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Preface

The International Conference "Mathematical Modeling and Computational Physics 2024" (MMCP 2024) is jointly organized by the Joint Institute for Nuclear Research (JINR), Dubna, Russia, the A. I. Alikhanian National Science Laboratory of Yerevan Physics Institute, Armenia, the Yerevan State University, Armenia, and Institute for Informatics and Automation Problems of the National Academy of Sciences of the Republic of Armenia, Yerevan, Armenia.

This year the MMCP conference is dedicated to the 80th anniversary of the birth of Academician Alexei Norairovich Sissakian (October 14, 1944 – May 1, 2010), an outstanding scientist in the field of elementary particle physics, theoretical and mathematical physics, director of the Joint Institute for Nuclear Research (2006 – 2010).

The MMCP 2024 follows the rich traditions of the previous conferences on mathematical modeling, numerical methods and computational physics that have been held in Dubna, Russia, since 1964, and, alternatively in Slovakia and Dubna since 2006, e.g., Computational Modeling and Computing in Physics 1996, Modern Trends in Computational Physics 1998, V. International Congress on Mathematical Modeling 2002, Mathematical Modeling and Computational Physics 2006, 2009, 2011, 2013, 2015, 2017, and 2019.

The Conference includes two kinds of contributions: invited plenary lectures, by invitation of the Organizing Committee, and original contributions, proposed by the participants and accepted by the Organizing Committee.

We welcome all the participants of the Conference, both the scientists having contributions included in the Book of Abstracts, and those who simply attend the Conference since they have found it attractive enough.

Conference Chairmen,
V. V. Korenkov (JINR Dubna)
G. Karyan (AANL Yerevan)

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Invited Plenary Lectures

Artificial Intelligence Driven Automatic Adaptive Quadrature

Gheorghe Adam[1,2] and Sanda Adam[1,2]

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The automatic adaptive quadrature (AAQ) rests on the additivity property of the Riemann integral. This feature asks for the use of an up-down approach to the derivation of the numerical solution of interest.

Therefore, the most appropriate method for the implementation of AAQ numerical algorithms should be based on the use of decision tree techniques. Since the tree nodes denote integration subranges, we deal with subrange decision tree (SDT) techniques.

Within the standard AAQ approach to the numerical solution of the Riemann integrals, provided by the QUADPACK package [1], SDT like decisions were implemented under heavy use of rules of thumb, mainly motivated by the scarcity of the available hardware resources. As a consequence, while the resulting code implementations showed the highest efficiency reported up to date [2], the existing code limitations enabled the solution of selected classes of Riemann integrals only. In particular, the QUADPACK AAQ codes cannot tackle large scale numerical experiments involving Riemann integrals characterized by properties that get defined during the numerical experiment only.

The decision tree analysis has become part of the artificial intelligence (AI) approach to the solution of the most intricate decision problems [3].

Based on our latest AAQ problem statements ([4], [5] and references therein), the present report makes a significant leap forward toward the development of flexible SDT techniques as AI tools for the numerical solution of Riemann integrals. Within this AI-AAQ method, the SDT decisions are prioritized at three distinct levels denoting respectively the *code robustness* (highest priority, which automatically checks and enforces the problem consistency), *code reliability* (next priority, enforcing truly computed output), and *code efficiency* (last but not least priority, able to exploit the existing hardware features to accelerate computations).

This flexible decision chain shows the features of an artificial intelligence approach able to solve all the distinct Riemann integrals, within precisely defined parameters following from the adopted floating point precision of the computations.

Acknowledgement. Work supported within the JINR project 06-6-1119-2-2024/2026.

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Dissipative Search of Unstructured Database

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The search of an unstructured database amounts to finding one element having a certain property out of N elements. The classical search with an oracle checking one element at a time requires on average $N/2$ steps. The Grover algorithm for the quantum search, and its unitary Hamiltonian evolution analogue, accomplish the search asymptotically optimally in $\mathcal{O}(\sqrt{N})$ time steps. We reformulate the search problem as a dissipative, incoherent Markov process acting on an N-level system weakly coupled to a thermal bath. Assuming that the energy levels of the system represent the database elements, we show that, with a proper choice of the spectrum and long-range but bounded transition rates between the energy levels, the system relaxes to the ground state, corresponding to the sought element, in time $\mathcal{O}(\ln N)$ [1].

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SANC for Higher Calculation: Application to e^+e^--Factories, $\gamma\gamma$-Colliders, $pp(p\bar{p})$-Accelerators

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The current state of the SANC (Support of Analytic and Numerical calculations for Colliders) computer system is under review. This system is developed for precise calculations of event distributions related to various decay processes and high-energy elementary particle interactions, specifically within the Next-to-Leading Order framework of the Standard Model. Currently, SANC implements a semi-automated calculation workflow that progresses from the SM Lagrangian to Monte Carlo event simulations. An overview of `SANC` tools, including `MCSANC`, `ReneSANCe` and `SANCphot`, has been performed.

Acknowledgement. This work was supported by the Russian Science Foundation, project No. 22-12-00021.

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Armenian National Supercomputing Center: Bridging Science and Technology through High-Performance Computing

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Supercomputing allows researchers, industry, and stakeholders to use computational models to simulate challenging or impossible conditions to replicate and measure in a laboratory setting [1]. National and regional supercomputing centers provide the computational power to tackle complex problems across various disciplines that require new programming paradigms and runtimes [2]. The paper provides an overview of the Aznavour supercomputer, as a national digital infrastructure leveraging existing high-performance computing Big Data infrastructures [3]. Its establishment accelerates scientific discovery and positions Armenia as a critical player in the global tech ecosystem.

The paper presents the prerequisites for establishing the supercomputing center, tracing its evolution from cluster [4] computing to cloud computing [5]. It also delves into the Aznavour supercomputer's architecture, detailing its software and hardware components, and highlights the various scientific and engineering communities driving demand for these high-performance computing resources.

Acknowledgement. The Aznavour supercomputer was established through the collaboration and support of the Armenian Government, the World Bank, the National Academy of Sciences of the Republic of Armenia (NAS RA), the Institute for Informatics and Automation Problems of NAS RA, the Toulouse Institute of Computer Science Research, the University of Paul Sabatier, Atos, and the Enterprise Incubator Foundation.

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The Crisis of Fundamental Computer Science and the Need to Create its New Mathematical Foundation

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Recently, the discrepancy between new components of computing systems and old programming and computing paradigms has become increasingly noticeable. Despite the launch of an increasing number of petaflop systems and the creation of exaflop systems, real performance on real tasks remains at the teraflop level. The same situation applies to data processing. With a naive view of Big Data, leading to the MapReduce paradigm, when for extremely large volumes of data they switch to programs like Hadup, transactions take more than 400–600 cycles of computing systems, which negates all the successes in the field of communications and new processor architectures. It seems to us that these problems lie in the outdated mathematical foundations of algorithmic paradigms, and more specifically, in the blurred connections between the implementation of continuous and discrete mathematical models.

To explain this, consider a typical example of solving a scientific or engineering problem, the mathematical model of which is described by a system of partial differential equations. To implement it on a computer, we must implement a discrete model (using the grid method, variational methods, expansion over a suitable basis, etc.). From a mathematical point of view, these are different models that are close only for completely continuous operators. However, modern nonlinear problems do not lead to such operators! The situation is especially dramatic for fully integrated systems. The original system has an infinite number of conservation laws, the solution exists and is stable. When the system is discretized, laws are violated, and during numerical implementation various kinds of artifacts arise, the suppression of which requires the introduction of fictitious boundary conditions, sources, transition to implicit schemes, etc. And this significantly lengthens the calculation time, leads to instabilities and strong connections between computational threads. As a result, none of the "Great Challenge" problems announced in the early 90s have yet been satisfactorily resolved.

These problems are partially resolved in the Natural Parallelization Paradigm, proposed for calculations in 1988, and for data processing in 2004. Its idea is simple and goes back to the theory of dynamical systems – if, after the transition to a discrete representation in the problem

matrix there are many large non-diagonal elements, a replacement of coordinates is required, which quasi-diagonalizes the matrix. This approach has proven to be very effective, but it has a significant difficulty. For each type of problem, the choice of coordinates is different, and its implementation requires quite a lot of work. Therefore, the question of creating a universal method for transforming coordinates in different tasks is very relevant, since without this, the use of such a paradigm in real systems is very problematic. Unfortunately, this issue is not resolved within the framework of standard approaches in the theory of dynamical systems.

It seems to us that the mathematical approach developed in the theory of gauge fields is very useful for creating such a method. It is called the method of functional integrals or path integrals. Such approaches were outlined at the beginning of the last century (Frechet, Levy, etc.). Since almost all of these mathematicians died in the First World War, it was forgotten for 30 years. The next important step was taken by Dirac, who solved the problem of constructing propagators for operator equations at short times (1936). Empirical justification for the use of path integrals for solving partial differential equations was given by Feynman in his Nobel speech. His approach, similar to Riemann's method in mathematical analysis, unfortunately did not allow for mathematical justification and led to divergences. Nevertheless, it turned out to be a very convenient tool for constructing perturbation theory and introducing collective variables. The idea of separating divergences and isolating delta functions associated with conservation laws was expressed in the pioneering work of Faddeev and Popov and strictly substantiated by Vasiliev. Somewhat later, three approaches appeared to strictly substantiate such integrals (Alimov, Bogdanov, Slavnov) in the spirit of the usual Lebesgue integral or even Lebesgue-Stieltjes. It is important that they were all constructive, i.e., allowed direct calculation of such integrals.

For application in fundamental computer science, the most constructive method seems to be the path integral reduction method, which reduces it through special canonical transformations to a Lebesgue integral of dimension equal to the dimension of the problem and the solution of first-order differential equations at each point of the integrand. A large number of fundamental and applied problems in physics have been approximately solved using these methods, but in the original formulation the method is accurate.

Lattice Study of Rotating QCD Properties

Victor V. Braguta

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In this report the influence of relativistic rotation on QCD properties will be considered. I am going to review the results which were obtained within lattice simulation of QCD. It has become commonplace to perform such studies in the reference frame rotating with the system under investigation. In this case there appears gravitational field and the problem is reduced to the study of QCD in external gravitational field. Within the report the following topics will be reviewed. The influence of relativistic rotation to QCD critical temperatures. Equation of state of rotating QCD and the moment of inertia of quark-gluon plasma. Inhomogeneous phase transitions in rotating quark-gluon plasma.

Modeling the Complexity of DNA Damage and Cell Survival Following the Exposure of Ionizing Radiations with Different Characteristics

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Research on the biological effects of ionising radiation is an actively developing field of interdisciplinary research having applications in many fields including radiation protection, nuclear medicine, and deep space exploration. In this report a review of biophysical models hierarchy to study early radiation effects in DNA and cells that are not available experimentally, and study on the problem of relative biological effectiveness of different types of ionizing radiation is presented.

In recent years a hierarchy of biophysical models incorporating physical, chemical, and biological events in a cell has been actively developed [1]. The key element of this hierarchy is the description of initial physical interaction with biological materials at the molecular level. Many dedicated track structure Monte Carlo simulation codes [2] have been developed for this purpose by simulating the transport of particles and the subsequent physical/chemical reactions with biological components of the cell that result in DNA damage. Finally, a set of biochemical reactions need to be simulated in order to study DNA repair and cell survival [3] that can be directly measured in the radiobiological experiments.

Presented model approach is based on recent version of Geant4-DNA simulation toolkit for computation of various types of DNA lesions, including single and clustered double strand breaks of different complexity. The model incorporates various structures of chromatin and reaction-diffusion events with damaging radyolityc species. Next stages of hierarchy incorporate the overall kinetics of DNA repair and its fidelity, to predict a range of biological endpoints including residual DNA damage, chromosome aberrations, and cell death. An extended example is given on the problem of radiation-induced effects in the central nervous system, where complex geometry of cells and heterogeneity of cell population increase the computational difficulty [4]. As a final endpoint of this partucular case the dose-dependence of sensitive cell survival was calculated in specific area of brain (hyppocampus) and projected on long-term effect of impaired neurogenesis [5].

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Modelling Quantum Randomness

Cristian S. Calude

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Quantum randomness is intensively studied because it is "believed" or "postulated" to be "true randomness". However, "true randomness" is a concept mathematically vacuous as Ramsey Theory proved long time ago. In the talk, we will describe mathematically a form of quantum randomness which is provably better than pseudo-randomness and present a photonic realization of it.

Computing Software Architecture for Distributed Processing of the BM@N Experiment Data

Konstantin V. Gertsenberger

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As in other large experiments on particle collisions, the topic of computing including distributed processing of physics events is extremely relevant in the BM@N experiment, the first ongoing experiment of the NICA project due to the heavy data flow, both from the operating experimental setup and from event generators in case of the simulation. Only in the last BM@N Run about half a petabyte of raw data was collected, and when the experiment reaches the design parameters, the amount of the data will increase by an order of magnitude. To quickly process all the hundreds of millions of events in hundreds of terabytes and perform necessary physics analyses with the publication of the results. a comprehensive computing software architecture has been properly designed for the BM@N experiment. It combines all distributed resources of the experiment into a single computing and data management system and automates job processing flows using well-proven software solutions and new developed information systems and services, both offline and online, which are presented in the report. The developed architecture has already been successfully used for mass data productions of BM@N experiment data, as will be demonstrated through concrete examples.

JINR Participation in the Construction and Upgrade of CMS Experiment

Vladimir Yu. Karjavine

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JINR contribution to CMS experiment is focused on the design, development, construction, operation and upgrade of the of the Endcap Hadron Calorimeter (HE) and the Forward station of the Muon system (ME1/1). Contributing to the CMS Computing, JINR provides robust operation of Tier-1 and Tier-2 centers. JINR staff take part in the experimental data taking, physical analysis and software development. During the first phase of CMS upgrade, aimed to the reliable work of detectors in the LHC design operating mode with energy $\sqrt{s} = 14$ TeV and instantaneous luminosity $L = 2 \times 10^{34}$ cm^{-2} s^{-1}, HE calorimeter segmentation was increased, and electronics were replaced. Detectors of the Muon system operating in the region of the high background rates, were equipped with new fast readout electronics. The second phase of the CMS upgrade, where JINR is participating in the High Granularity Calorimeter (HGCal) project and in the upgrade of the Endcap Muon system (ME), is aimed at ensuring reliable operation of the detectors in the High Luminosity LHC mode (HL-LHC) at energy $\sqrt{s} = 14$ TeV and instantaneous luminosity of $L = 5$–7×10^{34} cm^{-2} s^{-1}.

On Classical and Weakened Solutions of the Cauchy Problem for One Class of Nonlinear Parabolic Equations

Khachatur Khachatryan

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The report is devoted to the study of questions of the existence and uniqueness of the Cauchy problem for one nonlinear equation of parabolic type. Issues of constructing a weakened and classical solution to this problem will be discussed. For the corresponding nonlinear multidimensional integral equation, a constructive theorem for the existence of a positive smooth and bounded solution will be proven. Moreover, we will prove the uniform convergence of the corresponding iterations at a rate of decreasing geometric progression.

Methods and Technologies of Data Processing in Heterogeneous Computing Environments

Vladimir V. Korenkov

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The experiments at the Large Hadron Collider (LHC) at CERN (Geneva, Switzerland) played a leading role in scientific research. Data processing and analysis is carried out using high-performance complexes (Grid), academic, national and commercial resources of cloud computing, supercomputers and other resources. JINR is actively involved in the integration of distributed heterogeneous resources and the development of Big data technologies to provide modern large scale projects. JINR is actively working on the construction of a unique NICA accelerator complex, which requires new approaches to the implementation of distributed infrastructure for processing and analysis of experimental data.

The report provides an overview of methods and technologies for the development of a global computer infrastructure for storing, processing and analyzing experimental data at large scientific facilities (LHC, NICA, JUNO, neutrino program, etc.).

A brief overview of the projects in the field of the development of distributed computations performed by LIT in Russia, CERN, the USA, Europe, China, JINR Member States of JINR.

Nanobioelectronics: Applications in Information Technologies

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Bioinformatics is the area that develops methods and software tools for understanding of biological data, which includes sequence analysis, gene and protein expression, analysis of cellular organization, structural bioinformatics, data centers etc. A new and more general direction is to consider bioinformatics as informatics on the bases of nanobioelectronics and biocomputer technologies.

DNA molecular is an important example of data storage and biocomputing. The thermodynamics of DNA double strand in the Peyrard-Bishop-Dauxois model is considered [1]. Performing millions of operations simultaneously DNA – biocomputer allows the performance rate to increase exponentially. The limitation problem is that each stage of paralleled operations requires time measured hours or days. To overcome this problem can nanobioelectronics [2]–[4].

The central problem of nanobioelectronics is the realization of effective charge transfer in biomacromolecules. The most promising molecule for this goal is DNA. Computer simulation of charge transfer can make up natural experiment in such complex object as DNA. Such processes of charge transport as Bloch oscillations, soliton evolution, polaron dynamics, breather creation and breather inspired charge transfer are modeled. The supercomputer simulation of charge dynamics at finite temperatures is presented. Different molecular devices based on DNA are considered. These make the basis for solution of informatics problems on biomolecular technologies.

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Quantum-Quasiclassical Method for Few-Body Processes in Atomic and Nuclear Physics

Vladimir S. Melezhik

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In a series of works by V.S. Melezhik with co-authors [1], [2], [3], [4], [5], [6], a computationally efficient quantum-semiclassical method was developed for the quantitative analysis of various few-body quantum problems. The key idea of this approach goes back to works [7], [8] where it was applied to the molecular dynamics. In this approach, part of the variables (describing the quantum dynamics of a light particle) is described by the time-dependent 3D Schrödinger equation, which is integrated simultaneously with the classical Hamilton equations for the remaining variables of the entire few-body system of several interacting particles.

The main part of the report is devoted to recent results obtained with this method: the prediction of the possibility of obtaining accelerated and twisted atoms by using elliptically polarized strong short-wave laser pulses [9], [10] and the study of the spectral structure of halo nuclei during their Coulomb and nuclear breakup [11], [12]. We discuss the computational aspects of the method, its computational efficiency and possible applications.

Acknowledgement. This work was supported by the Russian Science Foundation under Grants No. 20-11-20257.

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On Overcoming the Crisis of Particle Tracking in High-Luminosity Experiments using Deep Learning Methods

Gennady A. Ososkov

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One of the key stages in the processing of experimental data of the HEP is the reconstruction of trajectories (tracks) of interacting particles from measurement data. For modern high-luminosity collider experiments, such as HL-LHC and NICA, a particular challenge for tracking is the very high, megahertz frequency of interactions, leading to an order-of-magnitude increase in the intensity of the data stream to be processed and, in addition, to a significant overlap of event track data when they are registered in track detectors. All these circumstances, recognized by physicists as the "Tracking Crisis", have shown that the tracking algorithms already in use are not efficient, accurate and scalable enough to handle data from high-luminosity experiments.

