Methods of Computational Physics for the Study of Complex Systems (06-6-1119-2-2024/2026)

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Project leaders: E.V. Zemlyanaya, O. Chuluunbaatar

Project deputy leaders: Yu.L. Kalinovsky, A. Khvedelidze

Participating JINR Laboratories: MLIT, VBLHEP, BLTP, FLNP, DLNP, LRB

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Three monographs were published on the basis of the results of research in applied mathematics and computational physics. The monograph [1] is devoted to developed iterative methods, algorithms and programs for solving systems of equations of various types using the finite difference method and the high-order finite element method (FEM). The monograph [2] focuses on developed iterative methods and algorithms for solving systems of nonlinear equations on top of the continuous analogue of Newton's method. In [3], the basic concepts, general techniques, and methods for working with matrices, including the calculation of determinants of various orders, are considered.

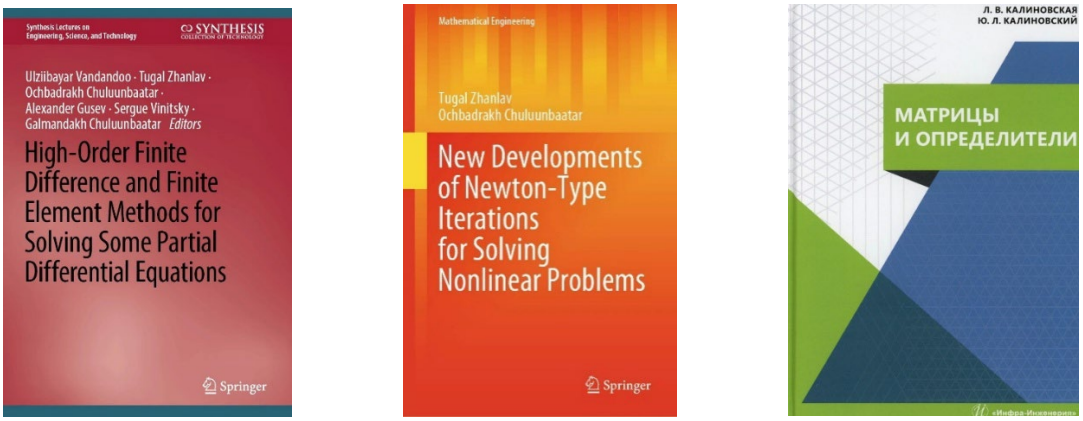

Fig. 1. Monographs [1-3] published in 2024.

To describe the collective quadrupole model of the atomic nucleus and compute the rotational-vibrational spectra and probabilities of quadrupole transitions, the GCMFEM program to solve boundary value problems for a system of two-dimensional elliptic differential equations with mixed derivatives was elaborated [4,5]. For the isotopes ^{190}Os and ^{154}Gd, the results are consistent with experimental data.

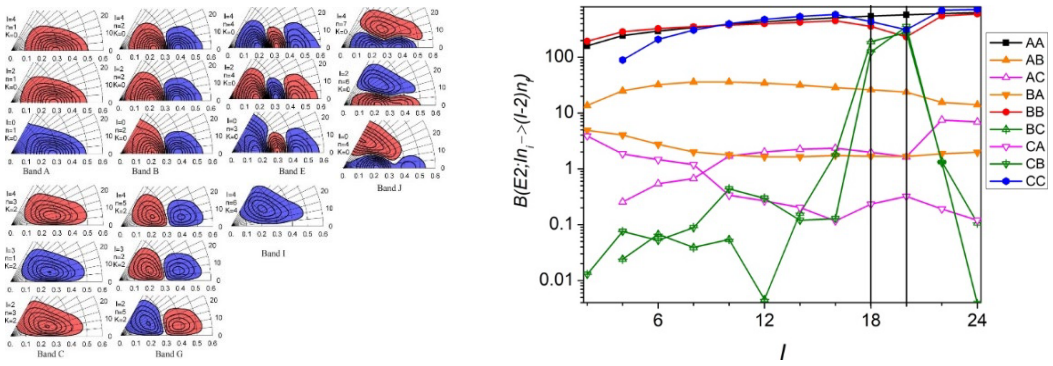

Fig. 2. Leading components of the eigenfunctions of the collective model of the ^{154}Gd atomic nucleus obtained in [5] (left) and computed quadrupole transitions B between the A, B and C bands in ^{154}Gd (right).

