievals relatively less accurate. In this poster presentation, the present GPM retrieval algorithm is presented which is contrasted with ground measurements conducted in the OLYMPEx ground validation experiment over the Olympic Mountains in the US in the winter of 2015-16. This experiment is presented in detail and preliminary results show less than desirable accuracy when comparing GPM measurements with measured reflectivity on the ground. Given these considerations, this poster provides an overview of present approaches to improve these retrievals which include special and generalized considerations of the Rayleigh-Gans approximation. It is surmised that better considerations of snow microstructure have the potential of improving snowfall retrieval from space based sensors such as the GPM.

9 Irreversibility and Quantum Information Flow under Global & Local Gauge Symmetries

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What is the structure of general quantum processes on composite systems that respect a global or local symmetry principle? How does the irreversible use of quantum resources behave under such symmetry principles? Here we develop an information-theoretic framework to address these questions and show that every symmetric quantum process on a system has an essentially unique decomposition in terms of the flow of symmetry-breaking degrees of freedom between each subsystem and its environment. The decomposition has a natural causal structure that can be represented diagrammatically and makes explicit gauge degrees of freedom between subsystems. Our framework also provides a novel quantum information perspective on lattice gauge theories and a method to gauge general quantum processes beyond Lagrangian formulations. This procedure admits a simple resource-theoretic interpretation, and thus offers a natural context in which features such as information flow and entanglement in gauge theories could be studied. The framework also provides a flexible toolkit with which to analyse the structure of general quantum processes. As an application, we make use of a ‘polar decomposition’ for quantum processes to discuss incompatibility in the use of quantum resources and to provide a novel perspective in terms of the geometry induced on the orbit of a local process under a symmetry action.

10 Modifying Effect of Released-Active and Initial Compound Forms: The Case of Contra-Directional Regulation of Model Processes

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In recent years, there has been an increased interest in high dilutions of various substances following the discovery of the released-activity phenomenon. The phenomenon is that released-active dilutions acquire a common property—the ability to modify the initial substance both inside and outside the organism.

The mechanisms of action of high dilutions are explained in the works of V.A. Tverdislov that experimentally describe the formation of two-dimensional quasi-crystalline structures, the pronounced effects of which are attributed not to the concentration dominance of separate components in a homogenous mixture, but to the local prevalence of chirally pure polarized clusters of a dilution component in the near-surface layers.

These conditions may well be associated with distinguishing the released-active forms of investigated compounds and their subsequent functional activity.

This study presents the results of research on compounds (antibodies to interferon-gamma, diclofenac, etc.) in released-active and initial forms describing their antiviral, anti-inflammatory and other types of activity that confirm the extent of their modifying effect, which is used in clinical practice.

11 Nekhoroshev Theorem for the Toda Lattice with Dirichlet Boundary Conditions

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In this paper, we prove a Nekhoroshev theorem for the Toda lattice with Dirichlet boundary conditions, i.e., fixed ends. The Toda lattice is a special case of a Fermi–Pasta–Ulam (FPU) lattice, and in view of the unexpected recurrence phenomena observed numerically in these chains, it has been conjectured that theory of perturbed integrable systems could be applied to these lattices, especially since the Toda lattice has been shown to be a completely integrable system. Whereas various results have already been obtained for the periodic lattice, the Dirichlet lattice is more important from the point of view of applications, since the famous numerical experiments have been performed for this type of system. Mathematically, the Dirichlet lattice can be treated by exploiting symmetries of the periodic lattice. Precisely, by considering the phase space of the Dirichlet lattice as an invariant submanifold of the periodic lattice, namely the fixed point set of a certain symmetry of the periodic lattice, the results obtained for the periodic lattice can be used to obtain similar results for the Dirichlet lattice. The Nekhoroshev theorem is a perturbation theory result which does not have the probabilistic character of other results such as those of the KAM theorem.