To overcome this crisis, in 2018 a group of physicists from CERN and other physics centers in the HEPTrkX project [1] staged a TrackML competition [2] to develop new solutions to tracking problems using deep neural networks. A dataset for their training and testing was prepared and published on the Kaggle platform [3]. The TrackML competition stimulated a number of important researches leading to the development of effective tracking algorithms using graph neural networks [4], transformers [5], as well as reanimation of tracking based on Hopfield neural networks, but with application of computational means of adiabatic quantum computers [6].

The experience in the development of tracking algorithms using machine learning methods, accumulated during the last decade by the specialists from MLIT JINR, allowed them to actively engage in research on overcoming the problems of the tracking crisis not only using information from already published publications, but also to propose their original innovations taking into account the specificity of domestic detectors in the high-luminosity experiments of the NICA megaproject at JINR [7]. In the present report a brief review of the ongoing work is made and their prospects are discussed.

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Anonymous Computation Scheme for Robust Authentication in Self-Organizing UAV Swarms

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UAV swarms operate autonomously using collective intelligence, where individual peers communicate and collaborate to make decisions as a group, share data in real time, and efficiently complete tasks like disaster response, search and rescue operations, environmental monitoring, and military missions. In our construction, the UAVs within the swarm carry out area surveillance and complete exchange of captured images during a quasi-random walk (rotor-router model). We also implement information full exchange (gossip-broadcast model) for seamless and continuous data sharing among the peers in the swarm. This communication ensures that every UAV has access to the most up-to-date information allowing for real-time decision-making and coordination. During mission execution, the the swarm autonomously completes its tasks in the absence of satellite communication, under active jamming, and without any direct external control thus exhibiting self-organization. Each peer follows simple rules based on local interactions, leading to efficient group behavior.

However, there are critical aspects in UAV swarm management. Ensuring the swarm safe and reliable operation requires addressing significant physical and information security challenges. Physical security concerns include unauthorized access or hijacking of the swarm, making it vulnerable to physical tampering or unauthorized takeovers, especially if they lack proper authentication measures. This can result in theft, loss of control, or even malicious repurposing of the peers. Other challenges include: data integrity and privacy risks, also malware and cyberattacks. The swarm's sensors and cameras collect sensitive information. Without strong encryption, this data can be vulnerable to unauthorized access.

Addressing these concerns requires implementing secure communication protocols and physical security measures to protect against tampering. We propose embedding unique authentication codes and confidential computing within the UAVs' individual hardware at their fabrication stage. Dedicated hardware devices will protect and manage cryptographic keys and ensure secure computation within secure enclaves. Anonymous computation will keep the identities of participants

and their data private. Depending on the swarm mission and associated energy consumption, approaches, such as: homomorphic encryption, secure multi-party computation, or zero-knowledge proofs may be embedded.

MPD Software Framework

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The software framework plays an important role in the HEP experiments. The major components of HEP computing are simulation, reconstruction and analysis. In JINR for the MPD experiment framework "mpdroot" has been developed since 2007. It is based on "Fairoot" package. and was most flexible and user friendly package at the time and now it is still fulfill all requirements for simulation and analyses tasks. Further advancement and implementation of modern tools and algorithms into "mpdroot" framework also is considering.

Sophisticated Techniques for Numerical Integration of Challenging Integrals: Extrapolation Methods and Asymptotics

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Integration by parts is one of the most popular techniques in the analysis of integrals and it has frequently been used to create divergent series or asymptotic expansions of integral representations. The product of the technique is usually a divergent series formed from evaluating boundary terms; however, sometimes the remaining integral is also evaluated. As an example, we consider the Euler series arising from integrating the Euler integral by parts:

$$\int_x^\infty \frac{\mathrm{e}^{-t}}{t}\,\mathrm{d}t \sim \frac{\mathrm{e}^{-x}}{x}\sum_{l=0}^{\infty}(-1)^l\frac{l!}{x^l}, \qquad x\to\infty, \tag{1}$$

where the remaining integral after n integrations by parts

$$(-1)^n n!\int_x^\infty \frac{\mathrm{e}^{-t}}{t^{n+1}}\,\mathrm{d}t$$

is often discarded and the divergent series has either been summed straightforwardly or through the use of sequence transformations.

Another example arises in molecular structure calculation. Through a reformalized integration by parts with respect to $x\,\mathrm{d}x$, the initial integral is transformed into the simple sine function integral:

$$\int_0^\infty x^{n_x}\frac{\hat{k}_\nu[R_2\gamma(s,x)]}{[\gamma(s,x)]^{n_\gamma}}\,\mathrm{d}x =$$

$$\int_0^\infty \left[\left(\frac{\mathrm{d}}{x\,\mathrm{d}x}\right)^\lambda\left(x^{n_x+\lambda-1}\frac{\hat{k}_\nu[R_2\gamma(s,x)]}{[\gamma(s,x)]^{n_\gamma}}\right)\right]\sin x\,\mathrm{d}x. \tag{2}$$

Due to the successive differentiation and anti-differentiation required to form the series or the remaining integral, the technique is difficult to apply to problems more complicated than the simplest. In this contribution, we explore a generalized and formalized integration by parts to create equivalent representations to some challenging integrals and we introduce a recursive algorithm based on the theoretically powerful

G transformation, which was handicapped by the lack of an algorithmic implementation. The recurrence relations reduce considerably the complexity of the algorithm, which is shown to be robust and leads to an unprecedented accuracy.

As a demonstrative archetype, we examine the infinite-range Fresnel integrals, the Twisted Tail, Airy functions, Bessel integrals, and the incomplete Bessel functions.

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Event Reconstruction in High-Energy Physics Experiments

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This report reviews methods of pattern recognition and event reconstruction used in modern particle physics experiments. It gives an outline of the event reconstruction chain of a typical large experiment, from the trigger to the physics object reconstruction. The concept is illustrated by two examples, LHC and NICA experiments, where algorithms for hit generation, local reconstruction, and global reconstruction are developed, followed by a discussion of the latest trends in high energy physics. Some emphases of particle identification and reconstruction of physics objects such as electrons, muons, photons, jets, τ leptons, and missing energy will be also underlined in this talk.

Offline Software and Computing for the SPD Experiment

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The SPD (Spin Physics Detector) is a planned spin physics experiment in the second interaction point of the NICA collider that is under construction at JINR. The main goal of the experiment is the test of basics of the QCD via the study of the polarized structure of the nucleon and spin-related phenomena in the collision of longitudinally and transversely polarized protons and deuterons at the center-of-mass energy up to 27 GeV and luminosity up to $10^{32}1/(\mathrm{cm}^2\mathrm{s})$. The data rate at the maximum design luminosity is expected to reach 0.2 Tbit/s. Current approaches to SPD computing and offline software will be presented.

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"Govorun" Supercomputer for JINR Tasks

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The "Govorun" supercomputer was created in 2018 on top of the experience gained during the operation of the HybriLIT heterogeneous cluster, which is part of the JINR MLIT Multifunctional Information and Computing Complex. HybriLIT has shown its relevance in solving tasks of QCD on lattices, radiation biology, applied research, etc. The continuous growth in the number of users and the expansion of the range of tasks to be solved entailed not only a significant increase in the computing capabilities of the cluster, but also the development and implementation of novel technologies, which resulted in the creation of a new computing system, the "Govorun" supercomputer. The "Govorun" supercomputer was built as a high-performance, scalable liquid-cooled system with a hyperconverged and software-defined architecture. The current configuration of the "Govorun" supercomputer involves computing modules containing GPU and CPU components, as well as a hierarchical data processing and storage system. The total peak performance of the "Govorun" supercomputer is 1.7 PFlops for double-precision calculations (3.4 PFlops for single-precision calculations) with a read/write speed of 300 GB/sec for the hierarchical data processing and storage system.

The created flexible architecture of the "Govorun" supercomputer and the hierarchical data processing and storage system included in it allow one not only to carry out calculations, but also to use the supercomputer as a research polygon for developing software-hardware and IT solutions for tasks underway at JINR. This feature made it possible to deploy polygons for quantum computing and LRB experimental data processing, to integrate the resources of the "Govorun" supercomputer into a unified heterogeneous environment based on the DIRAC platform for the NICA project and utilize its resources to implement the program of runs of data mass modeling within the MPD experiment.

The resources of the "Govorun" supercomputer have shown their relevance and effectiveness in solving such tasks as calculating the electronic structure of superheavy elements taking into account high-order relativistic corrections, investigating changes in the Periodic Law in the field of extremely heavy elements, studying the electronic structure of

elements of the end of the 7th and beginning of the 8th periods, modeling the kinetics of the excitation and relaxation of dielectrics irradiated by fast heavy ions, examining the structure of light exotic, heavy and superheavy nuclei and reactions with them, as well as analyzing the radiation safety of heavy ion accelerators at FLNR JINR using Monte Carlo modeling, etc.

The results obtained using the resources of the "Govorun" supercomputer from the moment it was put into operation in July 2018 until now are reflected in over 336 user publications, two of them in the Nature Physics journal.

At present, the resources of the "Govorun" supercomputer are used by scientific groups from all the Laboratories of the Institute. The number of users of the "Govorun" supercomputer is 350 people, of which 293 are JINR staff members, and 57 are from the Member States. Access to the supercomputer resources is provided only to those users who are directly involved in the implementation of the JINR Topical Plan.

Contributed Papers

Peculiarities of Buzdin and Chimera Steps in the IV-Curve of Superconductor Ferromagnetic φ_0 Josephson Junction

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In the presence of external electromagnetic radiation, the magnetization and current-voltage characteristics of superconductor-ferromagnet-superconductor φ_0 Josephson junctions have been studied. Due to the coupling of superconductivity and magnetism in this system, the magnetic moment precession of the ferromagnetic layer caused by the magnetic component of external radiation can lock the Josephson oscillations, which results in the appearance of a particular type of steps in the current voltage characteristics, completely different from the well-known Shapiro steps. These steps are called the Buzdin steps in the case when the system is driven only by the magnetic component and the Chimera steps in the case when both magnetic and electric components are present [1]. Unlike the Shapiro steps where the magnetization remains constant along the step [2], here it changes though the system is locked. We also, demonstrate the implementation of dieffrent types of dynamical states of magnetization[3]. These states in the synchronization region are distinguished by the type of magnetic moment precession and their Josephson oscillations have phase difference of π [3]. The possibility of switching between these states using a current pulse is demonstrated. Transitions between these states with increasing and decreasing bias current show hysteresis, which is reflected in the bifurcation diagram and the current-voltage characteristics. Additionally, we demonstrate how the results can be verified experimentally

by measuring the phase shift in voltage temporal dependence at fixed current values in both directions. Various applications of the results obtained can be found in the field of superconducting spintronics and quantum computing.

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Analytical Computation Software Module in Python for Automating the Representation of Equations for Further Numerical Modeling of the Chain of Nanomagnets Associated with the Josephson Junction

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The report will present the details of the development of a software module for studying the chain of nanomagnets associated with the Josephson junction, taking into account various types of interaction between elements to output equations in symbolic form for further numerical modeling. In this case, the equations are reduced to the form of a system of ordinary differential equations resolved with respect to the derivative. The implementation is is carried out using the SymPy library for symbolic calculations, which provides powerful tools for working with symbolic expressions, equations and systems of equations. Its advantages include easy integration with other Python libraries, such as NumPy and Matplotlib. This made it possible to carry out numerical calculations on a par with symbolic ones in the prepared Jupiter Notebook, and to visualize the results of these calculations.

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On Multipartite Generalization of X-states

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The notion of X-states of two qubits has proven to be an important object in itself for quantum information science, as well as a useful tool for the investigation of the entanglement space of two qubits, not least due to its acclaimed entanglement universality property. Although, generalizations of this notion are available for multipartite quantum systems these essentially are reduced to a generalization of the generalized GHZ-states. Thus, the hopes of their entanglement universality are obliterated, since all the proper subsystems of a system in such a state will be fully separable. In this report based on a recursive procedure we suggest a new generalization, which:

(i) encompasses the previously suggested generalization (the invariance group of these $G_N = G_{N-1} \times U(1) \times G_{N-1}$, with $G_2 = SU(2) \times U(1) \times SU(2)$ is a subgroup of the invariance group of our generalization $\mathfrak{G}_N = SU(2^{(N-1)}) \times U(1) \times SU(2^{(N-1)})$);

(ii) has a range of self-similarity properties.

The last provide us with a solid ground to conjecture the entanglement universality of the proposed generalization of X-states.

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Three-Loop Calculation of Dynamical Exponent z of φ^3 Theory

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We consider model A of critical dynamics [1] based on φ^3 model:

$$S(\varphi) = -\lambda\varphi'\varphi' + \varphi'\left[\partial_t + \lambda(\tau\varphi - \partial^2\varphi) + \frac{1}{2}g_3'\varphi^2\right]$$

Currently only 2-loop approximation is available for this model [2]. Nowadays new powerful methods developed among them are Sector Decomposition [3] and Hyperlogarithm [4] method. The main drawback and in the same time advantage of the Sector Decomposition method is that it is numerical method, so high accuracy require enormous time. From the other hand Hyperlogarithm method is analytical one, but it was used only once in dynamical problems, it was model of turbulence of infinite dimension [5], which contains drastic simplification. Thus we try to get result with both methods. For now we completed calculation of 3 loop approximation by Sector Decomposition and started calculation with hyperlogarithms. Scalar model itself does not play relevant role in physics, but may be easily transformed to different interesting multi-component models, e.g. percolation.

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Numerical Modeling of Thermodynamic Parameters for Hot Neutron Star Matter in Neutrino-Trapped Regime

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Understanding the thermodynamic properties and constituent composition of strongly interacting matter at various temperatures and baryon number densities is essential for comprehending the dynamics of high-energy heavy-ion collisions and for determining the properties and evolutionary future of proto-neutron stars.

We investigate the thermodynamic properties of the hot β-equilibrated hadronic matter which consists of neutrons (n), protons (p), electrons (e), electron neutrinos (ν_e), muons (μ), and muon neutrinos (ν_μ). To describe such matter, we use an improved version of the relativistic mean field (RMF) theory at a finite temperature, where, in addition to the effective fields of σ-, ω-, and ρ-mesons, the scalar-isovector δ-meson effective field is also taken into account. The numerical solution of systems of ten nonlinear algebraic equations allows us to obtain the meson mean-fields $\overline{\sigma}$, $\overline{\omega}$, $\overline{\delta}$, and $\overline{\rho}$, as well as the chemical potentials of the particles μ_n, μ_p, μ_e, μ_μ, μ_{ν_e}, and μ_{ν_μ}. This made it possible, for given values of temperature T and baryon number density n_B, to calculate the energy density ϵ, pressure P, and entropy density S of hadronic matter in the neutrino trapped regime.

For the thermodynamic description of the deconfined quark matter consisting of quarks (u, d, s), electrons (e), electron neutrinos (ν_e), muons (μ), and muon neutrinos (ν_μ) we used the local SU(3) Nambu-Jona-Lasinio (NJL) model. The problem in this case is reduced to solving a system of thirteen nonlinear algebraic equations. The numerical solution of the system of equations allows, for given values of temperature T and baryon number density n_B, to determine the constituent masses of quarks M_u, M_d, M_s, the concentrations of particles n_u, n_d, n_s, n_e, n_{ν_e}, n_μ, and also the chemical potentials μ_u, μ_e, μ_{ν_e}, μ_μ.

Knowledge of the constituent masses, for specified values of the baryon number density n_B and temperature T, makes it possible to determine the quark condensates σ_u, σ_d, and σ_s, as well as the other thermodynamic parameters of electrically neutral β-equilibrium quark matter in neutrino trapped regime.

The temperature dependencies of the parameters of the first-order phase transition from hadronic matter to strange quark matter are

studied. A phase diagram is obtained corresponding to the equilibrium coexistence of hadron and quark phases in (T–μ_B) and (T–n_B) planes. The thermodynamic parameters of the critical endpoint in the phase coexistence curve are found.

A more detailed description of the features of the model we used can be found in our publications [1]–[3].

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Flexibility Extension of the Event Picking Service for ATLAS Experiment

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ATLAS EventIndex [1] is a catalog of all recorded and simulated ATLAS events, one of four experiments at the LHC accelerator at CERN [2]. The Event Picking Service is one of the components of the Atlas Event Index. It is used when the user wants to collect interesting events from a huge amount of ATLAS data and reprocess them. The process of receiving an event can be split into separate tasks. The set of tasks may differ for different event types. Some tasks use external services, which can take a long time to receive results. An error may occur as a result of completing the task. Some of these errors can be corrected automatically by the service, but some require administrator intervention. Failed tasks must be restarted from the specified step after the problem is manually corrected by the administrator. This is critical if the error occurs after a long-running task has been completed. All of the above leads to the fact that the Event Picking Service must be flexible and be able to be customized for a specific situation. This article is dedicated to describing how elasticity is achieved in the Event Picking Service and how it improves during operation.

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Production of the Configuration Information System for the BM@N Experiment

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The collection, storage and processing of experimental data are an integral part of modern high-energy physics experiments. The Configuration Information System (CIS) is an essential element of a complex of information systems developed for the high-energy physics experiments. The CIS has been developed and implemented for the BM@N experiment to store and provide data on the configuration of the experiment hardware and software systems while collecting data from the detectors in the online mode. The CIS allows loading configuration information into the data acquisition and online processing systems, activating the hardware setups and launching all necessary software applications with required parameters on specified distributed nodes. The architecture of the CIS mainly contains the User Web Interface, Configuration Database to store configuration data, and continuously running Configuration Manager, which uses API of the chosen Dynamic Deployment System developed by the FAIR collaboration for managing a set of intercommunicating processes. The Web interface has convenient features both to add, view configuration data and monitor online tasks. The CIS provides rich error reporting and logging facilities for both individual tasks and whole work sessions.

Evolution of the Resource Manager of the ATLAS Trigger and Data Acquisition System

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The Resources Manager (RM) is one of the services provided by the Data Acquisition (DAQ) system of the ATLAS experiment the Large Hadron Collider (LHC). The ATLAS experiment contains many hardware and software resources which usage must be controlled to avoid conflicts during online operations. The purpose of the RM is to marshal multiple accesses to such resources. When new software process needs to be started or obtain exclusive permissions, the RM is queried to verify availability of the resources as they are described in the DAQ configurations database. This article talks about the evolution of the RM based on the operations experience and changes in the underlying DAQ system software towards improving of security, fault tolerance, error reporting, logging and test facilities.