Within the microscopic model of the optical potential, an analysis of proton-nucleus scattering data at energies of 200-1000 MeV was carried out. The estimates of the influence of the nuclear medium on the scattering amplitude depending on the energy of the incident proton and the atomic mass of the target nucleus were made [6,7].

A quantum-chemical cluster method to quantitatively substantiate effective spin models for various crystal structures of magnetic transition metal oxides was developed [8]. The method is applicable to wide families of new magnetic materials with complex chemical compositions.

A method for extrapolating perturbative expansions in powers of asymptotically small parameters to the region of finite or infinite values of variables was proposed [9,10]. The extrapolation is performed using self-similar factor approximants. In a number of cases, the method enables to accurately reconstruct the desired functions from their weak-coupling asymptotic expansions.

A study of the model of atomic optics with cold bosons was conducted [11]. It was demonstrated that when bosons were cooled in traps to temperatures at which the atomic cloud turned into a Bose-Einstein condensate, interference patterns, interference current, Rabi oscillations, harmonic generation, parametric conversions, and other effects could be observed.

The procedure for modeling fragmentation reactions was modernized on the basis of the transport-statistical approach in the BNV-SMM model [12]. It enabled to reduce the computation time and enhance the agreement with the experimental data of fragmentation reactions in comparison with other known approaches.

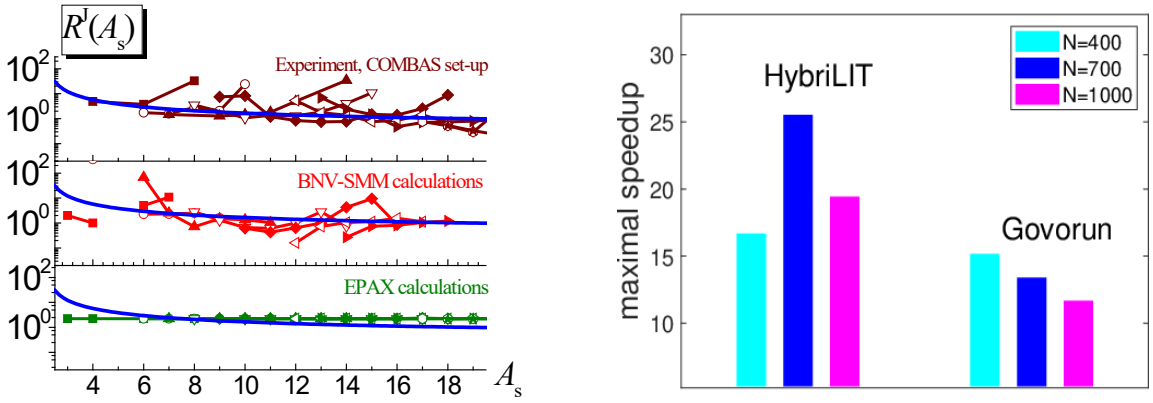

Fig. 3. Left: values of $R^J(A_s)=\sigma^J(A_s)_{Ta}/\sigma^J(A_s)_{Be}$ (σ^J is the cross section for the formation of the isotope of an element with number J, A_s is the mass number of the secondary fragment) calculated in [12] using the modified BNV-SMM procedure (solid blue line) for elements from He to Ne in the $^{18}O+^{181}Ta$ and $^{18}O+^{9}Be$ reactions at an energy of 35 MeV/nucleon in comparison with experimental data and with the calculation in the EPAX model (green curve). Right: maximum speedup of the parallel calculation of Floquet multipliers in the analysis of the stability of standing waves in the φ^4 model on the HybriLIT cluster and the "Govorun" supercomputer depending on the number N of terms in the Fourier expansion [13].

