05–6–1119–2014/2019	Priority: 1

Status: Being concluded

Methods, Algorithms and Software for Modeling Physical Systems, Mathematical Processing and Analysis of Experimental Data

Leaders: Gh. Adam
P.V. Zrelov

Participating countries and international organizations:

Armenia, Belarus, Brazil, Bulgaria, Canada, CERN, China, Czech Republic, France, Georgia, Germany, United Kingdom, India, Italy, Japan, Kazakhstan, Lithuania, Moldova, Mongolia, Poland, Romania, Russia, Saudi Arabia, Slovakia, South Africa, Switzerland, Tajikistan, USA, Vietnam.

Issues addressed and main goals of research:

Carrying out paramount advanced research in the field of computational mathematics and computational physics, directed to the creation of new mathematical methods, algorithms, and software for the numerical or symbolic-numerical solution of topics arising in experimental and theoretical studies, by using the newest computational tools, primarily the heterogeneous cluster HybriLIT. This subject area includes a wide spectrum of investigations underway at JINR in high energy physics, nuclear physics, condensed matter physics and nanotechnologies, biophysics, information technologies, etc., which demand the development of new mathematical methods and approaches for modeling physical processes, processing and analysis of experimental data, including the use of these studies in the NICA project, the neutrino programme and other strategic goals of the Institute. A distinctive feature of these investigations is the close cooperation of LIT with research groups from all the JINR laboratories and from Member State institutions.

Expected major results in the current year:

- Numerical investigation of model equations defining baryon behavior at NICA energies.

  Three-dimensional computer simulation of magnetic field distributions in superconducting dipole and quadrupole magnets for the projects NICA (JINR) and FAIR (GSI).

  Monte-Carlo simulations of gauge-invariant observables within the lattice SU(2) gluodynamics under various boundary conditions.

  Improvement of QGSM generator aimed at including experimental effects in the strange and dilepton particle yields.

  Development of numerical and analytical methods for computing the ionization spectra of hydrogen like hadronic atoms in the eikonal approximation.

  Modeling the extremely high energy electromagnetic showers analyzed in a number of ultra-high energy neutrino astrophysics projects such as Baikal, IceCube, and Antares.

  Analysis of interactions of stable and exotic nuclei with nuclei and protons on the basis of microscopic approach, including reactions $^{12,14}Be + ^{12}C$ and $^{12,14}Be + p$.

  Numerical investigation of complex physical processes described by multi-parameter systems of nonlinear equations.

  Transport approach based modeling of heavy-ion collisions in the Fermi energy range and its use in the analysis of COMBAS data.

  Numerical modeling of fast magnetization reversal due to the influence of external alternating fields on the effective magnetic anisotropy.

  Computer simulation of spin dynamics in dipole and spinor systems and numerical study of the influence of the quadratic Zeeman effect on spin dynamics.

Calculation of beam dynamics, measurement of the Smith-Garren curves and their recalculation as phase motion curves with the aim of evaluating the quality of formation of magnetic fields and their correction for the isochronous cyclotrons AIC-144 (Krakow, Poland), SC-200 (Hefei, China), DC-280 (FLNR, JINR).

Analysis of the measured magnetic field maps, calculations of beam dynamics and comparison of the results with those on simulated magnetic field maps (TOSCA, CST).

Development of numerical methods and algorithms for the study of phase transitions arising in materials under ion beam irradiation for parabolic and hyperbolic heat conduction equations.

Development and support of the primary data processing program "SAS" for the YuMO spectrometer at IBR-2M. Development and support of the new data converter "PSD2SAS" for position-sensitive detector in isotropic pattern scattering case. Development of algorithms for data analysis for anisotropic pattern scattering samples. Visualization and fitting of three-dimensional data records. Development of the basic elements method for solving problems of the contour analysis. Development of the basic elements method for solving problems of the contour analysis.

Development of methods, algorithms and programs for forecasting atmospheric pollution in the tasks of environmental monitoring based on machine learning.

Development of mathematical methods for resolving fine structure distributions with respect to mass and energy of the nuclear reaction products.

Least action control in Bayesian automatic adaptive quadrature.

Analysis of soliton-bearing PT-symmetric spinor systems of condensed matter physics.

Study of soliton solutions of the damped-driven repulsive nonlinear Schroedinger equation and their application to the analysis of the soliton-mediated frequency combs.

Calculation and optimization of the magnetic field configurations of the large superconducting magnet of the SPD setup within the NICA project.