HybriLIT Platform: Services and Environment for HPC Calculations, Mathematical Modeling, Data Storage and Analysis

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HybriLIT heterogeneous computing platform is a powerful computing component of the Multifunctional Information and Computing Complex of JINR, which was created and is being developed to provide resource-intensive and massively parallel calculations and data analysis for JINR tasks related to theoretical and experimental research. The platform consists of the GOVORUN supercomputer, education and testing polygon that includes ML/DL/HPC ecosystem, and a testing polygon for quantum computing. The development of the Platform is associated both with the general development of computing architectures and data storage systems, providing users with the latest solutions, and with active development of information technologies, the emergence of new tools for solving a wide range of applied problems and for creating scientific services.

The report will present a multi-level software and information environment of the Platform which includes a system, software and information level. This provides users with convenient tools for carrying out calculations using parallel programming technologies, machine and deep learning; it also provides opportunities for developing quantum algorithms using quantum simulators, as well as examples of developed scientific services.

Random Surface Growth in Random Environment: Renormalization Group Analysis of Infinite-Dimensional Model

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The influence of a random environment on the dynamics of a fluctuating rough surface is investigated using a field theoretic renormalization group. The environment motion is modelled by the stochastic Navier–Stokes equation. The surface is described by the generalized Pavlik's stochastic equation. As a result of fulfilling the renormalizability requirement, the model necessarily involves an infinite number of coupling constants. Despite this, the one-loop counterterm is derived in an explicit closed form and large-scale, long-time scaling behavior is investigated.

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Field Theoretic Renormalization Group Approach to a Problem of a Running Sandpile in Turbulent Environment

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We study continuous anisotropic model of self-organized criticality (running sandpile) [1] in turbulent environment modeled by the stochastic Navier–Stokes equation [2] using perturbative field-theoretic renormalization group analysis. We consider several possible random stirring forces for the Navier–Stokes equation: a white noise (fluid in thermal equilibrium) and a noise with a power-like correlation function (turbulent fluid).

In the first case, the field theory equivalent to the coupled stochastic equations is established to be multiplicatively renormalizable. Aside from the regime of ordinary diffusion above the upper critical dimension, the renormalization group equation reveals a semi-infinite fixed point curve in the four-dimensional space of coupling constants. Surprisingly, the entire curve is infrared attractive for realistic values of parameters. Its end point corresponds to a regime where the nonlinearity of the sandpile evolution (and, thus, anisotropy) becomes irrelevant. The critical exponents are calculated up to the leading one-loop order or exactly. The fixed points on the curve correspond to the same values of critical exponents but have different corrections. This might indicate that the curve might compress to a single point when higher order corrections are taken into account. There is no regime where the sandpile is not affected by the environment which makes isotropic fluid more "powerful" than anisotropic growth.

In the second case, additional small parameter appears, so the curve is defined by another condition: equality of the small parameters values, which makes it more exceptional than in the first case.

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ReneSANCe Event Generator for Precise Luminosity Determination

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We present precision calculations of processes for luminosity measurement at e^+e^- colliders: Bhabha scattering [1], dimuon production [2] and annihilation into photon pairs [3]. These processes are implemented in the `ReneSANCe` Monte Carlo event generator [4]. The `ReneSANCe` status and advantages are discussed.

Acknowledgement. This work was supported by the Russian Science Foundation, project No. 22-12-00021

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Iterative Solution of DGLAP Equations in QED

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An iterative solution of the Dokshitzer–Gribov–Lipatov–Altarelli–Parisi evolution equations in QED is realized in the FORM programming language [1]. Perturbative solutions for unpolarized QED parton distribution and fragmentation functions are presented explicitly in the next-to-leading logarithmic approximation [2]. The results are presented in terms of harmonic polylogarithms evaluated with the help of Mathematica package [3].

The obtained electron fragmentation functions are applied to calculation of higher-order QED radiative corrections to muon decay spectrum within the next-to-leading order logarithmic approximation. New analytical results are given in the $\mathcal{O}(\alpha^3 \ln^2(m_\mu^2/m_e^2))$. Earlier results in $\mathcal{O}(\alpha^2 \ln^1(m_\mu^2/m_e^2))$ and $\mathcal{O}(\alpha^3 \ln^3(m_\mu^2/m_e^2))$ orders are partially corrected.

The electron parton distribution functions are used to caculate initial-state radiative corrections to a general electron-positron annihilation process. Analytic results are presented [5] in the orders up to $\mathcal{O}(\alpha^4 \ln^3(s/m_e^2))$ where s is the square of the total energy in the center of mass system. These results are relevant for experiments at future electron-positron colliders including Super Charm-Tau Factory, CEPC, and FCC-ee.

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Cells Recognition of the Sensomotor Cortex on Histological Images

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The Sector of Radiation Physiology of LRB JINR studies the radiobiological effects of ionizing radiation on the central nervous system (CNS) of small laboratory animals [1], [3]. One of the methods for assessing the severity of CNS lesions is the morphological analysis of brain cells. On the photographic images of histological samples, all objects of nervous tissue are manually marked and classified by an expert. Achievements in the application of machine learning and neural network models will make the analysis process easier and faster.

The paper describes approaches to solving the problem from the stage of data annotation to the final results, that demonstrate the prospects for using machine learning models. Thereby we can increase the speed of obtaining results and reduce the subjectivity of the approach to the processing of experimental data.

Acknowledgement. This work was supported by RUDN University Strategic Academic Leadership Program, project No. 021934-0-000. Data annotation and algorithm development were carried out based on the ML/DL/HCP ecosystem of the HybriLIT Heterogeneous Platform (MLIT JINR).

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Reconstruction of Neutron Star Mass Distribution from Cooling Evolution

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Based on observations of the surface temperature and age of neutron stars, possible mass values of the observed objects were investigated across various cooling models. The results showed that these values strongly depend on the compressibility and superconductivity of nuclear matter. It was found that the masses of the observed stars primarily range between 1.2 and 1.7 solar masses. Additionally, the dependence of the temperature range of neutron stars on their age was studied for different cooling models.

Fast Reconstruction of Programmable Integrated Interferometers

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Programmable linear optical interferometers are vital for applications in classical and quantum information processing. Accurately predicting the interferometer matrix given a set of control parameters is challenging due to manufacturing imperfections, which necessitates the experimental reconstruction of these errors. However, the integrated design of these devices prevents the separate analysis of internal elements, complicating the reconstruction procedure. Traditional methods rely on global optimization, which is slow and computationally intensive. In contrast, in [1][2] we have introduced an optimization-free algorithm based on linear algebra that enables fast and accurate characterization of high-dimensional interferometers. In the report we will discuss the further method speed-up, its limitations, and extension to the Clements architecture of the optical interferometers.

Acknowledgement. This work was supported by the State Program No. FFNN-2022-0016.

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A Computer Model of Microstrip Coordinate Detectors for the Hybrid Tracker of the BM@N Experiment

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The study of dense baryonic matter formed as a result of relativistic heavy-ion collisions is one of the important researches in High Energy Physics (HEP) [1]. The nuclear matter in this phase, called a quark-gluon plasma (QGP), is a mixture of quarks, antiquarks, and gluons when they are freed of their strong attraction for one other under extremely high energy densities. It is expected that the study of the quark-gluon plasma will help physicists understand the formation features of the universe shortly after the Big Bang. One of the appropriate experiments that can create the most optimal energy conditions for the formation of this matter is Baryonic Matter at Nuclotron (BM@N) [2].

A unique experimental setup consisting of various detector subsystems was developed for this experiment. The core of the setup is a hybrid tracker made up of different types of microstrip coordinate detectors to register the trajectories of charged particles produced as a result of primary heavy-ions collisions. All tracker detectors can be divided into three groups. The first group located in front of the target and consists of Silicon Profilometers (SiProf) and Silicon Beam Tracker (SiBT) for monitoring and tracking the ion beam. The second is detectors inside the analysing magnet SP-41, such as Vertex Silicon Plane (VSP), Forward Silicon Detector (FSD) and Gas Electron Multipliers (GEM). The detectors of the third group are Cathode Strip Chambers (CSC) located behind the magnet.

The aim of the work was to develop the computer model of the aforementioned detectors and prepare the software based on this model for realistic response simulation and reconstruction of spatial coordinates from microstip readout planes. The results given in the report refer to the configuration of the latest experimental run conducted in 2024 and also for the upcoming run preliminary scheduled for 2025.

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Terahertz Oscillating Kinks in Microtubules

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The dynamics of microtubules is considered in the frameworks of the longitudinal model. Using the approximation of the slowly varying envelopes, the systems of nonlinear equations describing this process are derived. The approximate solutions of the derived systems of equations in the form of oscillating kinks are obtained. The obtained solutions are compared with the results of the numerical simulation.

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Web Service for the Trajectory Analysis of Laboratory Animals in the "Morris Water Maze"

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The behavioral test "Morris Water Maze" is a useful device to study spatial learning, behavioral reactions and memory of small laboratory animals exposed to irradiations.

Within the framework of the joint project between MLIT and LRB JINR aimed at developing an information system, we have designed a web service to automate the analysis of experimental data related to the behavioral test "Morris Water Maze". In data analysis, the automation tasks are concerned about the analysis of video data. Meanwhile, the development of convenient tools can significantly reduce the research time and human factor influence. Here we present the results of web service developing which is designed to annotate and classify the data for the trajectories of rodents' movements in the "Morris Water Maze" behavioral test. The functionality of the service enables a person to monitor the correctness of the constructed trajectory, classify the trajectory based on deep learning approach and obtain a number of characteristic parameters of the rodents' movements during the experiment. The web service is available at `http://bio-dashboards.jinr.ru/morris/Morris_tracking`.

The web service was developed and deployed based on the ML/DL/HPC ecosystem of the HybriLIT Heterogeneous Computing Platform.

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An Investigation of Two-Level Data Processing for Packet Transmission Time Analysis Using Machine Learning Methods

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This paper examines the impact of two-tier data processing on RTT analysis in computer networks using machine learning methods. Effective data processing plays a key role in the successful training of machine learning models, especially in network environments. The study proposes a methodology involving two-tier data processing, which consists of pre-processing and post-processing using machine learning methods. This approach aims to improve the accuracy and performance of RTT analysis by optimizing the quality and relevance of data. The results of the study show that the use of a two-tier data processing strategy can significantly improve the performance of machine learning models in analyzing network performance metrics. This study contributes to the development of network data analysis technologies and the optimization of machine learning applications in network management.

Radiative Corrections to $W^{\pm}$ Boson Hadroproduction with Longitudinal Polarization of Initial States

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The effects of complete one-loop electroweak radiative corrections to $W^{\pm}$ boson hadroproduction were studied for the case of longitudinal polarization of initial particles [1]. Different types of asymmetries for typical energies and degrees of polarization for `RHIC` experiment were analyzed. Numerical results were obtained using the Monte Carlo generator `ReneSANCe` [2].

Acknowledgement. This work was supported by the Russian Science Foundation, project No. 22-12-00021.

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Two-loop Corrections for $2\gamma \to 2\gamma$ Polarized Process

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Two-loop corrections from fermion loops in the four photon polarized process are discussed. The analytic results for 4γ are used to upgrade the SANCPHOT code to investigate results for modern photon colliders.

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Hadron Cluster Finding in the SPD/NICA

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The possibility of observing jet of hadrons in proton-proton collisions at an energy of $\sqrt{s}$= 27 GeV in the SPD experiment was studied. The study was performed on the simulation processes with partons using the anti-k_T, k_T and Cambridge–Aachen jet reconstruction algorithms. The results include an analysis of the kinematic characteristics of the jets and an estimation of the expected statistics.

Automatic Build and Distribution of Software for MPD of the NICA Project

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For physicists participating on the heavy-ion collision experiments studied via the Multi-Purpose Detector (MPD) [1] of the Nuclrotron-based Ion Collider fAcility (NICA) [2] the main access point to data is going to be the MPDRoot [3]. It is a off-line software framework for simulation, reconstruction, and physics analyses for both simulated and experimental data. Unfortunatelly, compilation and installation of this package and its dependencies can be an insurmountable barrier for users without sufficient experience in IT.

In this talk, we will show, how we were able to adapt the approach introduced in CERN [4] not only to automate the process of building MPDRoot and its dependencies, but also how we have made available the compiled software to the general public.

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Basic Tasks of Artificial Intelligence in Multidisciplinary Research

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The article's concept divides sciences into predictive and descriptive, emphasizing their differences. Descriptive sciences focus on describing phenomena and laws, while predictive sciences aim to forecast phenomena based on identified patterns. The central idea is that predictive sciences work with models, whose accuracy determines the precision of the predictions themselves. Depending on the possibility of creating universal models, sciences can be classified as formalized, such as physics, or weakly formalized, such as geology and ecology.

A systemic approach plays a crucial role in modern scientific research, necessary for solving multidisciplinary problems. This approach includes emphasizing the significance of meta-scientific questions and reconsidering the relationships between goals, problems, tasks, models, and theories. Applying a systemic approach in science involves consistent methodologization, formalization, theorization, mathematization, and computerization of the problems under study.

Particular attention is given to multidisciplinary research, which requires the involvement of specialists from various scientific fields. To successfully address such challenges, a general framework for problem formulation and resolution has been developed. This framework includes stages such as problem formulation, formalization, choice of solution method, and analysis and interpretation of results. This scheme allows for a coordinated approach to solving complex problems involving multiple scientific disciplines.

Artificial intelligence is playing an increasingly significant role in science, especially in the context of solving multidisciplinary problems. The development of AI tasks includes processes such as identifying research objects, describing and comparing them, forecasting, and ordering by uniqueness. Machine learning methods and neural networks are becoming important tools that automate data analysis and model creation processes, significantly facilitating researchers' work.

The article also provides examples of applying these methods in practice. For instance, the K-means clustering method and hierarchical

taxonomy are used for grouping data. Neural networks are applied for classification and prediction of objects, while Principal Component Analysis (PCA) helps rank objects by their degree of uniqueness.

In conclusion, the authors emphasize the importance of a systemic approach and the use of AI as powerful tools for solving complex scientific problems, particularly in the context of multidisciplinary research. These tools not only enable effective formulation and modeling of scientific problems but also successfully resolve them based on data provided by various scientific disciplines.

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Optimization of the Neutron Spectrum Unfolding Algorithm Based on Tikhonov Regularization and Shifted Legendre Polynomials

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An algorithm for unfolding the neutron spectrum from the results of measurements with the Bonner multi-sphere spectrometer is proposed. Measurements are related to the spectrum through a system of Fredholm integral equations of the 1st kind. The proposed algorithm is based on decomposition of the spectrum into shifted Legendre polynomials [1]. To solve the system of Fredholm equations Tikhonov regularization is used. The construction of a stabilizing functional containing derivatives of several orders is proposed. A weight matrix with condition numbers of the Gram matrices of the detector's response functions is added to the stabilizing functional. This weighting matrix ensures statistical equalization of contributions from measurements with spheres of different diameters. The proposed method was used to unfold the spectra at the IREN facility at JINR.

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PI-Type Fully Symmetric Quadrature Rules on the 3-, ..., 6-Simplexes

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In this talk we present fully symmetric quadrature rules with positive weights, and with nodes lying inside the $3, \ldots, 6$ dimensional simplex (so-called PI-type). PI-type fully symmetric quadrature rules up to 20-th order on the tetrahedron, 16-th order on 4-simplex, 10-th order on 5- and 6-simplexes are presented. The number of nodes of the presented quadrature rules for the corresponding orders does not exceed the known ones, and most of them are new. In the calculation we applied the modified Levenberg-Marquardt methods for solving nonlinear equations with convex constraints. The corresponding programs are implemented in MAPLE-FORTRAN environment, and the weights and nodes are first calculated using a FORTRAN program with an accuracy of 10^{-25} and refined up to accuracy of 10^{-50} using a MAPLE program.

This talk is based on [1].

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Application of the KANTBP 3.1 Program and its Modifications to the Study of Some Nuclear Reactions Processes

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The KANTBP 3.1 program [1] for calculating the energies, reflection and transmission matrices, and the corresponding wave functions in the coupled-channels approximation of the adiabatic approach was applied to study several nuclear fusion reactions [2]–[5]. The effectiveness of the KANTBP 3.1, with respect to the widely used programs of NRV [6] and CCFULL [7] essentially at low and large collision energies, is mainly determined by the correct formulation of boundary conditions.

In this talk we discuss about application of KANTBP 3.1 program to solve multichannel scattering problem with complex potentials for studying nuclear fusion and quasielastic reactions. A comparison of the results obtained using the KANTBP 3.1, R-matrix [8] and modified version of the Numerov method within the CCFULL model [9] is presented.

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Prediction of Flows with Porous Inclusions Using the Generalized QGD-System of Equations

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Many engineering applications and technological processes deal with flows in porous media. In many practical cases, it is necessary to study systems consisting of a free flow of a clear liquid and solid inclusions that can be treated as a saturated porous body. To predict flows in such complex domains, a new mathematical model was developed and verified in the present work. In this model, the generalized governing equations were obtained by averaging the quasi-gasdynamic (QGD) system of equations [1] over a small representative elementary volume [2] in the whole domain involving both free and porous body flow subdomains. In doing so, the Darcy-Forchheimer terms appear only in the porous body subdomain whereas all other terms of the equations include the variable porosity. Thus, these new generalized equations are reduced to the standard QGD-system of equations in the free flow subdomain, while the Darcy-Forchheimer law is included in the porous body subdomain. Such a one-domain approach allows constructing homogeneous numerical algorithms without using any domain decomposition techniques.

To verify the proposed model and to evaluate its possibilities, two test problems were investigated numerically and compared with available numerical data. In both cases, the Darcy flow regime was considered for an isotropic porous medium at the Mach number $M = 0.1$ and the Reynolds number $\mathrm{Re} = 1$. In the first test, a flow in a plane channel containing a porous plug was calculated. The porous plug is located at the middle of the channel and significantly affects the impinging flow. The impact of the porous plug on the developed parabolic velocity profile specified at the inlet of the channel was studied in our predictions. Flows in a lid-driven cavity partially filled with a porous medium were predicted in the second test. Various values of the permeability of the porous layer were considered and compared in our calculations. In both cases, a good enough agreement with similar calculations by other authors was obtained.