As part of the cooperation program with the University of Cape Town, a study of the spherically symmetric time-periodic standing waves of the φ^4 model in a ball of finite radius was carried out [13,14]. They are considered as an approximation of weakly radiating oscillons. For the 3D case, coexisting types of standing waves were found, and the dependence of the energy and stability intervals of the waves on the radius and frequency was investigated. Calculations were performed on the HybriLIT platform and the "Govorun" supercomputer. The frequency range where the variational method provides an accurate description of the (1+1)-dimensional oscillon was defined [15].

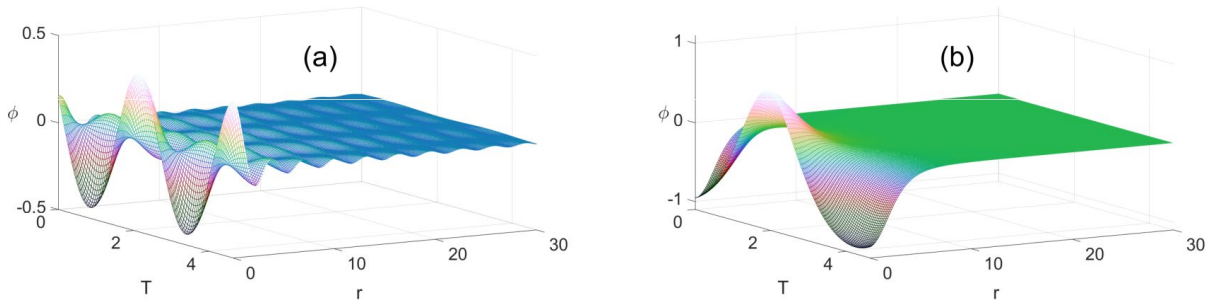

Fig. 4. Coexisting spherically symmetric standing waves in the φ^4 model obtained in [13,14].

Based on the non-stationary heat conduction equation in a coordinate system associated with a moving evaporation front, as well as within the two-temperature thermal peak model, the dynamics of the laser ablation of materials under the action of ultrashort laser pulses was investigated [16].

A method for the refined calculation of the spread of energy losses in crystal lattices under irradiation with heavy ions with relativistic energies was proposed, it has an advantage in accuracy compared to existing approaches in the case of irradiation with highly charged ions [17].

Molecular dynamics methods were employed to simulate the interaction of beta-amyloid peptide 25-35 with DMPC phospholipid membranes in the presence of a large number of K^+ and Cl^- ions in the solution. The results provide information on possible processes occurring during membrane destruction in the presence of peptides [18].