12 Novel Symmetry and Symmetry-Breaking Induced Complexity in Cosmological Evolution

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Scale-Running of the propagator coupling-constants can induce complexity phenomena [1] involving novel symmetries and symmetry-breakings with antiscreening/screening effects. In the context of cosmological evolution, such effects can yield new insights with dark matter consequences. Starting from the nonperturbative, one-particle irreducible renormalization-group differential generator with coarse-graining transformations due to intrinsic fluctuations, explicit Lifshitz-like complexity may be demonstrated analytically for the crossover phenomena involving helically ordered states in gravitational evolution at large scales [2]. Interesting explicit examples will be described to demonstrate such phenomena. These ideas can easily be extended to a variety of dynamic and condensed matter systems.

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13 On Modified Symmetries for the Boltzmann Equation

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In this contribution, we are using Lie group theoretical methods and a generalized modified symmetry for solving a second-order partial differential equation. In particular, we determine the new Lie point symmetries using modified symmetries for the Boltzmann equation and deduce the corresponding group-invariant solutions.

14 Potassium Channel Gating Mechanism Modeled by Harmonic Oscillators

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Potassium channels are integral membrane proteins that selectively transport K^+ ions across cell membranes. They function through a pair of gates, which work in tandem to allow the passage of the ions through the channel pore in a coupled system, to which I refer here as the “gate linker”. To closely examine the role of the gate linker in channel functioning, I mutated the amino acids in the cDNA of this region, either alone or together with amino acids of adjacent regions. The functional effects of these mutations suggest that the gate linker functions analogously to a triad of coiled springs arranged in series. Accordingly, I constructed a physical model of harmonic oscillators and analyzed it mechanically and mathematically. The operation of this model indeed corresponds to the phenomena observed in the mutations study. The harmonic oscillator model shows that the strength of the gate linker is crucial for gate coupling and may account for the velocity, direction, and efficiency of ion transfer through the channel. Such a physical perspective of the gating process suggests new lines of investigation regarding the coupling mode of potassium channels and may help to explain the importance of the gate linker to channel function.

15 Realization of a Torus as Generic Lattice Structure in All Three Dimensions from Lax Pairing Transformation of the Conventional Minkowski Spacetime

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The Hubbard model and its extended versions which have important applications in condensed matter physics depend on the lattice structure. This often leads to edge effect making some lattice sites not to be on equal footing with the others and finite size effect resulting from applying the model to small lattice sizes. It is proposed here that transforming these lattices in all three dimensions into a torus will help to resolve the edge effect as well as aid in resolving of the finite size effects as they become scale invariant. Our approach is to use the knowledge that since in the past the Lie groups, Lie algebras and some of their applications were mainly concerned with the space-time of special relativity with metric $(+++ -)$ with respect to the real contravariant bases (x,y,z,ct) , it can be shown that a Minkowski spacetime with the inclusion of ellipsoidal and toroidal deformations of a sphere in Sophus Lie's original group of continuous transformation of a sphere can lead through the application of the *principle of duality* between points, lines and planes in 3-dimensional projective geometry to explicit realization of generalizations of the conventional Lie algebra as deformation of the conventional Minkowski spacetime. Thus by considering in geometric algebra terms, we use the Lax pairing with appropriate symmetric and nonsymmetric parameters to transform the quadratic form in 4-dimensional space of the conventional Minkowski space-time into a "unified field" tensor, with a torus as the "generic" geometric structure. We then demonstrate how to obtain the variational ground state energy from generic lattice structures for the Hubbard model and its versions important for strong correlations in condensed matter physics.

16 Spontaneous Symmetry Breaking Related to the Onset of Instabilities in Low-Temperature Plasma

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The study of plasma instabilities is still a hot topic because of their consequences for the development of applications. Here, we report on the experimental investigation and theoretical modeling of the onset of low-temperature plasma instability, as a consequence of the nonlinear dynamics of some complex space charge structures. The obtained results show that the onset of the instability takes place by spontaneous symmetry breaking, which involves transitions between measurable Lie groups. In this situation, a parallel transport in the Levi–Civita sense can be defined, preserving only the direction of the vector and not its modulus. This situation was explained by the phase correlation of the plasma particles.