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Algorithm for Identification of the Equilibrium Position of a Marine Object in the Conditions of Sea Waves

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The equilibrium parameters of any physical object are easily determined in static conditions, when there are no disturbing influences. However, in conditions of oscillatory motion of the object, measurement or determination of such parameters is impossible. At the same time, knowledge of equilibrium parameters can be very important. For example, for a ship in storm conditions, especially in an emergency situation, knowledge of equilibrium parameters of roll, pitch and draft are decisive in making a decision on controlling the object and fighting for its survivability.

In operational conditions, judgment about the equilibrium position can be made only on the basis of indirect measurement data. These include records of ship motion under the action of external excitations, as well as a priori information on the parameters of the ship itself. The technical problems arising in the development of the equilibrium position identification algorithm are as follows:

1. The recorded processes are generally non-stationary both due to changes in the object parameters under emergency conditions (e.g., due to water inflow into the compartments) and due to non-stationarity of external excitations (e.g., wind gusts)

2. The averaging characteristics of the motion cannot be considered as an equilibrium position, especially in the case of nonlinear asymmetric oscillations.

The report proposes an approach to solving these technical problems on the basis of taking into account the physics of ship motion and using the dynamic characteristics of the object. The constructed algorithm is used in onboard decision support systems of marine objects.

Computational Simulation as a Tool of Investigating the Behavior of a Marine Object in Storm Conditions

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Controllable ship motion in conditions of intense storm waves is a very indicative problem of practical hydromechanics. The design of surface ships requires a large complex of engineering solutions to ensure safety of navigation and unconditional fulfillment of the functions assigned to the ship. Over the past century and a half, the complex nature of marine technology has caused to carry out complex and expensive model tests of designed objects in towing tanks, since it was impossible to achieve the result by computational methods alone. The disadvantages of this way are well known. They are the influence of the scale effect, impossibility to reproduce all external excitations of interest, especially extreme situations, difficulties in variation of technical solutions of the object itself (geometric shapes, change of ratios of ship dimensions: length, width, draft, freeboard, etc.).

Now all details of the physics of the behavior of marine objects are well investigated and understandable. The level of detail and accuracy of computational models that are possible for implementation on modern hardware is so high that they can be considered as a replacement for not only a model, but also a full-scale experiment. This allows the use computational simulation as a means of studying ship behavior in complex hydrometeorological conditions.

For these purposes, a universal programming environment has been developed in the realization of a unified set of computational simulation. It is created with the help of special tensor mathematics, which provides a visual and extremely effective modeling of the spatial motion of a ship with a rapidly changing wetted hull surface, rebuilding the spatial velocity distributions of currents and moving surfaces in a storm conditions. Various hydrodynamically adequate models of wind waves are used: ARMA, trochoidal progressive and standing waves [1]. The modeling is based on the general laws of conservation of mass, momentum, and energy. The computational simulation boils down to integration of pressures over the hull volume immersed in water.

All methods in the developed modeling environment are implemented in a single interactive complex. The choice of modeling mode is selected or changed dynamically. When changing the sea wave mode, the simulation is automatically resumed with the introduction of a smoothly developing wave packet into the computational domain [2].

Thus, the presented environment of mathematical modeling of ship hydrodynamics gives the possibility of conducting a comprehensive computational simulation, which gives the opportunity to completely replace the physical experiment.

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Rule of the Second Normal Form

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This paper is devoted to inference rules for dependencies (functional and multivalued) in relational model of data.

First, we introduce definitions of functional and multivalued dependencies starting with the relation.

Then, we list and unify rules for dependency reasoning collected from several sources [1], [2], and [3]

Third, we introduce the new rule of the Second normal form. This new rule is proved for functional and multivalued dependencies.

Finally, we comment applicability of discussed rules.

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Effect of Oxidative Stress on the Structure of Glutamate Receptors and Membranes in Neural Cells

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Amino acid residues such as cysteine, methionine, tyrosine, histidine and tryptophan, as well as the carboxyl group in the structure of phospholipid membranes are most likely to undergo changes as a result of oxidative stress in the structure of the NMDA glutamate receptor [1], [2], [3]. In this work, the modeling of the network activity of neurons with damaged glutamate receptors and POPC (1-palmitoyl-2-(9'-oxo-nonaoyl)-gycero-3-phosphocholine) lipid membranes was carried out in two stages. At the first stage, 100 ns molecular dynamics modeling of NMDA receptors containing modified amino acid residues was carried out. Based on a comparative analysis of the dynamics of the ion channel radii of the damaged and native forms of molecular systems, the ratio of receptor conductances $g = G/G_b$ was determined, where G is the ion channel conductance of the damaged system receptor, G_b is the ion channel conductance of the native system.

In the second stage, the local potential of the neuronal population and the power spectrum of the EEG signal were calculated using the NEURON program for the model [4], where the necessary parameters of the receptor ion channel were changed in accordance with the obtained data on the conductivity of the receptor ion channels. The ionic current of the glutamate receptor in the neural network model is represented as:

$$I_{\mathrm{NMDA}} = G_{\mathrm{NMDA}} P(V_{\mathrm{pre}})(V - V_e)/(1 + [\mathrm{Mg}^{2+}] \exp(-qV)/K_d), \quad (3)$$

where G_{NMDA} is the maximum conductance of the NMDA receptor for a certain type of ion, $P(V_{\mathrm{pre}})$ is the probability of channel opening depending on the presynaptic potential and the macroscopic kinetics of the receptor states, V is the postsynaptic membrane potential with equilibrium voltage V_e, q is a phenomenological constant reflecting electrochemical properties [5], K_d is the dissociation constant [6], $[\mathrm{Mg}^{2+}]$ is a magnesium binding parameter.

In the course of the present study, the values of collective rhythms (theta and gamma) of the hippocampal neural network were determined during oxidative modification of the system and changes in the local potential of the neural population of the model were revealed depending on the localization of damage in the structures of the receptor and phospholipid membrane.

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Some New Algorithms for Monte-Carlo Event Generators

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Monte-Carlo generators of events are important for modeling processes on colliders. Unlike numerical integration case a special treatment needed to achieve unit weight of events. We propose two algorithms of different kind to reach this goal. One of them based on interval arithmetic [1], [2] and another on fast-converging Chebyshev approximations.

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Coupling of UrQMD 3.4 and SMM Models for Simulation of Neutron and Nuclear Fragment Productions in Nucleus-Nucleus Interactions

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The UrQMD model is widely applied for simulation of nucleus-nucleus interactions at high energies. It allows one to generate multi-particle production in the interactions in the so-called "cascade" mode. We check that the model reproduces experimental data by the NA61/SHINE collaboration on $\pi^{\pm}$-meson, K-meson, proton and anti-proton production in $^{40}Ar + {}^{45}Sc$ interactions at P_{lab} = 13, 19, 30, 40, 75, and 150 GeV/c/nucleon. The model results for K^+-mesons are below experimental data. A coupling of the model with the Statistical Multi-fragmentation Model (SMM) allows one to simulate neutron and nuclear fragment productions using the EoS mode. In the mode, molecular type propagation of nucleons is used accounting potential interactions, stochastic scatterings and multi-particle productions. We choose evolution time 100 fm/c. At the end of the evolution, the well-known clustering algorithm is applied for creation of nuclear pre-fragments in the equal velocity reference frame. An excitation energy of a pre-fragment is calculated as a difference between sums of kinetic and potential energies of nucleons, and a ground state mass of the pre-fragment. Then, SMM is starting to work. We check that the combination of UrQMD and SMM allows to describe neutron spectra in the reactions – p+C, Al Fe, In, and Pb [1], [2]. Fragment mass distributions in nucleus-nucleus interactions are also analyzed. The UrQMD model enlarged by SMM can be applied at FAIR and NICA experiments.

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Nanoroughness Induced Anti-Reflection and Haze Effects in Opaque Systems

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How to make a material anti-reflective without changing its high refraction index? Achieving anti-reflection in high-refractive-index materials poses challenges due to their high reflectivity (Fresnel equations). Based on theory with new boundary conditions, we propose modifying surface properties on a nanoscale to tackle this. Our study on weakly rough opaque surfaces reveals significant changes in specular and diffuse scattering, predicting anti-reflection where roughness matches light penetration depth for the first time. Experimental validation on nano-roughened Si films (at wavelengths 300-400 nm) supports our findings. We also analyze angular and polarization dependences of nanoroughness-induced haze, showing predominant p-polarization and minimal haze at nanoscale, yet impactful specular reflection reduction.

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Quantum Thermodynamics of Single-Particle Systems from First Principles

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A microscopic theory of quantum thermodynamics has been developed for a multicomponent ensemble of reacting particles, which significantly expands our previous work on this topic [1]. The medium is considered as a selected sub-ensemble consisting of single-particle or $4D$ isotropic oscillator systems immersed in a random environment, which, as a result of evolution in the limit of thermodynamic equilibrium, with different probabilities pass into topologically different final quantum states. Within the framework of a stochastic differential equation (SDE) of the Langevin-Schrödinger (L-Sch) type, which describes the quantum state of a selected particle in a reacting environment, the problem of self-organization of a single-particle system with its environment is investigated. By the help of a low-dimensional reference SDE, the original L-Sch equation is reduced to an autonomous form, which is then solved explicitly in an orthogonal basis of random processes in Hilbert space. Assuming that the interaction of a single-particle system with the environment is described by a complex Gauss-Markovian random processes, taking into account the reference SDE, a Fokker-Planck (F-P) type equation for the distribution of environmental fields is derived. The geometric and topological properties of the resulting additional space are studied in detail. Using the F-P equation, the measure of the functional space and, accordingly, the mathematical expectation of the time-dependent wave function of a single-particle system are constructed. In the limit of statistical equilibrium, the time-dependent entropy and complexity of the selected sub-ensemble are studied in detail, taking into account the influence of its environment. It is shown that all thermodynamic potentials of a selected sub-ensemble can be constructed in the form of functional integrals, which are then calculated exactly using the generalized Feynman-Kac theorem and reduced to double-integral representations with solutions of second-order partial differential equations (PDE). It is proved that when imposing an additional constraint on the wave function of a $4D$ isotropic oscillator,

the representation describes the quantum thermodynamics of a multicomponent ensemble of particles, the selected-particle of which is a reacting hydrogen atom.

The developed model of quantum thermodynamics is also interesting because it does not imply restrictions on the power of interactions with the environment, which makes the approach suitable for studying atomic-molecular processes far from the state of thermodynamic equilibrium of the environment, in critical states, when elementary processes occur under the strong influence of collective effects, including with a topological change in the structure of the original single-particle quantum systems that make up the selected sub-ensemble. Finally, the obvious advantage of the presentation is the possibility of a universal description of all processes occurring with the selected particle - scattering, restoration and capture, and that it is very important to create a mathematical algorithm for carrying out mass calculations of the parameters of the system from the first principles of quantum mechanics.

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The General Three-Body Problem in Conformal-Euclidean Space: Hidden Symmetries and New Properties of a Low-Dimensional System

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The twentieth century is notable for two revolutionary concepts in physics – the theory of relativity and quantum theory. The application of these theories has led to significant advances in the development of technology and engineering, despite the existence of a number of contradictions between them. In particular, the question of a natural explanation for the quantum-classical transition, wave function collapse, etc. remains open. Note that to solve the problem of the quantum-classical transition, the answer to the question is important: is irreversibility fundamental to the description of the classical world? To answer this question, we examined the classical three-body problem, formulating it in conformal Euclidean space and rigorously proving its equivalence to the Newtonian three-body problem. It is shown that a curved configuration space with a local coordinate system allows one to discover new hidden symmetries of the internal motion of a dynamic system, which allows one to reduce the three-body problem to a 6th-order system instead of an 8th-order one. The most important result of such consideration is that the chronologizing parameter of the motion of the center of mass of a system of particles, which we call internal time, is in general irreversible, which should be typical for a general three-body problem. An equation for the evolution of a flow of geodesic trajectories is derived, with the help of which its entropy is constructed. The connection between the geometry and topology of space and internal time is examined in detail, its features are analyzed – multidimensionality, heterogeneity and the arrow of time. New criteria for assessing the complexity of a small-sized dynamic system and the dimension of emerging stochastic fractal structures are obtained. An effective mathematical algorithm has been developed for the numerical

simulation of the general three-body problem, which is traditionally a difficult-to-solve system of stiff ordinary differential equations.

Details of the work can be found in the papers [1]–[2].

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Kinetic Modeling of the IEC Device in Order to Predict the Number of Produced Ions

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An Inertial Electrostatic Confinement (IEC) is often referred to as a portable neutron source. This device can be used as a research reactor due to its simple structure and low cost. This device includes two electrodes and a feed-stalk. By using a power source, a voltage difference is applied between two electrodes, by means of a feed-stalk connected to the inner electrode. A lot of experimental and simulation research has been done all over the world. In this work, the IEC device is kinetically modeled using the particle-in-cell (PIC) method. This modeling has been done at a constant voltage of 25 kV and a normal pressure range (10^{-4} torr to 10^{-2} torr). According to the obtained results, the number of ions increases with decreasing pressure. At 10^{-2} torr pressure, the number of ions is equal to 1.03×10^{11}, while at 10^{-4} torr pressure, this value increases to 9.35×10^{12}. This increase in ions shows that the mean free distance increases with the decrease in pressure, and the probability of collision between ions and neutrals decreases.

Pythia Generator Parameters Tuning with Professor2 Package Oriented for Belle2 Physics

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This study focuses on optimizing the Pythia8 Monte Carlo event generator parameters using the Professor2 package, tailored for Belle II physics applications. Pythia8, a widely used tool for simulating hadronic events, features numerous tunable parameters that affect the modeling of particle interactions, including hadronization and parton showers.The accuracy of these simulations is essential for the Belle II experiment in investigating various physics phenomena.

By utilizing the Professor2 package for multi-parameter optimization, we systematically adjust Pythia8 parameters to achieve the best alignment between Monte Carlo simulations and experimental Belle II data. The tuning process includes automated sensitivity analysis, comparison with both on- and off-resonance Belle II data, and validation against previous Belle II Pythia6 tunes. All steps of the process, including parameter testing, optimization, and comparison, were automated to ensure efficiency and reproducibility. This comprehensive approach guarantees that the Pythia8 generator produces highly accurate simulations, improving the reliability of event reconstruction and subsequent analyses in Belle II physics.

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Implementations of the Finite Element Method for the Collective Model of Atomic Nuclei

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We propose new computational schemes, algorithms and programs of the finite element method for solving elliptic multidimensional boundary value problems in a polyhedral d-dimensional domain.

To reduce the boundary value problems to an algebraic one, the desired solution is sought as an expansion over the basis of piecewise polynomial functions constructed by joining Hermite interpolation polynomials and their derivatives at the boundaries of adjacent finite elements in the form of d-dimensional parallelepipeds.

The performance of the developed finite element schemes, algorithms and programs is demonstrated by solving benchmark boundary value problems for the five-dimensional harmonic oscillator used in the collective model of atomic nuclei. Calculations of the spectrum, quadrupole momentum and electric transitions of ^{154}Gd and ^{238}U isotopes is discussed.

This talk is based on [1]–[3].

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Dynamic Isotropic Percolation Process: Three-Loop Approximation

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The field-theoretic model of dynamic isotropic percolation process is studied. In particular, the topic of obtaining higher-order results within the framework of field-theoretic renormalization group is discussed and both analytical and numerical algorithms for calculation thereof are presented. The model is studied near the upper-critical dimension $d_c = 6$ and preliminary results for selected topologies of three-loop Feynman diagrams are presented.

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Turbulent Dynamo as Spontaneous Symmetry Breaking: α-Effect

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We investigate developed turbulence in stochastic magnetohydrodynamics (MHD) in the absence of mirror symmetry. In our study, the model is formulated as a certain statistical field theory, within which a general scenario of generation and renormalization of a homogeneous magnetic field arising in the turbulent regime (the turbulent dynamo) is formulated. This scenario is associated with the instability of the initial turbulent system and consists of its stabilization through the generation of an average homogeneous magnetic field B_0 via the mechanism of (dynamic) breaking of rotational symmetry. For the model in this regime, the turbulent electromotive force (EMF) is proportional to B_0 (the so-called α-effect), and the corresponding proportionality coefficient α is calculated in the one-loop approximation.

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A Class of Symmetric Three-Body Periodic Free-Fall Orbits

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In this work we consider a special class of symmetric periodic orbits for the free-fall equal mass three-body problem. For free-fall periodic orbits the bodies shuttle back and forth in a plane between two "stopped" triangles (bodies are with zero velocities at two instants) [1]. If the first "stopped" triangle is at time $t = 0$, then the second is at the half period – at $t = T/2$, where T is the period of the orbit. We are interested in a special class of free-fall periodic orbits with central symmetry, which have the additional property to fulfill the Eulerian half-twist conditions at $t = T/4$ and $t = 3T/4$. Using this property we conduct a specialized numerical search targeted only for this class of orbits. The search is based on Newton's method and uses high precision floating point arithmetic in order to overcome the sensitive dependence on the initial conditions.

Acknowledgement. The computations were performed in the "HybriLIT" platform and on the resources of the JINR Member States distributed information and computing environment (called the JINR DICE for short), Dubna, Russia. The work of I.H. is partially supported by the European Union-NextGenerationEU, through the National Recovery and Resilience Plan of the Republic of Bulgaria, project number BG-RRP-2.004-0008-C01.

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Optimization of the Accelerator Control by Reinforcement Learning: A Simulation-Based Approach

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Optimisation of the accelerator control is a critical challenge for the experimental particle physics. Such optimisations require substantial human effort in both real-life experiments and simulation-based studies. Finding the optimal tuning for the accelerator systems is complex, time-consuming, and resource-intensive task.

The primary goal of this study is to develop a library that would act as a co-pilot for physicists, by facilitating the accelerator control process. This solution is intended to reduce tuning time, improve operational efficiency, and save resources.

To address these challenges, we employed a simulation-based approach using Elegant [1] as a simulation backend. We developed a Python wrapper that enables seamless integration with Reinforcement Learning (RL) [2] algorithms, streamlining input management, simulation execution, and output processing. This wrapper is also suitable for other simulation backends like MAD-X, SixTrack, and Xsuite.

Using this wrapper, we created a custom RL environment specifically designed for accelerator optimization. Within this environment, we trained various RL models, such as [3] and [4], to tackle the particle transport problem, by focusing on improving the beamline transmission efficiency.

In this presentation, we demonstrate the application of our RL approach to an accelerator control problem and highlighte the improvements of efficiency and performance achieved through our methodology. We discuss how the integration of simulation tools with a Python-based RL framework may provide a powerful resource for the accelerator physics community, showcasing the potential of machine learning in optimizing complex physical systems.