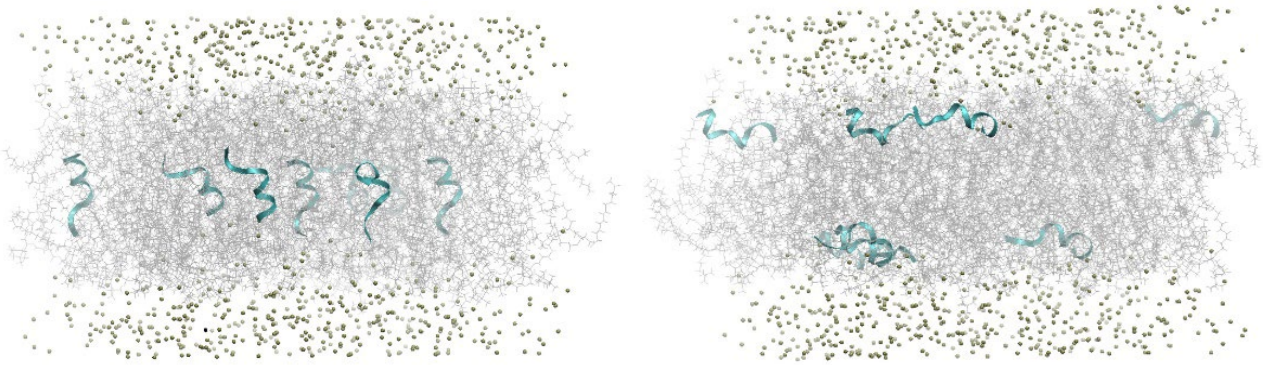

Fig. 5. Localization of peptides in the center of the membrane (left) and in the head groups of the bilayer (right) [18].

The FITTER_WEB web application, developed and deployed on the cloud infrastructure, was adapted to investigate the structure of phospholipid vesicular systems of various types using small-angle neutron and X-ray scattering data on the basis of the separated form factor model [19].

The method for modeling the formation of hydrated electrons in a liquid was modernized. By taking into account the Coulomb potential, it enabled to expand the frequency range of the scanning laser, for which the calculation results are consistent with the experiment [20].

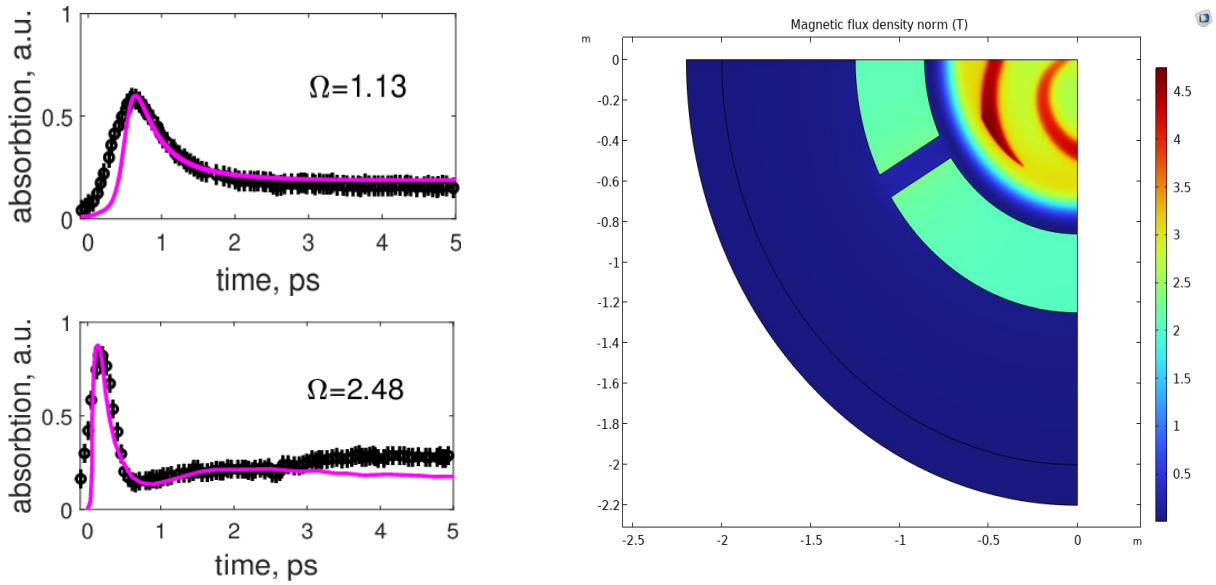

Fig. 6. Left: formation of a hydrated electron in water, a comparison of the calculation from [20] with experimental data. Right: magnetic field distribution for a dipole magnet calculated on the basis of the approach proposed in [21].

A combined FEM-based procedure [21] was proposed, it allows reducing computational costs without loss in accuracy when solving 3D magnetostatics problems with complex geometry using a magnetic vector potential.