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17 Suppression of Magnetization Tunneling in Rare-Earth Atoms on Surfaces of Various Symmetry

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In the classical world, it is easy to store a bit of information. One needs a bistable system with a high enough barrier between the two ground states. Such a system is exemplified by a magnetic cluster with uniaxial anisotropy, so that the direction of the magnetic moment encodes the information.

On the nanoscale, a high barrier is not enough. Fourteen years ago, P. Gambardella et al. found that single Co atoms on Pt(111) have high enough anisotropy energy to have stable magnetization at low temperatures [1]. Later investigations [2,3] showed, however, that the magnetization of those atoms and similar systems switches on nanosecond timescales. Interaction with the electron bath of the substrate allows “magnetization tunnelling”, where the system switches between two ground states aided by elastic electron scattering.

The probability of such switching depends on the symmetry of the ground state wavefunctions, which in turn is determined by the symmetry of the adsorption site and the total angular momentum of the magnetic atom. An appropriate combination of these symmetries leads to a first-order suppression of the tunneling process, stabilizing the magnetic state.

We classify the possible symmetry combinations and analyse recent experimental reports of magnetically stable rare-earth atoms in light of this theory.

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18 Symmetric Maps on the Plane: Mathematical Properties and Numerical Experiments

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We consider a class of discrete time two-dimensional dynamic systems that are symmetric, i.e., $(x', y') = T(x, y)$ such that $ToS = SoT$, where $S: (x, y) \rightarrow (y, x)$ is the reflection through the diagonal. Symmetry implies some properties in terms of qualitative and quantitative dynamics, for instance there exist synchronized trajectories, while fixed points and other invariant sets are symmetric w.r.t. the main diagonal or they are invariant as well. Synchronization may also emerge. After showing some of the main features related to this kind of systems (such as attractors and their basins), some numerical examples obtained using software MatLab will be presented and the related algorithms will be discussed.

19 Symmetry Analysis of the Hamilton-Jacobi-Bellman Equation Arising in Financial Mathematics

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We outline symmetry analysis on the Hamilton-Bellman-Jacobi equation presented by Heath in [1] as an equation for mean-variance hedging and analysed by Leach in [2] using classical symmetry analysis. We further apply modified symmetry analysis on this equation and compare our analytic results with numerical solutions. We do this by introducing a new infinitesimal parameter into the group generators [3]. This helps us solve the unintegrable solutions usually appearing in invariant solutions.

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20 The Symmetric and Antisymmetric Eigenvalue Problem for Electromagnetic Equilateral Triangular Waveguides via Plane Wave Reconstruction

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A plane wave reconstruction technique is presented for the solution of Helmholtz's equation governing wave propagation in equilateral triangular electromagnetic waveguides in order to aid in the classification of symmetric and antisymmetric modes as well as to resolve the problem of excitation of triangular patch antennas. The case of transverse magnetic (TM) modes of a patch antenna with magnetic wall boundary conditions is discussed as representative of problems with Neumann boundary conditions. The technique sheds light on how these antennas may be excited and is applicable to problems with Dirichlet boundary conditions as well as to other triangular shapes including the right isosceles triangle, the 30° – 90° – 60° , the 30° – 120° – 30° , and the 15° – 90° – 75° triangles. The solutions are classified into two major categories: triaxially symmetric with eigenvalues that are harmonic multiples of $4m\pi/(a)$, and solutions that are symmetric or antisymmetric with respect to only one median of the equilateral triangle. The triaxially symmetric solution is a result of sources at the centroid sending out waves perpendicular to the sides of the triangle in a Y configuration, while the latter are a result of two sets of waves traveling in opposite directions (clockwise and anticlockwise) parallel to the sides of the triangle in a Δ configuration. The solutions symmetric/antisymmetric with respect to only one median divide into two groups: one group with eigenvalues that are harmonic multiples of $4m\pi/(3a)$ and another group whose eigenvalues are not harmonic multiples of one another (solutions become triaxially symmetric/antisymmetric if m is a multiple of 3). These cases will be discussed in light of Lamé's solution [1–3] as detailed by McCartin in a series of papers [4,5].

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