Acknowledgement. This work was supported by the HSE Basic Research Fund.

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Adsorptions of Hg, Cn, Pb and Fl Elements on Trigonal Selenium Surface from Periodic DFT Calculations

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Recently, Chiera and coauthors [1] reported the experiment focused on adsorption behavior of elemental Hg also on the trigonal Selenium (t-Se) using gas chromatographic methods. This was done in order to prepare sensitive chemical separation and characterization of the transactinides Copernicium (Cn, Z = 112) and Flerovium (Fl, Z = 114).

To assist this experiment with the corresponding molecular modeling, we constructed several slabs made of trigonal Selenium with few different surface cuts. We calculated the adsorption energies of Group-12 (Hg, Cn) and Group-14 (Pb, Fl) elements using periodic DFT with relativistic effects included.

Our theoretical results show that the adsorption energies of Hg, Cn elements are close to each other, as well as are the adsorption energies of Pb, Fl elements. But adsorption energies Group-12 elements are substantially lower than the adsorption energies Group-14 elements. Therefore, in the future experimental separation and characterization the elemental Cn should be clearly distinct from the elemental Fl on the t-Se surface.

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Nonrelativistic Approximation in the Theory of a Spin 2 Particle with Anomalous Magnetic Moment

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We start with the 50-component relativistic matrix equation for a spin 2 particle in presence of external electromagnetic fields. This equation describes the particle with anomalous magnetic moment, the complete wave function consists of 2-rank symmetric tensor and 3-rank tensor symmetric in two indices.

We apply the general method for performing the nonrelativistic approximation, which is based on the structure of the 50×50 matrix Γ^0 of the main equation. With the use of the 7th order minimal equation for matrix Γ^0, we introduce three projective operators. They permit us to decompose the complete wave function into the sum of three parts, one is large, and two other are small in nonrelativistic approximation. We have found independent 5 large variables, and 45 small ones. In order to simplify the task, by eliminating the variables related to the 3-rank tensor we have derived relativistic system of 2nd order equations for 10 components related to symmetric tensor, and then take into account decomposition of these 10 variables into linear combinations of large and small ones. In accordance with general method, we separate the rest energy in the wave function and specify the orders of smallness for different terms in arising equations.

Further, after performing the needed calculations, we derive the system of five linked equations for five large variables. It is presented in the matrix form which has the nonrelativistic structure, where the term of additional interaction with external magnetic field through three spin projections is presented. The multiplier before this interaction contains the basic magnetic moment and an addition due to anomalous magnetic moment. The last characteristics is a free parameter of the theory.

Application of Minimax Optimization for Solving the Dirac Equation of an Electron in the Field of Two Fixed Attractive Coulomb Centers

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In this talk we present our variational solution of the two-center Dirac problem using a basis constructed by linear combinations of relativistic Slater type spinor wave functions with non-integer powers of the radii r_1 and r_2 on the two centers. The solutions are obtained by a minimax procedure that we have developed with a new iterative scheme. We use independent large and small components of the Dirac spinor. This permits us to take control of the spurious solutions, and gives us the possibility to avoid them by the appropriate choice of the wave function parameters. We investigate the behavior of the electron in its $1s\sigma g$ level of the diatomic homo-nuclear systems $A_2^{(2Z-1)+}$, where A represents the heavy element and Z its atomic number (up to $Z = 121$). Our approach has the advantage of needing small basis sets (maximal number of basis set is 62) for a relative error of the of $10^{-7} - 10^{-8}$. Our results are comparable to those obtained by the standard minimization procedure and the kinetic balance condition, for which several hundred basis sets should be used.

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Method for Alignment of Multilayer 2D Coordinate Detectors

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A method for track based alignment of the layers of 2-coordinate detectors is presented. Strait tracks from charged particles leave traces in 2D multilayer detectors. Having coordinates of those tracks in each layer we can estimate shifts and rotations of layers in common reference frame. Positions of the layers can be used to correct measured tracks for better spacial resolution of the detector. Also manufacturing quality can be estimated this way.

Parameterizing the Entanglement Body of a Qubit Pair

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A knowledge of the geometry and symmetries of states of finite-dimensional quantum models affords us to make not only generic statements about their physical content, but can strongly simplify many computational issues [1]. The symmetries of quantum models are realized exploiting the freedom of unitary changes of the basis of the Hilbert space associated to the quantum system. Such unitary operations, performed on the state space $\mathfrak{P}_n$ of an $n-$level quantum system comprised of two subsystems with n_A and n_B levels respectively, are divided into three categories [2]:

(i) *The global unitary transformations* $\mathrm{G} = SU(n)\,, \quad n = n_A n_B$;

(ii) *The local unitary transformations* $\mathrm{G_L} = SU(n_A) \times SU(n_B)\,$;

(iii) *The nonlocal unitary transformations* $\mathrm{G}/\mathrm{G_L} = SU(n)/SU(n_A) \times SU(n_B)\,.$

The operations (i) represent adjoint transformations of a density matrix $\varrho \in \mathfrak{P}_n\,,$

$$\mathrm{Ad}_g\, \varrho = g\varrho g^{-1}\,, \qquad g \in SU(n)\,. \tag{4}$$

The adjoint action (4) ensures an existence of equivalence relations between the states, $\varrho_1 \overset{SU(n)}{\sim} \varrho_2\,,$ and hence provides a global orbit type

stratification of $\mathfrak{P}_n$ with strata classified according to their isotropy groups $[H_\alpha] \subset G$:

$$\mathfrak{P}_n = \bigcup_{\mathrm{G-orbit\ type}} \mathfrak{P}_{[H_\alpha]} \,. \tag{5}$$

The second operations (ii) $g_L \in G_L$ act independently on the partially reduced density matrices $\varrho_A = \mathrm{tr}_B \varrho$ and $\varrho_B = \mathrm{tr}_A \varrho$, each describing the subsystem states:

$$\varrho_A \mapsto \mathrm{Ad}_{\mathrm{SU(n_A)}} \varrho_A \,, \qquad \varrho_B \mapsto \mathrm{Ad}_{\mathrm{SU(n_B)}} \varrho_B \,, \tag{6}$$

and therefore preserve all local characteristics of each subsystem. Finally, using the transformations (iii), a further classification of the states is achieved by "merging" together those states having the same local properties. After factoring out this local equivalence, the resulting structure containing information about the system's nonlocality is given by the *entanglement space*:

$$\mathcal{E}_{n_A \times n_B} = \mathfrak{P}_n / SU(n_A) \times SU(n_B) \,. \tag{7}$$

The components $\mathfrak{P}_{H_\alpha}$ in (5) are given locally as the following direct product of two factors:

$$\mathfrak{P}_{[H_\alpha]} = \Delta_n^{(\alpha)} \times G/H_\alpha \,, \tag{8}$$

where $\Delta_n^{(\alpha)}$ is a subset of the ordered $(n-1)$-simplex of eigenvalues of the states with a given algebraic degeneracy corresponding to the isotropy group H_α. Particularly, for the states with a non-degenerate spectrum, the isotropy group is the maximal torus $H_1 \simeq T^{n-1}$, and $\Delta_n^{(1)}$ is the interior of the simplex Δ_{n-1}. Using (8) we arrive at the entanglement space decomposition taking into account a double coset decomposition of $SU(n)$,

$$\mathcal{E}_{n_A \times n_B} = \bigcup_{\mathrm{orbit\ type\,[H_\alpha]}} \mathcal{E}_{n_A \times n_B}[H_\alpha] \quad = \bigcup_{\mathrm{orbit\ type\,[H_\alpha]}} \Delta_n^{(\alpha)} \times G_L \backslash G / H_\alpha \,. \tag{9}$$

In our report we consider in detail the generic component, $\alpha = 1$, of (9) for a pair of qubits ($n_A = n_B = 2$), i.e., a subset of $\mathfrak{P}_4$ which consists of maximal rank states with a non-degenerate spectrum and isotropy group $T^3 \subset SU(4)$,

$$\mathcal{E}_{2\times 2}[\mathrm{T}^3] = \Delta_3 \times \mathbb{B} \,, \tag{10}$$

where $\mathbb{B}$ denotes the 6-dimensional double coset:

$$\mathbb{B} = SU(2) \times SU(2) \backslash SU(4) / T^3 \,. \tag{11}$$

Based on a recently proposed parameterization of $SU(4)$ group [3], we prove that $\mathbb{B}$ admits the coordinate chart given by the direct product of two regular octahedrons $\mathcal{O}_h \times \mathcal{O}_h$ with the edges length $2\pi\sqrt{2}$. The algebraic structure of the entanglement body (10) is described and a related problem of the separability of mixed states of two qubits is discussed within the algebraic framework (cf. [4], [5] and references therein). Using the Peres-Horodecki separability criterion of quantum states [6],[7], the system of inequalities in nine independent Singular Value Decomposition (SVD) variables of the density matrix is obtained. The SVD variables include the eigenvalues of $\varrho \in \mathfrak{P}_4$ and 6 out of the 15 angles which parameterize the diagonalized $SU(4)$ matrix in SVD of ϱ. The introduced six SVD angles are the moduli parameters of the double coset $\mathbb{B}$.

Apart from this, the system of inequalities determining the separable states of a qubit pair is also rewritten in terms of the Bloch vector length r and two angles on the spherical triangle on $\mathbb{S}_2(\sqrt{\frac{3}{4}}\, r)$ [8] and six coordinates on the double coset $\mathbb{B}$.

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Speaker Tagging Correction with Non-Autoregressive Language Models

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Speech applications dealing with conversations require not only recognizing the spoken words but also determining who spoke when. The task of assigning words to speakers is typically addressed by merging the outputs of two separate systems, namely, an automatic speech recognition (ASR) system and a speaker diarization (SD) system. In practical settings, speaker diarization systems can experience significant degradation in performance due to a variety of factors, including uniform segmentation with a high temporal resolution, inaccurate word timestamps, incorrect clustering and estimation of speaker numbers, as well as background noise. Therefore, it is important to automatically detect errors and make corrections if possible. We used a second-pass speaker tagging correction system [1] based on a non-autoregressive language model to correct mistakes in words placed at the borders of sentences spoken by different speakers. We first show that the employed error correction approach leads to reductions in word diarization error rate (WDER) on two datasets: TAL and test set of Fisher. Additionally, we evaluated our system in the Post-ASR Speaker Tagging Correction challenge [2] and observed significant improvements in cpWER compared to baseline methods.

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Small-Angle Scattering and Neutron Reflectometry Methods in the Study of Magnetic Nanoparticles in Magnetic Fluids and Their Composites

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The possibility of using neutron and X-ray scattering methods for nanoscale structural investigations will be discussed in detail, drawing on our extensive experience over the last 10 years. Namely, results from neutron reflectometry [1] and small-angle neutron scattering for nanoscale characterization of magnetic nanoparticles (MNPs) in bulk and at interfaces will be presented. The structural analysis of various magnetic fluids (MFs), MNPs with bio-macromolecules (e.g., magneto-ferritin, amyloids, and magnetosomes), textile-based nanocomposites with MNPs [1], and ferronematics (composite systems of liquid crystal (LC) with MNPs) will be described. A special focus will be on MNPs clustering in an LC matrix and their alignment in different LC phases [3]. Additionally, the interaction between surfactant/polymer molecules used in the stabilization of MFs were investigated, which is crucial for synthesizing stable MFs with controllable properties. The effect of external magnetic and electric fields on MNPs behavior based on neutron scattering data will also be presented. The structure of

all studied systems will be modeled and presented using neutron and X-ray data.

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Three-Body Problem and Precision Physics

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A review of the modern methods in the Coulomb three-body problem will be presented. Variational methods for the nonrelativistic Schroedinger equation, relativistic corrections, and the Nonrelativistic QED will be discussed.

Application of the methods developed to various fields of physics like physics of exotic atoms (antiprotonic/pionic/kaonic helium, μCF), or precision spectroscopy of the hydrogen molecular ions H_2^+ and HD^+. Impact on the fundamental physical constants, precision determination of masses of particles and antiparticles, search for new physics will be given.

Polarization Drift Compensation Using Supervised and Reinforcement Learning

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Quantum key distribution (QKD) systems are widely used to secure the communication channels. Due to temperature fluctuations and mechanical deformations, the refractive index of the optical fiber can fluctuate, thereby causing random changes in polarization states on the receiver side. A polarization controller on the receiver side is used to compensate these distortions.

To minimize QBER the polarization controllers (PC) are used on receiving side. In general they are controlled by rule-based [1] and coordinate descent systems [2]. In this work we propose a framework of PC modeling and method of PC real-time tuning using different machine learning approaches: supervised and reinforcement learning (RL).

We find that the QBER stores the information about the way to adjust the actuators of the PC to minimize the error rate and compensate distortions in quantum channel. Using this observation, we create dataset for supervised learning and environment for RL. Then we train simple multilayer perceptrons to predict voltages of actuators of PC, taking as input QBER values. As a result, using RL model we achive the convergence to 2.5 % of QBER in modeling and 10 % of QBER in real-time setup tuning in 10 steps.

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A Web Application for Fitting Experimental Data Using JINR Cloud Infrastructure and ROOT Package Tools

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The FITTER_WEB application was developed to solve the problems of fitting experimental data with multiparameter theoretical functions reflecting model representations of the objects under study [1]. The user is given full control over the fitting process, as well as the ability to use the built-in ROOT mechanisms of parallelism. The contribution describes the structure of the web application, the software tools used for its development, and the specifics of deployment to the JINR cloud infrastructure. The results of the FITTER_WEB analysis of the small-angle scattering data on a samples of polydispersed populations of phospholipid-based unilamellar vesicles are presented [2]. The issues of optimizing the web application related to the allocation of computing resources in the JINR cloud, as well as multi-user calculations, are discussed.

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Machine Learning for Cyclotron Magnetic Field Isochronization

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This article explores the application of machine learning techniques to the isochronization of the magnetic field in the MSC-230 isochronous cyclotron. The primary objective is to reduce the computational effort typically required for adjusting the magnet geometry to achieve isochronicity. By predicting the necessary modifications to the magnet's geometry, our approach aims to streamline the iterative process. We compare several machine learning models against traditional methods, demonstrating their potential to reduce the number of iterations needed.

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Finite Difference Models of Dynamical Systems with Polynomial Right-Hand Side

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One of mathematical models most widespread is a dynamic system described by a system of ordinary differential equations

$$\frac{d\vec{x}}{dt} = \vec{f}(\vec{x})$$

with polynomial right-hand side. As a rule, from physical reasons a few integrals of motion are known, but they are not sufficient to reduce the system of differential equations to Abel quadratures. Unable to reduce the system to quadratures, we are forced to solve it numerically. Having solved the many-body problem using the explicit Runge-Kutta method, we can only sadly watch as the mechanical energy of the system changes, and closed trajectories turn out to be open.

From general considerations, it follows that any mechanical system should define a one-to-one correspondence between the initial and final positions of the system. In order to construct a difference scheme that imitates this property, we can try to approximate the original Hamiltonian system by equations that define a birational correspondence between the initial and final points.

It is easy to see that this can always be done for systems with a cubic Hamiltonian, using a method that arose in the field of solitonics [1]; some authors associate it with the name of W. Kahan, others with the names of Hirota and Kimura [2], [3]. We came to it when searching for a discrete analogue of the Painlevé theory [4].

As an example of such a dynamic system, a top fixed at its center of gravity is considered in detail, see also [5]. In this case, the discrete theory repeats the continuous theory completely:

1. the points of the approximate solution lie on some elliptic curve, which at $\Delta t \to 0$ turns into an integral curve;

2. the difference scheme can be represented using quadrature;

3. the approximate solution can be represented using an elliptic function of a discrete argument.

The general solution of the elliptic oscillator defines a birational transformation on the integral curve, which does not extend to a birational transformation of the entire phase space. Using Kahan's method we approximate this solution by a birational transformation of the entire space, for which we correct the integral curve, preserving its genus. Thus, Kahan's scheme imitates the elliptic oscillator, but does not reproduce its properties exactly.

Transferring the developed technique to the case of equations with a polynomial right-hand side does not cause significant difficulties, since back at the beginning of the 20th century G. G. Appelroth [6] proposed a method that allows, by increasing the number of unknowns, to reduce a system with a polynomial right-hand side to a system with a quadratic right-hand side. This procedure was later called quadratization [7].

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Molecular Dynamics of the FUS Protein Fibril: Phosphorilation Effect

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Polymerization and phase separation of proteins containing low-complexity (LC) domains are important factors in gene expression, mRNA processing and trafficking, and localization of translation. We performed the all-atom Molecular Dynamics (MD) simulation to address the stability and spatial dimensions of self-assembling fibrils formed by the LC domain of the fused in sarcoma (FUS) RNA-binding protein. The 214-residue LC domain of FUS (FUS-LC) is destabilized by phosphorilation of the specific amino acid residues. We have estimated the radius if gyration of the FUS-LC fibrils, the number of intra-molecular hydrogen bonds, and other characteristics describing the structure of fibril. These studies offer a structural basis for understanding LC domain self-assembly, phase separation, and regulation by post-translational modification. The obtained results are qualitatively agreed with the experimental ones [1].

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Neural Networks in the Baikal-GVD Experiment: Selection of Neutrino Events and Neutrino Energy Reconstruction

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Baikal-GVD is a neutrino telescope with an effective volume of approximately 0.6 km^3 located in Lake Baikal. To facilitate observations within the framework of neutrino astronomy, two critical event processing challenges should be addressed:

1) the isolation of the neutrino-induced events from background events caused by extensive air showers (EAS), and

2) the reconstruction of ν event parameters, such as the energy of the corresponding muon.

This study presents a machine learning approach, specifically utilizing neural networks, to address these challenges. For the first problem, Monte Carlo simulations demonstrate that convolutional neural networks can preserve 50 % of neutrino-induced events while achieving the desired background suppression factor of 10^6. Regarding the second problem, we develop a neural network model that predicts both the energy and its associated uncertainty for a given event, employing a specialized loss function. On Monte Carlo simulated data we achieve an error factor of 3 for a wide range of energies (from 10 GeV and above) and a factor of 2 for high energies (from 10 TeV and above).

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Hypernuclei Signal Reconstruction in the BM@N Experiment

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One of the main physics tasks at the NICA complex is the analysis of strange particles and hypernuclei, the increased yield of which can be a sign of the phase transition between nuclear matter and quark-gluon plasma. The report presents the results of the analysis of hypernuclei birth in the BM@N experiment. Algorithms for extracting particle energy losses in tracking detectors to separate double-charged fragments from single-charged particles are shown. The first observations of the hypernuclei signals are shown.