A numerical integrator of ordinary differential equations based on a combination of the methods of Appel'rot dynamic system quadrature and Kahan discretization was investigated [22]. The proposed approach opens up the possibility of creating difference schemes whose algebraic properties significantly differ from the properties of the original dynamic system.

A study on the possibility of employing artificial intelligence to optimize and increase the speed of computations when modeling magnetic fields of accelerators was conducted [23]. The prospects for using computer vision and artificial intelligence to optimize beam motion within the CORD (Closed ORbit Dynamics) program, which implements calculations on the effect of betatron oscillations and phase motion of beam particles on the magnetic field of the MSC230 cyclotron, were analyzed.

A matrix-free method of preconditioned conjugate gradients, adapted for multi-core computers, was developed to solve finite element systems with high-order approximation [24]. The main advantage of the method is the absence of the need to store a 3D sparse finite element matrix, which significantly enhances the efficiency of computations.

Within the work on the creation of superconducting magnets for charged particle accelerators, the modeling of superconducting windings with a coaxial cable, an important element of modern magnetic systems, was performed together with VBLHEP and DLNP physicists [25]. Based on 2D and 3D modeling with varying the location of current windings in the magnetic system, the characteristics of the Nuclotron superconducting dipole magnet were optimized. A computer model of the current winding of the MSC-230 cyclotron from the superconducting coaxial cable with a new version of its winding was

developed. Based on the separate modeling of nine superconducting cores of the coaxial cable, a winding model oriented towards a power source with a current of 0.5 kA was elaborated.

An algorithm for calculating multidimensional integrals with pole-type singularities was developed on the basis of the identification and bypass of singularities during integration using the Monte Carlo method [26].

Conditions that ensure a simple elementary input of the problem parameters, resulting either in a decision tree defined by a single interval or in a forest of decision trees defined by a set of adjacent intervals, were established for a two-rule Bayesian adaptive quadrature, critically dependent on a priori input data provided by the user, to calculate one-dimensional Riemann integrals [27].

A scheme for the parallel numerical integration of the three-dimensional non-stationary Schrödinger equation in the representation of a discrete variable, providing a significant reduction in the computation time for problems with a large number of grid nodes, was proposed and implemented [28].

The interaction of the spinor and electromagnetic fields and their influence on the evolution of the Universe were investigated within the Bianchi type-I and FLRW cosmological models. For the Bianchi type-I model, it was established that the interaction of these fields softened the restrictions arising from the non-zero off-diagonal components of the energy-momentum tensor [29]. In the FLRW geometry, the role of the nonlinear spinor field for various curvatures was studied, restrictions on the field parameters were identified, and the numerical solutions of the corresponding equations of state were obtained [30].

The non-classicality indicator of a state in a finite-dimensional quantum system based on an assessment of its remoteness from the set of “classical states” was investigated. It was shown that classical states determined by the non-negativity of the Wigner function were concentrated in a convex polyhedron of the simplex of the eigenvalues of the state density matrix [31].

A new scheme for the factorization of transformations of the SU(4) group into factors that allow constructing a double coset corresponding to the left action of its SU(4)×SU(2) subgroup and the right action of the maximal torus of the SU(4) group was proposed [32,33].

A method that increases the computational efficiency of assessing the nonlocal characteristics of a pair of qubits was proposed. Within this approach, a subset of separable 2-qubit states of rank 4 is described as a semi-algebraic manifold defined by a system of polynomial inequalities of the 3^{rd} and 4^{th} order on the eigenvalues of the density matrix with polynomial coefficients in the form of trigonometric functions established on the direct product of two regular octahedra [34].

Within the generalized Stratonovich – Weyl formulation of quantum mechanics, the question of the dichotomy between the elementary and composite nature of a finite-dimensional quantum system was investigated. It was demonstrated how information about the possible realization of a virtual two-level subsystem was encoded in the properties of the Wigner function of a complete four-level system [35].

A version of quantum formalism in which finite (or countably infinite) sets are used instead of continuously infinite ones was studied. An analysis of the decompositions of a quantum system into subsystems, based on the structure of a finite cyclic group, showed that quantum behavior was significantly manifested only in subsystems whose Hilbert space dimensions were powers of prime numbers [36].

Using the example of the problem of searching for the ground state in the Ising model with an longitudinal magnetic field, the quantum approximation optimization algorithm (QAOA) was simulated on the Cirq quantum computing simulator of the JINR HybriLIT quantum polygon. Computations illustrated that the connection of the cuStateVec package considerably enhanced the efficiency of computations [37,38].

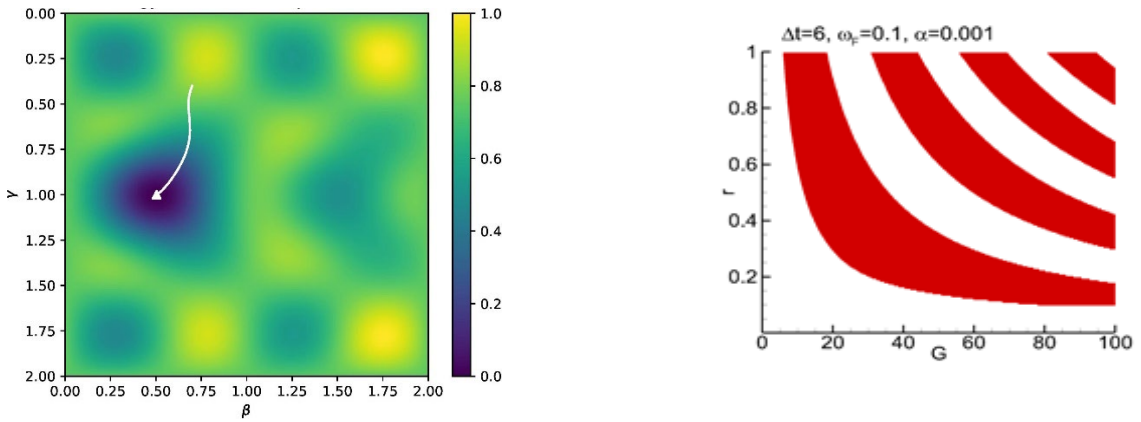

Fig. 7. Left: dependence of the energy on the values of variational parameters in the Ising model with an external magnetic field, calculated on the quantum polygon [37]. The white arrow shows the trajectory of the gradient descent. Right: example of the structure of the arrangement of magnetic moment reversal domains on the plane of parameters of the superconductor – ferromagnet – superconductor model of the φ0-junction with weak dissipation, calculated in [39].

The simulation of domains of reversal in the superconductor – ferromagnet – superconductor model of the φ0-junction with weak dissipation depending on the parameters that regulate the action of the external current was conducted. The parallel implementation enabled to reduce the computation time by up to 30 times [39].

The ecosystem for modeling Josephson structures based on the Jupyter Book platform was complemented with materials to investigate the dynamics of a superconducting quantum interferometer (SQUID) with two Josephson junctions. A computational scheme for constructing the current-voltage characteristics of the SQUID under the influence of a magnetic field was developed. The parallel implementation using the Numba library provided a significant speedup of calculations [40,41].

An algorithm for searching for stable configurations with a minimum energy for a system of similarly charged particles in a two-dimensional region was developed, it allows the value of the global minimum in energy to be calculated with high accuracy in a minimum amount of time compared to other known approaches [42]. A new approach to a quantitative analysis and search for signals of phase

transitions “crystalline – hexatic – liquid phase”, based on the multifactor correlation analysis and analysis of topological characteristics of stable configurations at zero temperature and a fixed number of particles in the system, was elaborated [43].

Two methods of point approximation in 3D space by a set of parallel planes based on the orthogonal least squares method were tested using the Newtonian scheme for solving the corresponding nonlinear problem proposed by the authors in one of the approaches [44].

Key publications within the project for 2024

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