Mathematical Analysis of Interactions in Ferronematics

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Ferronematics are magnetically active anisotropic fluids. They are a manifestation of the idea of Brochard and de Gennes, who suggested that doping liquid crystals by magnetic particles may enhance their sensitivity to magnetic fields. They have developed the continuum theory of magnetic suspensions in nematic liquid crystals [1]. The ability of liquid crystals to become oriented by electric or magnetic fields is due to the anisotropy of their dielectric permittivity (ε_a) or diamagnetic susceptibility (χ_a). The influence of the field is usually tested experimentally in sandwich cells, where a nematic or ferronematic layer fills the gap of thickness D between two parallel flat glass plates. In order to calculate the threshold fields one has to consider the free energy density of the system. The situation is becoming slightly more complicated if the liquid crystal is subjected to both electric and magnetic fields, as the two fields may be either perpendicular or parallel with each other.

Though the first theory of ferronematics [1] pretended $\boldsymbol{m} \parallel \boldsymbol{n}$, experiments in some thermotropic ferronematics [2] have proved that in the studied case the presence of a parallel orientation of $\boldsymbol{m}$ and $\boldsymbol{n}$ can be excluded. Therefore the theory has been revised and expanded by Burylov and Raikher [3, 4] considering a finite value of the surface density of anchoring energy W at the nematic–magnetic particle boundary. The anchoring energy, as well as the parameter ω defined as the ratio of the anchoring energy to the elastic energy of the liquid crystal ($\omega = Wd/K$, where d is the size of the magnetic particles and K is the orientational-elastic Frank modulus), characterize the type of anchoring of the nematic director on the surface of the magnetic particle. The condition $\omega \gg 1$ corresponds to the rigid anchoring. When $\omega \leq 1$ the anchoring is soft which, unlike the rigid anchoring, permits both $\boldsymbol{m} \parallel \boldsymbol{n}$ and $\boldsymbol{m} \perp \boldsymbol{n}$ boundary conditions. By these extensions the Burylov–Raikher theory could be successfully applied for ferronematics. In its frame the destabilization of the uniform texture of ferronematics exposed to external magnetic or electric field (the Fréedericksz transitions) could be described and the expressions for their critical fields in different geometries could be derived. Their results were used for interpretation of our experiments.

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Modified Transport Approach for Description of Fragmentation Reactions in Heavy-Ion Collisions

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Nuclear reactions in which the projectile is fragmented in two of more pieces are widely used to study the characteristics of nuclear matter, to produce secondary beams and to obtain new isotopes. It is important to be able to predict the isotope distributions of fragments obtained in these reactions. Different transport approaches are used to get the results [1]. In this report calculations in Boltsman–Nordheim–Vlasov approach are presented [2], it is shown that transport type calculations produce excited fragments and the statistical codes should be used to obtain cold fragments to be able to compare the results of calculations with experimental data. In this report we show how to take into account the dependence of excitation energy of the fragment on its mass number and how to find the balance between the time of model calculation and their precision. The comparison with the QMD predictions [3] are given and the difference of two approaches is discussed.

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Construction of Fisher Information Matrix for Multiparametric Problem in Super-Resolution Optical Fluctuation Imaging

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Diffraction of light limits the spatial resolution of classical optical microscopes. Recently, a number of super-resolving techniques have been proposed: stimulated-emission depletion microscopy, super-resolving imaging based on fluctuations of fluorescence markers, structured illumination microscopy, quantum imaging. Development of new approaches forced the researchers to revisit the notion of optical resolution. Instead of quantifying visual distinguishability of small features (such as Rayleigh criterion) or analyzing Fourier components transfer, one can perceive the collected images (raw datasets) as abstract sources of information about the investigated sample and define the spatial resolution as the smallest size of the sample details, such that the input signal (image) provides enough information for their reconstruction [1]. A powerful tool for quantification of the information content of signal datasets is Fisher information [2]. It describes sensitivity of the acquired signal (image) to variation of the sample parameters of interest and is connected to the errors of their estimation by Cramer-Rao bound.

Construction of Fisher information matrix (FIM) includes integration over all possible values of the multivariate random signal. The number of components in the signal equals at least the number of detector pixels, but may be much higher if correlation functions (photon coincidences) are used. In quantum imaging, FIM calculation is feasible since the signal components are independent and obey Poisson distribution [3]. The problem becomes much harder for super-resolution optical fluctuation imaging (SOFI) — a technique based on collecting series of frames for stochastically fluctuating fluorescent emitters and constructing cumulant images. Due to image blurring and emitters' fluctuations, the signal components become statistically dependent and include non-Poissonian noise components. Construction of FIM for SOFI has been reported for a single-parameter problem of estimating separation of 2

point-like emitters [4]. Here, we address multiparametric SOFI problem: estimation of positions and intensities of multiple fluorescent emitters. The solution is based on multivariate normal approximation of the signal distribution and includes: 1) automated expansion of the expressions for the expectation values and covariances of the cumulant image components in terms of emitters' signal moments; 2) numerical estimation of the requested moments by sampling emitters' fluctuations and shot noise; 3) construction of the FIM for a specific sample model. The calculations were performed at HPC system Shaheen III in KAUST (Saudi Arabia) and demonstrated successful construction of FIM up to the 4th order of cumulative images in SOFI.

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Quantum Field Renormalization Approach to Magmethydrodynamics: Analysis in Elsasser Variables

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We are interested in the stochastic magnetohydrodynamics (MHD) process define by the Elssaser variables which is more advantage for noncompressible MHD description. The stochastic process is rewritten into a quantum field model using the Martin-Siggia-Rose formalism. We proceed by using the renormalization group (RG) approach to study large-scale (infrared) behavior of the physically interesting correlation functions. The RG investigation is carried out up to the second order of perturbation theory and the stable infrared fixed points, the area of stability are determined. The RG analysis is performed using a small expansion parameter ε, which describes deviation from Kolmogorov scaling law. Finally, the critical dimensions of physically interesting functions in the inertial range interval are presented.

Computational Environment for the Numerical Modelling of Hybrid Superconductor/Magnetic Nanostructures

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The successful study of hybrid superconductor/magnetic nanostructures requires the utilisation of advanced computing technologies, software environments, data analysis and visualisation tools, and parallel programming to accelerate calculations on hybrid computing architectures. A notable reduction in the time required for the study of magnetization control mechanisms and the properties of magnetic excitations can be achieved through the adaptation of algorithms for use in high-performance computing architectures. One of the tools that increases the efficiency of such researches is the JupyterHub-based computing environment developed at MLIT JINR. This environment provides opportunities for solving problems of numerical simulation of hybrid superconductor/magnetic nanostructures on ML/DL/HPC HybriLIT platform, convenient organization of calculations and visualization of simulation results.

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An Approach to Quantum Channel State Estimation Based on Machine Learning Models

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Quantum key distribution (QKD) systems require a post-processing procedure to form a common key, with error correction (EC) being one of the most computationally complex and time-consuming stage. For EC using low-density parity check codes, one of the parameter selection approaches relies on a priori quantum bit error rate (QBER) estimation [1], [2]. Existing algorithm utilizes physical equations and statistics for error rate estimation, which can be unstable and sensitive to distribution outliers.

Precision of the estimation is crucial for optimal code rate choice. We thus propose a novel approach to predict the QBER using machine learning and time series forecasting. We develop several machine learning algorithms for time series forecasting, including deep learning [3] and gradient boosting with autoregressive components [4], along with a Python module for training and evaluation on real data samples. The objective of the study is to integrate the models into QKD systems using microservices for online forecasting and investigate whether these methods outperform classical approaches in experiments on real transmitters.

Our study demonstrates that the proposed forecasting techniques improve the quantum key correction speed in a series of experiments. The result of this study helps advance the research in quantum cryptography, increasing quantum key generation speed in high-performance QKD systems.

Acknowledgement. This work was supported by the HSE Basic Research Fund.

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A Fourier-Modal Approach to Free-Form Simulations of Diffractive Optics

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The simulation of coherent monochromatic light scattering on a periodic structure is a ubiquitous problem in science and technology. There are a variety of mathematical approaches to solve it. In the context of periodic nanostructures, a Fourier modal approach is a natural choice for the computations. However, this approach is limited to structures that are uniform in the direction normal to the surface. Conventionally, this problem is solved by approximating the structure by a stack of vertically uniform layers: a lamellar approximation, solving the Maxwell equations for each layer, and stitching the solutions across the stack. This requires first creating a geometric model of the structure and then discretizing it. Therefore, each new type of structure requires reinventing the geometric model, which is tedious.

An idea to extend the Fourier modal approach to the vertically non-uniform structures was proposed by Huang et.al [1]. They found the Fourier modal solution for the 1D photonic crystal periodic in the direction normal to the surface without discretizing it on uniform layers. In our work, we have extended this idea to a 2D structure. Namely, we consider the diffraction grating as a 2D photonic crystal periodic in both the lateral and vertical directions. We found the solution of the time-harmonic Maxwell equations for such a structure. We then set the boundary conditions so that the thickness of the structure is exactly one period in the vertical direction. This allows us to simulate diffraction gratings by considering only a Fourier transform of the scattering potential in a primitive cell, and no discretization on layers is required. Furthermore, it allows to consider the grating without explicitly defining the geometry. An example of such a calculation is shown in the Figure 1. Instead of solving the equations in each layer, the new approach allows to consider the structure by its form factor and solve the near-field problem in one go. The mathematical details of this approach will be discussed in the talk.

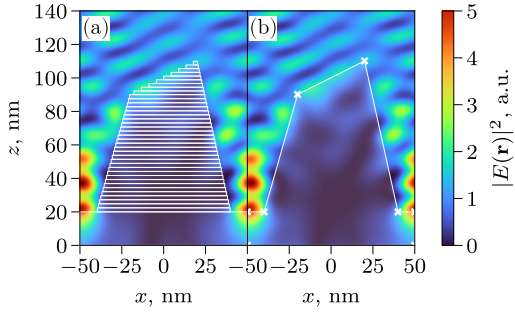

Figure 1: Near-fields calculated using the Fourier modal approach in (a) the conventional lamellar approximation and (b) using the free-form approach. Calculation parameters: silicon grating with 100 nm period, incident photon energy $\hbar\omega = 500$ eV, angle of incidence $\alpha_i = 5°$, calculated for conical mount.

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Track Reconstruction Transformer: A Scalable Deep Learning Approach for Particle Tracking in High-Energy Physics

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Particle track reconstruction is crucial for high-energy physics, particularly in high-luminosity environments where traditional methods encounter limitations in scalability and efficiency. To overcome these challenges, we introduce the Track Reconstruction Transformer (TRT), a novel deep learning model inspired by the Detection Transformer (DETR) that offers significant advancements in particle trajectory prediction [2]. TRT leverages a Transformer architecture to process detector hits and directly predict particle track parameters, generating a set of potential tracks, each with an associated probability indicating the likelihood that it represents an actual track to account for the variable number of tracks per event. This approach adopts the parallel processing efficiency of DETR, offering significant speed and scalability advantages compared to conventional methods. The TRT model is based on the Point Cloud Transformer backbone [1] [2] and has been evaluated using a toy dataset with helical track approximations and uniform noise hits. We present details on the model's implementation, training, and performance, including strategies to address the $O(N^2)$ complexity of transformers. While current tests focus on processed hits, we also discuss the potential for adapting TRT to raw detector data (avoiding the hit reconstruction phase) in future work, leveraging the flexibility of transformer architectures for even broader applicability.

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On Precursors of Topological Phase Transitions of Interacting Particles Confined in a Disk Potential

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Phase transitions in quasi-two-dimensional systems of interacting particles play an important role in the physics of nanomaterials. The physical and chemical characteristics of such systems depend on their structural properties, that can change during phase transitions under the influence of external conditions (e.g., temperature). Until now, the main attention is paid to the search of phase transition in infinite two-dimensional systems [1], [2]. One of the central issues of such an analysis is the illumination of the conditions for onset of the hexatic phase, accompanied by the appearance of defects in the Wigner crystalline phase at a certain temperature. However, a fundamental question arises on the critical number of particles at which the symmetry of the crystal lattice in the system under consideration begins to be broken as well [1], [2].

In this work, we investigate two-dimensional systems of interacting particles confined by an infinite lateral potential with a circular symmetry [3]. Using the approach developed by the authors, we propose a computational algorithm for searching of precursors of phase transitions with an increase in the number of particles in the considered system. This approach is focused on a simultaneous study of the topological characteristics of the system and a joint orientation-translational correlation analysis of structural changes occurring with an increase of the number of particles.

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Plasma Diagnostics in High Magnetic Fields

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The determination of the magnitude of magnetic field occupies an important place in the diagnostics of higher temperature hydrogen plasmas in external magnetic fields. The use of spectroscopic methods in hydrogen plasmas is extremely difficult because of the large Doppler and Stark broadening of spectral lines [1]. The measurement of the magnetic field by observation of the Faraday rotation of the polarization plane of light by the conduction electrons is applicable only for fairly dense plasmas in high magnetic fields [2].

Here we examine theoretically the possibility of determining the magnitude of the magnetic field in a hydrogen plasma based on the resonant Faraday rotation of the polarization plane of light by residual natural atoms in the plasma (or by specially introduced impurity atoms). We note that this method can also be used to determine the density of neutral component in a plasma when the magnetic field is known. In our earlier studies [3], [4] the average and local magnetic field and neutral atom density were found in plasma.

The Faraday effect is closely coupled to the splitting and shifting of the energy levels of hydrogen atoms in a magnetic field (the Zeeman and Pashen-Back effects). Usually the hydrogen plasma is in a magnetic field $H \geq 10^3$Oe. For such fields the magnetic splitting parameter $\mu_0 H$ in hydrogen becomes comparable to the fine structure interval ($\delta E \approx 10^{-1}\text{cm}^{-1}$) so that the Pashen-Back effect appears.

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Hockey Stick Model Reveals a Dose Threshold for the Residual Foci of DDR Proteins

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Ionizing radiation (IR) is commonly used in the diagnosis and treatment of cancer, affecting not only cancer cells but also normal fibroblasts. Depending on the IR dose, dose rate, and its physical properties, fibroblasts may experience cell death, senescence, or excessive protein production. This can lead to negative tissue effects such as inflammation and fibrosis.

DNA double-strand breaks (DSBs) are the most critical type of DNA damage caused by IR. The repair of these breaks determines the cell's fate: proliferation, senescence, or death. Cells with unresolved DNA damage may become cancerous. The most sensitive method for analyzing DNA DSBs is immunocytochemical analysis of DNA damage response (DDR) proteins, including γH2AX, 53BP1, and pATM. These proteins form DNA damage foci, which are crucial for DNA repair. The protein p53, phosphorylated at serine 15 (p-p53 Ser-15), also forms foci and is involved in DDR. In irradiated fibroblasts, the number of γH2AX, 53BP1, and pATM foci increases dose-dependently, peaking 0.25 to 1 hour post-radiation, then decreases, though some residual foci may persist for 24 hours or longer. Residual γH2AX foci can indicate cell viability loss and serve as a prognostic tool for radiation-induced cell death.

This study aims to investigate the dose responses of residual yH2AX, 53BP1, pATM, and p-p53 (Ser-15) foci in human fibroblasts 24–72 hours after exposure to 0.1–5 Gy of X-rays.

The experimental data analysis performed with the hockey stick model showed the presence of a dose threshold for the residual foci of all proteins studied. The threshold dose varied from 1.19 (24 h) to 0.79 (72 h) Gy for yH2AX foci, from 1.04 (24 h) to 0.84 (72h) Gy for 53BP1 foci, from 0.77 (48 h) to 0.43 (72h) Gy for pATM foci and from 1.28 (48 h) to 0.17 (72 h) Gy for p-p53 (Ser-15) foci. The estimated threshold doses are close to the quasi-threshold dose ($Dq = 0.99 \pm 0.09$ Gy) calculated from the cell survival curve.

Summarizing our findings, we show, for the first time, that the residual foci curve in X-ray irradiated normal human fibroblasts has a dose threshold. The values of the threshold dose and Dq in irradiated fibroblasts are very close. The excellent agreement between the calculated values of the threshold dose and Dq in irradiated fibroblasts proves that residual foci are sites, where cells are still attempting to repair potentially lethal DNA damage.

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Machine Learning for Particle Identification at MPD

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One of the significant tasks (at the offline analysis stage) at the MPD experiment is charged particle identification (PID). There are conventional PID algorithms based on direct measurements of energy loss in the Time Projection Chamber and mass measurements provided by information from the Time-of-Flight system. Over the last ten years, machine learning approaches have become widely used in high energy physics problems in general and in PID in particular. This is due to the fact that conventional PID algorithms have poor performance in the high momentum range. This work is devoted to the machine learning application for PID in the MPD experiment. Current research results will be demonstrated.

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Production System of the SPD Experiment

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The SPD experiment at the NICA collider at JINR is under construction. But despite this, processing requests for simulation and reconstruction algorithms tuning already require significant computing resources, and the results of data processing occupy a fairly large disk space. For example, a standard request for the generation of 20 million events involves two calculation steps (simulation and reconstruction) and the generation of 10 terabytes of data and 15 thousand output files, not taking into account service files with processing logs. It is clear that in order to quickly generate the required data sets, it is necessary to create a system that would automate the generation of jobs, distribute them across available computing resources and manage the output data. To solve this problem, a production system for the SPD experiment is being developed. This system is created in line with the data streams recorded in the TDR, and should ensure their reliable storage and processing. The current status of work on the creation of a production system for the SPD experiment is presented in this report.

Acknowledgement. The study was carried out with the financial support of the Russian Science Foundation No. 22-12-00109, `https://rscf.ru/project/22-12-00109/`.

Shifting from Slurm to Kube-Scheduler for Efficient Cloud-Native HPC Workloads with the Shoc Platform

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This paper introduces an innovative approach to executing High-Performance Computing (HPC) workloads using serverless methodologies in the cloud, specifically by leveraging the Kubernetes scheduler as an alternative to the traditional Slurm[1] scheduler. The Shoc[2] (Serverless HPC Over Cloud) system is extended to utilize Kubernetes for optimal scheduling of various workflows, including single-node tasks and clustered workloads such as MPI[3] jobs. By modeling Slurm's resource allocation, scheduling, and batching concepts within Kubernetes, this work demonstrates the feasibility and advantages of this paradigm shift.

Slurm, the de facto standard for HPC workload management, offers advanced resource management and sophisticated scheduling algorithms tailored to HPC environments. It provides fine-grained control over CPUs, memory, and GPUs, supporting complex job constraints and affinity rules. In contrast, Kubernetes focuses on containerized applications, managing resources at a higher abstraction level. The kube-scheduler provides flexibility and scalability, with enhanced orchestration, containerized execution, and cloud-native integration, though it traditionally lacks Slurm's hardware-specific granularity.

Through comparative analysis, this paper shows how the Kubernetes scheduler, when controlled by the Shoc system, can mimic and extend Slurm's capabilities. It highlights real-world examples to illustrate the additional benefits Kubernetes offers, such as improved resource utilization, seamless scalability, and increased workflow flexibility. The results indicate that using Kubernetes for HPC workloads provides a compelling alternative for future HPC environments, combining the strengths of container orchestration with the demands of high-performance computing.

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Electron-Hydrogen Compton Scattering at High Momentum Transfer: Calculations of Second Born Singular Integrals

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The quasielastic collisions of electrons with atoms and molecules at high momentum transfers attract now the interest of scientists (see for example [1] and references within). Account of the nucleus motion after a kick with a few keV electron leads to unexpected effects in shapes of differential cross sections, calculated with the first and second Born approximations (see Fig. 1).

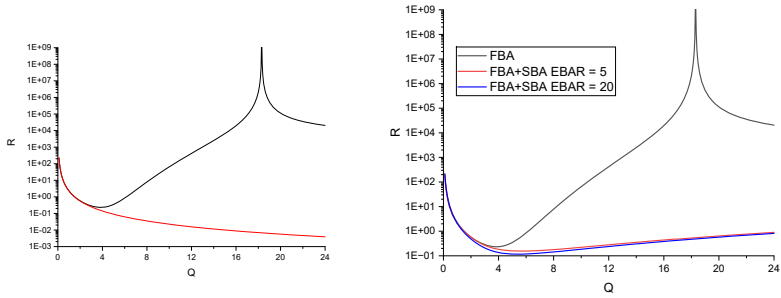

Figure 1: Left panel: FBA (black curve, $m_N = 1836$ a.u., red curve, $m_N = \infty$). Right panel: SBA with different closure approximation parameter $\bar{\varepsilon}$.

We consider the atomic scattering reaction $e+H(1s) \to e+H^*(2s, 2p)$ and calculate the value $R = \sigma(2p)/\sigma(2s)$ versus the momentum transfer $Q = |\vec{k}_0 - \vec{k}_s|$, i.e ratio of differential cross sections with different final excitation.

In this talk we discuss the way of calculation of singular SBA integrals with use of the closure approximation. The results show a noticeable contribution of the SBA if the parameter is disposed in the range of intermediate continuum excitation.

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Numerical Scheme for Relativistic Boltzmann Equation with Spherical Geometry

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We present our numerical method for solving relativistic Boltzmann equation for relativistic plasma of electrons, positrons and photons adopting spherical symmetry. We consider collision integral for binary processes between electrons, positrons and photons. All binary processes are calculated from QED matrix elements in the Born approximation. We the transport term we apply second order piecewise linear reconstruction scheme. The scheme is conservative and satisfies both energy and particle.

Acknowledgement. This work was supported by BRFFR grant № F23IKR-001.

Fluence and Absorbed Dose Calculations for the Biological Samples Irradiated with Heavy Ion Beams at the Long-Term Modes

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Applied research program at NICA accelerator complex assumes a wide range of experiments in life sciences dealing with various outcomes in living organisms as a result of the heavy ion exposure. Planning of these experiments requires simulation of radiation conditions for samples be irradiated. This study is focused on determination of necessary fluence and absorbed dose values for the experiment with exposure of yeast cells to heavy ions in order to select mutants with increased accumulation of squalene. Squalene is an important polyunsaturated triterpene with wide applications in the food, pharmaceutical and other biotechnology industries [1].

Currently, the main methods for squalene production are extraction from oil-producing plants, microbial fermentation with Saccharomyces cerevisiae, but the scale economic viability are limited. Radiation-induced mutagenesis is one of the alternative ways to obtain mutant strains with improved squalene production. In this regard, the use of heavy ions as a mutagen is of great interest because of their high biological effectiveness [2].

To calculate the fluence and absorbed dose values, we assume that Petri dishes with yeast cultures on solid media are placed perpendicular to ion beam and that Petri dishes are stacked to a pack of 1–8 pieces. As a test data set, we use data taken in long-term exposure mode during the adjustable run of NICA complex and LTS ARIADNA facility in December 2022 – January 2023. The beam intensity was analysed as it was done for the solid materials previously, assuming different energy losses in pack of the biological samples [3], [4].

Dosimetry calculations were done for the set of absorbed doses expected to be most effective in terms of for producing mutant cells.

Geometry of ion beam having a uniform central part and halo is taken into account in calculations. Beams of 54Xe131 ions with the energy of 500–4000 MeV/nucleon were selected for the analysis. The particle fluence and absorbed doses were calculated taking into account the intensity of the ion beams extracted from Nuclotron accelerator of the NICA complex.

The results of calculations provide a necessary input for planning experiments with radiation exposure of yeast cells aiming at obtaining a novel biotechnology method for increased production of squalene.

The study is performed within the ARIADNA collaboration [4].

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Chaotic Features of a Stack of Long Josephson Junctions with Inductive and Capacitive Couplings

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We have studied the chaotic features of the high temperature superconductors numerically. This structure is simulated as a stack of long Josephson junctions with inductive and capacitive couplings between different junctions in the stack. It is found that the chaotic features are triggered by the moving fluxon and interjunction coupling. It is well known that usually an external radiation produces the chaotic effects in the single junction. We expect that even in the absence of the external radiation the periodic motion of fluxons in long Josephson junction leads to the appearance of chaotic dynamics in the stack of long Josephson junctions. The chaotic features of the stack of coupled long Josephson junctions are analyzed by calculations of the Lyapunov exponents. We compare results for a stack of junctions with the case of a single junction and discuss the origin of the observed chaos and effects of the coupling between the junctions.

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Simulation of a Controllable Magnetization Reversal in a Chain of Phi-0 Junctions by an Alternating Voltage Pulse

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In φ_0 Josephson junctions, the spin-orbit interaction in a ferromagnet layer provides a mechanism for direct coupling between the magnetization and the superconducting current, which makes it possible to control the magnetic properties by means of the Josephson current, as well as the effect of magnetization on the Josephson current. Recently, the possibility of developing cryogenic memory based on the magnetization reversal in the φ_0 junction has been studied. However, when using several φ_0 junctions in a single chip, it becomes necessary to realize the magnetization reversal in a selected φ_0 junction. We propose a solution to this problem based on mathematical modeling of the dynamics of a system consisting of three φ_0 junctions connected via LCR-circuits, which is reduced to solving the Cauchy problem. It is shown that by applying an external alternating voltage pulse with a frequency coinciding with the eigenfrequency of the LCR-circuit, it is possible to realize the magnetization reversal in a selected φ_0 junction, i.e. the possibility of controlled reversal of magnetization is demonstrated. The influence of system parameters on the dynamics of magnetization in each of the φ_0 junction is studied in detail. We have developed a software module for the performed calculations.

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Specifics of AI Generative Models When Used for Particle Physics

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AI development brings a revolutionary changes to our life and our society. The practical use of AI approaches for scientific studies is slightly behind the general use. This lag is driven by a specific requirements to the machinery imposed by scientific use. Using AI based fast simulation for particle physics experiments is a popular trend nowadays.

In this presentation we will discuss typical approaches [1],[2],[3] to developing fast models for simulating responses of different detectors, limitations of such AI based approaches and possible ways [4],[5] to overcome those limitations.

Acknowledgement. The research leading to these results has received funding from the Basic Research Program at the HSE University and was supported through computational resources of HPC facilities at the HSE University.

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Deep Learning Methods in High Luminosity Track Reconstruction Scenario: Applying TrackNET to TrackML Challenge

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Particle track reconstruction is a pivotal task in modern high-energy physics experiments. Traditional methods like the Kalman filter, though effective, face significant challenges in scalability and computational efficiency in environments with high track multiplicity and noise. To address these limitations, the TrackML competition was established to discover new, effective approaches for reconstructing particle trajectories with both high performance and quality [1]. In this work, we introduce TrackNET, a deep learning model based on a GRU recurrent neural network architecture that reconstructs particle tracks by concurrently processing multiple seeds, beginning from hits on the first detector layer and iteratively predicting the region on the next detector layer where subsequent hits are likely to appear, thereby constructing the track. Unlike the Kalman filter, TrackNET avoids complex algebraic computations and has a minimal memory footprint, processing only a small subset of hits at a time [2], [3]. This efficiency enables the parallel execution of hundreds of models to generate a list of track candidates with high recall. These candidates are then ranked based on a relevance criterion to identify the most accurate tracks. When applied to the TrackML dataset, TrackNET achieved promising results in both processing speed and reconstruction accuracy. These results highlight TrackNET's potential as a scalable, efficient solution for particle tracking, with promising implications for future collider experiments and high-energy physics research.

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Numerical Modeling of Gamma Sources Based on Nonlinear Compton Scattering

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Linear and Nonlinear Compton scattering (L- and NCS) represents a crucial mechanism for generating high-energy gamma rays in intense electromagnetic fields [1], [2]. This process, wherein electrons interact with ultra-intense laser pulses, results in the emission of high-energy photons, offering promising avenues for advanced narrow-band gamma-ray source development. However, accurately modelling these interactions poses significant challenges due to the complex nonlinear dynamics and the necessity for high-fidelity numerical simulations.

This talk presents a comprehensive approach to the numerical modelling of gamma sources based on NCS, highlighting the development and application of state-of-the-art computational techniques. We discuss advantages and disadvantages of several well-known numerical approaches: 1) semi-analytical methods; 2) Monte-Carlo simulations; 3) simulations based on calculation of radiation based on particle trajectory. Comparison of results obtained with these methods will be presented. Our developed framework utilizing modern GPUs will be discussed. Results are relevant for many ongoing projects aiming on development of ultra-bright narrow-band X- and gamma-ray sources based on interaction of lasers with electron beams, for example, ELI-NP in Romania and INOK project in Russia.

Acknowledgement. This work was supported by the joint SIOM-Skoltech Laboratory.

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Polarized Photon-Photon Collisions in ReneSANCe Monte Carlo Generator

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We describe the implementation of processes of photon-photon collisions with arbitrary polarization in ReneSANCe [1] Monte Carlo generator. Numerical results for a number of Standard Model processes will be shown for different energies (in the range from MeV to TeV) of colliding photons.

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Textile/Iron Oxide Nanozyme Composites: Preparation, SANS/SAXS Characterization, Modelling of Structural Arrangements and Environmental Technology Applications

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Magnetic iron oxide nano- and microparticles (MPs) have a great potential in biochemical, biomedical, clinical, biotechnology and environmental applications. In the year 2007 the presence of intrinsic peroxidase-like activity similar to horseradish peroxidase was described; the term "nanozyme" was introduced to define nanomaterials with enzyme-like activities.

Immobilization of (bio)catalysts to a solid carrier enables their simple separation from the reaction mixture and repeated application. Textile materials represent low-cost carriers applicable for immobilization of wide variety of molecules or particles.

Cotton textile was modified by direct application of acid magnetic fluid or by microwave synthesized magnetic particles. Peroxidase-like activity of textile bound iron oxides enabled decolorization of selected organic dyes such as crystal violet.

Cotton textile and cotton textile with MPs were measured by SANS and SAXS. Due to the different behavior of the experimental SANS curves for various samples by means of appropriate modelling it was

concluded that addition of nanoparticles to textile changes the structural organization at nanoscale. At SANS curves two power laws regions could be seen which points out that there are two kinds of scattering objects in the samples. At intermediate q-region power-law behavior of scattering intensity close to ˘1 corresponds well to cylinder-like objects while in small q-region power exponent is -2.7 or -3.4 depending on the sample [1]. SANS and SAXS data give similar results about structural organization of textile and (nano)particles. Sketch of the different behavior of MPs was proposed according to the analysis of SAS curves [1].

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From Black Holes to Data Pipelines: A Physicist's Journey to Tech Innovation

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The scientific mindset and analytical skills honed in academia prove invaluable in navigating the complexities of the modern tech landscape. By embracing data-driven methodologies and fostering a culture of experimentation, we can unlock new levels of efficiency, productivity, and success.

At 10Web, we've harnessed machine learning (ML) to develop our patented technology for "Generating higher-level semantics data for development of visual content".

Our current product suite leverages generative AI and other cutting-edge technologies to streamline website creation, management, and optimization. It utilizes the power of generative AI to automatically generate high-quality content, images, and even entire website designs. This eliminates the need for extensive manual labor and allows users to create visually stunning and engaging websites in a fraction of the time.

At the core of our data-driven approach lies the strategic utilization of Google's BigQuery and BigQuery Machine Learning (BQML). These advanced tools empower us to navigate and analyze vast amounts of data efficiently. By leveraging their capabilities, we uncover hidden patterns, detect anomalies, and discover emerging trends in a timely manner, enabling informed decision-making. BigQuery, a cloud-based data warehouse, provides us with a scalable and flexible platform to store and manage petabytes of data. BQML simplifies the process of building, training, and deploying machine learning models on BigQuery. It supports a wide range of machine learning tasks, including classification, regression, clustering, and anomaly detection, allowing us to uncover valuable insights from our data.

By combining scalable storage, powerful analytics capabilities, and machine learning capabilities, these tools are transforming the way scientific research can be conducted, opening up new opportunities for groundbreaking discoveries.

Modeling Quantum Simulations with Various Methods

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This study investigates accurate modeling for modeling quantum systems, particularly emphasizing qutrits – quantum units with three states.

Modeling these systems requires large-scale simulations to accurately capture their complex behaviors and interactions. Different methods are utilized, each with specific scalability, performance, and computational complexity strengths. The use of Monte Carlo methods [1], classical numerical methods [2], and machine learning optimization algorithms [3] on high-performance computing systems significantly reduces the time required for theoretical calculations and improves the reliability and stability of the modeled systems. These approaches collectively enhance the accuracy of modeling and the prediction of quantum system behavior.

The study also develops an approach to optimize differential equations for the simultaneous execution of multi-task quantum operations, such as XOR, AND, and OR [4]. This method aims to achieve high accuracy in operations and optimize quantum logic elements, contributing to the advancement of quantum computing. Comparative analysis of these methods reveals their strengths and weaknesses, which helps increase computational efficiency – an essential step toward the practical application of quantum technologies. The results confirm the feasibility of the proposed approaches and their potential in quantum computing, accelerating technological progress and overcoming technical challenges. This research significantly contributes to the development of quantum informatics, opening new possibilities for the practical use of quantum computing.

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CAST: Center of Advanced Software Technologies

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I will present the research and development conducted at our center, covering several topics related to compiler technologies and software security analysis. Within the framework of compiler technologies research, we will explore code obfuscation and optimization approaches. Our software security analysis direction includes the development of various methods for static analysis, fuzzing, and symbolic execution. We will discuss methods for detecting memory leaks and other software defects, including known vulnerabilities. Additionally, we will introduce several methods for improving fuzzing efficiency and directed symbolic execution. We will also present potential research directions regarding the application of AI for software analysis and optimization. Furthermore, a brief introduction to our research in natural language and speech processing, autonomous systems, and ECG analysis will be provided.

Supercomputing Centers and Their Impact on Research Output: Multinational Comparison

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Scientific communities and industry widely use supercomputing resources for large-scale simulations and modeling. Due to high capital and operational costs make evaluating the return on investment critical. There is a growing interest in understanding whether proximity to these centers is linked to higher research productivity and quality, as measured by academic publications. The research question addressed in the article is whether there is a correlation between the number of academic publications and the amount of resources. The study analyzed the relationship between supercomputing centers and academic research output using bibliometric data from the Web of Science. The study collected 221,271 publications based on twenty-four selected keywords related to high-performance computing and supercomputing. Pearson correlation, Spearman's rank correlation, and cross-correlation analysis were analyzed to determine the strength and direction of these relationships. The consistently high Pearson correlation coefficients over different periods confirm a robust linear relationship between the availability of supercomputing centers and the volume of corresponding scientific publications. While moderate Spearman correlation coefficients suggest some nonlinearities or outliers, other factors — such as the maturity of the research environment, regional differences, and institutional policies — could also shape the dynamics between supercomputing infrastructure and research productivity.

CVE, CWE and CPE Use Case

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In an ever-changing information space, many companies face increasingly complex challenges in ensuring the security and integrity of the confidential data they manage. This paper discusses how cybersecurity risks can be taken into account, that is, which resources and tools should be initially applied before purchasing or developing software.

The research is aimed at the possibilities and examples of the use of such NIST information systems as CPE, CVE, and CWE. CPE (Common Platform Enumeration) is a structured naming scheme for information technology systems, software, and packages. CPE is used to identify platforms to which CVEs are applicable [1] The aim of CVE (Common Vulnerabilities and Exposures) is to identify publicly disclosed cybersecurity vulnerabilities [2]. CWE (Common Weakness Enumeration) is a category system for hardware and software weaknesses [3]. We can say simplifying the terms, that weakness which is exposed to attacks is vulnerability.

The authors used CPE, CVE, and CWE, in a use case for new Moodle system acquisition to demonstrate how in reality cybersecurity requirements can be managed.

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Simulation of Dark Matter Production within the Extended 2HDM Models

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We present the results of a modeling of dark matter production in association with a leptonically decaying Z boson and large missing transverse momentum in proton-proton collisions at $\sqrt{s} = 13.6$ TeV.

The results of a full modeling of detector response for the signal are shown. Background events are estimated and event selection strategy is determined. Proton-proton collision data at a center-of-mass energy of 13.6 TeV collected by CMS during the machine's third run (Run 3) is being analyzed.

Stochastic Voter Model Driven by Avalanche-Like Perturbations

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A voter model, first proposed to describe of territorial competition among biological species [1], has been successfully used to study a wide range of collective phenomena such as the transition to consensus in social groups, price formation in financial markets, language dynamics in populations and so on. In the original version of the model, the identical voters (agents) form a network. At each step of the system evolution, a randomly chosen agent switches between two states by copying the state of its neighbor, also chosen at random. Later, to account for the specificity of real systems, a number of variants of the basic model have been proposed [2].

Here we present a modification of the noisy voter model [3] that allows us to study not only the dynamics of the voters' binary states, but also the reasons that lead to this process. In our model, the changes in the binary state (opinion) of the voters (agents) are caused by the avalanche-like dynamics of the threshold variables (pressure) assigned to them [4]. Examples of such behavior include a two-way voting process in a community of people influenced by their environment, and the decision-making process in a group of traders under market pressure.

The system under study is considered as a scale-free network in which the nodes depict elements (agents, voters), and the edges represent possible interaction between them. The structure of the inter-voters links is not static. Its temporal evolution is due to the agents' "activity". This characteristic determines the probability for the agent to be linked with its nearest neighbors at a given time moment. According to the proposed rules for opinion changes, an agent that is not linked to neighbors can change its opinion to an opposite one, regardless of the opinions of other agents. A linked agent can copy the opinion of its neighbor during an avalanche process.

Analytically and numerically, we show that the system-averaged agents' "activity" completely determines the mode of opinion dynamics. When the averaged "activity" is larger than its critical value, the system

switches between two consensus states. In the opposite case the system tends to the state where the opposite opinions coexist and the system-averaged opinion is equal to zero. The critical value of the system-averaged "activity" defines the state where all values of the common opinion occur with equal probability. We show that the analytical and numerical results are in a good agreement. This fact demonstrates the possibility of controlling the system dynamics by manipulating the "activities" of the agents.

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Dunkl-Relativistic Particles in the Presence of External Fields with Non-Constant Ricci Scalar

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In the past few decades, some problems in quantum mechanics have led to the suggestion of changing its form. Considering that ordinary quantum mechanics cannot fully cover some of the experimental data in different fields of physics, raised to propose new forms for quantum mechanics. These changes have been studied using different approaches such as structural transformations, transformations of operators, or unusual potentials. One of the cases of transformations is related to the Dunkl operator, which looks like a fancier version of the regular derivative including the parity operator. The present work takes a closer look at how the Dunkl operator can improve quantum mechanics. The outline of this research is as, we investigate the relativistic particles with non-constant Ricci scalar in the presence of Dunkl derivative, the generalization of a cosmic string space-time. Here, the Klein-Gordon equation as well as a quantum particle described by the Klein-Gordon oscillator in the curved background space-time are investigated in the presence of external fields in the proposed framework. It is seen that the energy eigenvalues get modified in comparison to the results obtained in a cosmic string space-time in the absence of the Dunkl operator. In each step, the results are compared with the results of our initial theories in the limit state where Dunkl's parameter tends to zero.

A Deep Learning Model for Automated Quantification of DNA Repair Foci in Somatic Mammalian Cells

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Double-strand breaks (DSBs) are the most lethal DNA damages induced by ionising radiations. Here, we present a DSB quantification method based on the analysis of DNA repair foci (γ-H2AX and 53BP1) in somatic mammalian cells as the most reliable biomarkers of DSBs. Human dermal fibroblasts and human mesenchymal stem cells were irradiated with 1, 2, and 5 Gy of X-rays and their fluorescent immunocytochemistry microscopy images were captured at 24 hours after the irradiation. The captured images were annotated in CVAT platform and the exported data were obtained in Yolo (You-Look-Only-Once) format. The deep learning approach consisted of two stages; a computer vision algorithm and a neural network were used to extract the cells from each image thus providing our features (cell images) and corresponding labels, then these data were split as the required train/test/validation set for the deep learning model based on a Yolo algorithm to count the number of the two mentioned foci per cell. The results of our model were compared with the biologists' manual counting and DARFI program.

The developed algorithm and training models were based on the ML/DL/HPC ecosystem of the HybriLIT Heterogeneous Computing Platform.

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On the Effectiveness of Computer Visual-Language Models in Medical Image Analysis

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Recently, large language models have been in the focus of attention in the field of natural language processing [1]. In addition, their integration with computer vision systems allows users to conduct research on multimodal data. Computational visual-language models such as LLaVA [2], Flamingo [3] or CLIP have demonstrated impressive performance in a variety of visual-linguistic tasks. Computational visual-linguistic models (VLM) have a huge number of applications that can potentially be used in the field of biomedical visualization [4]. In this paper, studies have been conducted to show the effectiveness of VLM in detecting anomalies in biomedical images such as MRI brain images, histological blood cell images and chest X-rays.

CNN-based methods achieved the best performance on all datasets, which is understandable since CNN-based methods are pre-trained on the training set while VLM are not. However, the pre-trained VLM still show impressive performance, and at no cost to the training phase - using only the pre-trained models. In addition, with CNN-based methods, users need to train three separate model instances for three different datasets, while only one VLM instance is required for all datasets. Among the visual-linguistic models, BiomedCLIP, ChatGPT and OpenFlamingo perform best in predicting diagnosis. In general, BiomedCLIP achieves the best performance when averaged over three datasets.

Although visual language models allow users to create interesting and useful applications, there is an urgent need to develop a fully automated artificial intelligence system that can perform appropriate task solving. VLMs are extremely effective in language tasks such as machine translation, grammar checking, question answering, or information retrieval, but they are not yet ready to replace humans in specific applications such as analyzing and predicting diseases from medical images. Data collection and utilization is another limitation for VLM. The performance of AI models is data-dependent because the quality of output data is highly dependent on the quality of input data. More recently, the use of training data has increasingly raised privacy concerns in recent times as it may inadvertently leak. Despite the fact

that visual-language models are not yet able to outperform classical deep learning models on benchmark datasets, it is worth noting that they can serve as voice assistants for pre-diagnosis.

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Computer Algorithms for Synthetic Images Modelling Based on Diffusion Models

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Deep neural networks have enabled significant breakthroughs in medical image analysis. However, due to their high data requirement, small datasets in medical imaging tasks may prevent them from reaching their full potential. Synthetic data generation is a promising alternative to augment training datasets and enable medical image research on a larger scale. Recently, diffusion models have attracted the attention of the computer vision community because of their ability to generate photorealistic synthetic images. In this paper, we explore the possibilities of using diffusion models [1]–[4] and develop computer algorithms for creating high-resolution synthetic images.

Acknowledgement. This work was supported by the RUDN University Strategic Academic Leadership Program, project No. 021934-0-000.

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CMS Open Data: Dimuons Lessons

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The report will present the experience of using the CERN Open Data portal with the data collected by the LHC experiments. The results of a study on the production of muon pairs in the Drell-Yan process during proton-proton collisions at the LHC with a center-of-mass energy of 13 TeV are presented. The work is based on open data from the CMS experiment, collected during the second LHC run in 2015, with an integrated luminosity of 2.67 pb^{-1}. Differential cross-sections of the studied process as a function of the invariant mass of muon pairs were obtained, and the kinematic distributions of muons and muon pairs were examined. A comparison of the CMS open data analysis results with Standard Model predictions and previously published results from the CMS collaboration was conducted. The measurements were shown to be consistent with first-order electroweak theory and second-order QCD perturbation calculations.

Technology for Selecting Deep Learning Models Based on Actualized User Experience Using the Auto-ML Approach

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In the contemporary era of significant advancements in photo and video processing, object recognition and classification algorithms find extensive application in both personal and professional domains3 [1]. However, the expansion of their usage areas brings an increase in factors influencing the diversity of computer vision tasks and the quality of image processing, including object dynamics and deformation within the frame. The growth in the number of neural network architectures complicates the selection of effective models for solving such tasks, posing new challenges for developers of these algorithms [2].

Our approach to addressing this issue involves creating a recommendation system (`https://saaresearch.github.io/`), based on the logic of production rules formed from the analysis of previous research and scientific data [3]. During our study, methods and technologies for creating recommendation systems, as well as methods for extracting statistical data and metadata from raster image sets, were analyzed. This work discusses the development of a framework that serves as a library of implemented algorithms for solving machine learning tasks. Special attention is given to the technology of selecting deep learning models based on updated user experience using the Auto-ML approach. The production rules will take into account the metadata of image dataset and the performance metrics of machine learning models, such as FPS, mAP50, Precision, and Recall [4], [5]. Thus, the framework enables more efficient selection of deep learning models under various conditions of object detection tasks, including the original datasets of users, and also facilitates the training of selected models in different modes (on CPU, GPU, multi-GPU) with specified parameters.

The main goal of this work is to create a tool that automates the process of selecting optimal machine learning models, taking into account the user's experience and preferences, thereby significantly improving the efficiency and accuracy of model development in various applications. The results presented in this work demonstrate the high efficiency of the proposed technology, emphasizing the importance of

an integrated approach to data analysis and machine learning in creating recommendation systems to solve a wide range of computer vision tasks, including those in industry.

Acknowledgement. This work was supported by ITMO University.

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Asymptotic Method for Modeling Electromagnetic Wave Propagation in Irregular Waveguides

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The paper describes a method for modeling electromagnetic wave propagation in irregular waveguides, where the solutions of Maxwell's equations are expressed as an asymptotic expansion for a reverse angular frequency as a small parameter. This approach allows use of computer algebra systems for symbolic investigation of such solutions.

For the zeroth approximation of the proposed method the symbolic solutions were obtained [1] and further work conducted to investigate the results [2], [3]. In a case of two-dimensional three-layer smoothy-irregular waveguide, a system of linear algebraic equations is constructed from the conditions between dielectric media and solved to determine a symbolic form of electromagnetic field components in each layer of the waveguide [4].

In this paper the first order approximation of the method is discussed. Maxwell's equations are investigated symbolically to formulate a problem of finding waveguide modes and are reduced to a system of inhomogeneous differential equations. This system is solved symbolically using Python's SymPy library. A symbolic form of electromagnetic field for two-dimensional three-layered irregular waveguide are also calculated in symbolic form for the first order approximation of the asymptotic method.

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Development and Visualization of Cellular Automata Models for Predicting Heterogeneous Traffic Flows

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Nowadays the traffic flow theory is an independent scientific direction based on the physics of traffic and involving mathematical modeling. Traffic models are used both in research and in practice as the core of intelligent transportation systems, so requirements for the model adequacy are increasing. Over the years, two approaches to the traffic simulation, namely, the macroscopic hydrodynamic models and the microscopic cellular automata (CA) models have been developing at KIAM RAS [1]. The aim of the present work is to create tools for predicting heterogeneous traffic flows within the CA approach. Many factors can be identified to characterize the flow heterogeneity. In this investigation various types of vehicles (passenger cars, minibuses, buses or trucks) are distinguished. CA models consider individual traffic participants with their own properties and are well suited for accounting the flow inhomogeneity. CA models are discrete in space and time. The road is represented as a lattice whose cell states are updated at each time step. Multi-cellular models are of interest: they allow one vehicle to occupy more than one cell.

A generalization of the well-known Nagel-Schreckenberg (NaSch) model [2] for the heterogeneous case is developed: a vehicle can occupy from 1 to 3 cells (a cell length is 7.5 m) depending on its type, a longer vehicle has a lower maximal speed (from 5 to 3 cells per time step). Using the traffic light test problem as an example, the obtained flow dynamics is compared with the prediction by the Helbing-Schreckenberg (HS) model [2] which is a discrete variant of the optimal velocity (OV) model. Different OV-functions are suggested for various vehicle types. The length of a cell is 1.5 m, thus in the current HS model a vehicle occupies from 5 to 15 cells. The use of small cells increases "the resolution" of an automaton — greater velocity discreteness ensures more realistic simulation of movement. The preference for further development is given to the NaSch model. A version of the multi-lane NaSch

model for heterogeneous flows has already been created. In the future, it will be implemented on small cells.

One of key points of the work is the visual dynamic presentation of the simulation results. Software for modeling traffic flows including a visualization system is being developed at MADI [3]. The visualization system is based on Unity 3D [4] — a free cross-platform game development engine that is highly compatible with CA models. The system allows creating lattices with cells of various shapes in three-dimensional space and studying traffic even at multi-level junctions with complex road geometry.

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Geant4 Hadronic Models

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Geant4 is a package for simulation of particle's and nuclei penetration through various materials. It is used by a large number of experiments and projects in a variety of application domains, including high energy physics, astrophysics and space science, medical physics and radiation protection. In high energy experiments, it is used at detector constructions, for simulations of detector responses, developments of reconstruction algorithms and other aims. Very often Geant4 is included in a computational framework of experiments (MPD, SPD, BMN, CBM and others). There are in the core of the package various codes for simulations of various physical processes: Binary cascade model (BIN), the Bertini cascade model (BERT), the Fritiof model (FTF), and the Quark-Gluon String model (QGS), and so on. Usually, they are used in frameworks of experiments. Though, they can be used directly in the so-called stand-along mode, what allow to analyze physical processes. Most of the core models will be shortly considered in the report.

NDMSPC – EOS and N-Dimensional Analysis with ROOT, Enhanced by Web Interface and VR Visualization

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This talk delves into the synergy of NDMSPC (NDiMensional SPaCe), EOS at CERN, and N-dimensional histograms via the ROOT framework. Discover how a web interface serves as a powerful analysis tool, enabling dynamic queries on projections in N-dimensional space. Interact and visualize the data seamlessly with JSROOT and VR (aframe), ushering in a new era of immersive exploration in high-energy physics.

Optimum Number of CUDA Streams for the GPU Implementation of the Tridiagonal Partition Method

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The parallel partition algorithm for solving systems of linear algebraic equations (SLAEs) with tridiagonal coefficient matrices suggested in [1] is a simple, but quite an efficient numerical approach for solving SLAEs with tridiagonal coefficient matrices, splitting the matrix into sub-matrices and then solving smaller SLAEs in parallel. The algorithm was initially intended for a large number of processors and so up to 250 are used in the computational experiments in [1].

The development of HPC applications usually involves two major steps – developing correct code, and improving the code for performance. Here, we are going to present one of the optimizations made to our CUDA implementation of the partition method, namely building a heuristics for finding the optimum number of CUDA streams.

A time complexity model for the GPU realization of the partition method is built. A refined model of the time complexity model for the partition method being executed on multiple CUDA streams is formulated.

Computational experiments for different SLAE sizes were conducted, and the optimum number of CUDA streams for each of them was found. Based on the collected data a model for the sum of the times for the non-dominant GPU operations (that take part in the stream overlap) is formulated using regression analysis. A fitting non-linear model for the overhead time connected with the creation of CUDA streams is created. Statistical analysis is done for all the built models.

An algorithm for finding the optimum number of CUDA streams is formulated. Using this algorithm, together with the two models mentioned above, predictions for the optimum number of CUDA streams are made. Comparing the predicted values with the actual data, the algorithm is deemed to be acceptably good.

Acknowledgement.

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Mathematical Model of Fractal Thermodynamics and Analysis of Produced Particle Tracks within the MPD Experiment of the NICA Collider

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The MPD experiment [1] is planned to start at the NICA accelerator complex in 2025 in order to investigate hot and dense baryonic matter produced in the collision of heavy nuclei up to Au after their interaction in the MPD detector at an energy of $E = 11.5$ GeV/nucleon.

The main objective of our work is to identify the fractal properties of the set of tracks produced by emitted particles during the collision of beams of Au atomic nuclei within the MPD experiment.

The computer reconstruction of particle tracks resulting from the interaction of Au heavy ion beams is demonstrated in five figures simulated with different event topologies.

The parameter $\delta^{(l)}$ was used as a criterion for the proximity of the studied images to fractals. If $\delta^{(l)} \ll 1$, then the studied sample is close enough to a fractal and a mathematical model of fractal thermodynamics can be used to study it [2], [3]. This mathematical model describes the relationships between the major fractal thermodynamic parameters, namely, fractal entropy $S_f^{(l)}$ and fractal temperature $T_f^{(l)}$.

The fractal parameters were calculated using Gwyddion, a modular program for graphic data analysis.

The values of $\delta^{(l)}$ are equal to: $\delta^{(1)} = 0.02701$, $\delta^{(2)} = 0.02336$, $\delta^{(3)} = 0.02109$, $\delta^{(4)} = 0.02172$, $\delta^{(5)} = 0.02448$, i.e., less than 3 %, which gives grounds to employ the fractal thermodynamics model for analyzing the fractal thermodynamic parameters $S_f^{(l)}$ and $T_f^{(l)}$ of produced particle tracks within the MPD experiment.

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On a Method for Numerical Solution of a Time-Dependent Schrödinger Equation Based on Lee-Trotter-Suzuki Formula

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The report is devoted to the results of investigation a methods for numerical solution a time-dependent Schrödinger equation. A brief overview of a family of numerical solution methods based on the application of the Lee-Trotter-Suzuki product formula [1] to the approximation of an evolution operator is presented. The problem of reducing a number of exponential operator in high-order accuracy approximation schemes by optimizing the sequence of multipliers is discussed.

Two tenth-order accuracy algorithms to approximate the evolution operator are constructed based on the idea proposed by Yoshida [2]. The results of numerical tests that demonstrate the stability of the algorithms and their order of accuracy are presented. The constructed algorithms make it possible to significantly reduce the number of exponential factors in the circuit compared to the Lee-Trotter-Suzuki formula. The application of the Lee-Trotter-Suzuki method to solving some non-stationary problems is demonstrated.

Acknowledgement. This work was supported by the Russian Science Foundation, project no. 20-11-20257.

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Application of Modern Consolidation Methods for Processing Complex Medical Data

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According to the International Organization for the Fight against Alzheimer's Disease, currently around 55 million people worldwide suffer from dementia and the number of such people is projected to only grow. The identification of early signs of incipient dementia remains quite difficult, preclinical and pre-clinical diagnosis of cognitive impairment is significantly complicated by the slow, imperceptible progression of cognitive impairment characteristic of neurodegenerative diseases with the development of symptoms, which in the early stages can be regarded as a normal age-related cognitive decline. The use of several examination methods provides a chance to increase the accuracy of early diagnosis of Alzheimer's disease. However, modern methods of computer analysis (spectral, autocorrelation, cross-correlation, the method of complex mutual spectra, etc.), methods of functional neuroimaging (single-photon emission tomography (SPECT), positron emission tomography (PET), etc.), magnetic resonance imaging (MRI) used for diagnosis reveal such a large heterogeneity of patient examination results, what becomes clear is that none of them can be so precise and specific as to be the basis for a diagnosis of Alzheimer's disease. The paper proposes an approach based on modern consolidation methods for processing medical examination data of patients.

ϕ^4 Oscillons as Standing Waves in a Ball: A Numerical Study

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Weakly radiating spherically-symmetric oscillons in the ϕ^4 theory can be approximated by standing waves in a ball of a finite radius [1]. We determine the temporally periodic standing waves as solutions of a boundary-value problem on the two-dimensional domain $[0, T] \times [0, R]$ where T is the period of oscillations and R radius of the ball. Numerical solution implements the Newtonian iteration with the 4th order finite difference approximation. The stability of standing waves is classified by evaluating the associated Floquet multipliers. The multipliers are calculated, in parallel, using resources of the JINR Multifunctional Computing Complex [2],[3]. Details of the numerical approach and parallel implementation are described, numerical results are presented. Dependence of structure and properties of standing waves on R and T is discussed.

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