Numerical analysis by quantum chemistry methods of exchange interactions in crystalline iridium-oxide compositions with varying geometry of local bonds. Development and use of a program package of the quasi-phonon model of the nucleus for the study of the properties of heavy exotic nuclei. Development and use of a program package of the quasi-phonon model of the nucleus for the study of the properties of heavy exotic nuclei.

- Improvement of the FTF model of the Geant4 package and refinement of its parameters for simulation of proton-nuclear and core-nuclear interactions at intermediate energies within the joint project of PANDA and HADES collaborations - Phase-0 and Phase-1 (GSI).

  Simulation of proton-proton and deuteron-deuteron interactions at nucleon-nucleon collision energies of 3-15 GeV (in the center of mass system) in the framework of the FTF model of the Geant4 package for the NICA/SPD experiment. Adaptation of the FTF model for inelastic interactions in the computing environment of the NICA/SPD experiment - SPDRoot.

  Development of Geant4 FTF model for modeling nuclear-core interactions in a wide range of energies and analyzing experimental data at BM@N (JINR) and NA61/SHINE, and planning experiments for CBM (GSI) and MPD (JINR/NICA).

  Participation in design of data bases for NICA project. Participation in design of online DAQ system for NICA project.

  Commissioning the Geometry Database for the CBM experiment. Development of a database concept for useful events selected in the CBM experiment.

  Software support of ATLAS experiment, agreed with the ATLAS computing team: support of online TDAQ ATLAS components that was implemented in LIT; support and improvement of tool for ATLAS network monitoring dashboards; creation and support of Monitoring for ATLAS EventIndex project; participation in modernization of ATLAS condition databases for RUN3, design and implementation conversion tools from COOL data to CREST data.

  Development of algorithms for processing experimental data acquired with the planes of microstips tracking detectors (GEM and SILICON) for the current configuration of the BM@N/NICA setup.

Development of software for detailed simulation of physics processes occurring in gaseous and semiconductor detectors of the main tracking system in the BM@N/NICA experiment. BM@N: Reconstruction of trajectories and identification of charged particles using tracking and time-of-flight detectors.

Investigations on the possibility to construct effective neural net algorithms for event reconstruction in TAIGA experiment.

Experiment NUCLEON: Development of a program for the analysis of data on the anisotropy of the cosmic rays. Investigation of additional possibilities of modified data analysis schemes of records from heavy leaky calorimeters.

BM@N experiment: Experimental data processing of GEM detector data under improved impulse reconstruction of charged particles. Use of the obtained results for the reconstruction of the decays of short-lived strange and multistrange baryons.

CMS: Further development and testing of the algorithm of overlapped signal separation in CSC and its implementation into official CMS release; assessment of CSC performance (efficiency and resolution) with new LHC data; completion of CSC ageing studies on muon beam tests with radiation source (CERN Gamma Irradiation Facility (GIF++)).

Investigation of structure and properties of polydispersed vesicles of phospholipids by analysis of experimental data on the small angle acattering of neutrons and x-rays.

High order mean-square piecewise polynomial approximation based analysis of the slow noise changes of the power of the IBR-2M reactor.

BAIKAL project: Development of the data acquisition software. Development of alert system.

Further development of VMRIA software package for large data set automatic analysis in experiments carried out on the High Resolution Fourier Diffractometer at IBR-2M.

Development of methods and software for automatic calibration of multi-detector systems.

Further development of statistical non-parametrical methods for parameter estimation and hypothesis testing under low data statistics and process observation incompleteness.

Development of methods for the simulation of the reflection of neutrons from layered nanostructures.

Development of criteria and methods for selection of exotic nuclei in the CBM experiment.

Development of triggers for recording rare decays of J/ψ in the dielectron and dimuon channels in the CBM experiment.

Investigation of statistical features of the Internet traffic. Analysis of external impact on the statistical characteristics of the information traffic.

Development of FPGA programs as part of reading and data acquisition electronics for CBM experiment.

Go4 user library upgrade for the data aquisition system for the experiments at the fragment-separator ACCULINNA-2 at FLNR.

Development of the FAIRroot based package EXPERtroot for simulation and data analysis for the experiments at the fragment-separator ACCULINNA-2 at FLNR.

Calculation of electrostatic potentials for Zn protein transcription factors.

Development of new methods for computation of kinetic, thermodynamic, and optical parameters of intermediate compunds in reactions of transition metal ions with heterocyclic compounds.

- Development and support of the information-computing environment of the heterogeneous platform HybriLIT including installation and maintenance of specialized libraries and application software packages.

  Optimization and analysis of the performance of developed packages of parallel programs using various parallel programming techniques.

  Modeling processes of single and multiple ionization/photoionization of the water molecule.

  Study of helium single ionization by fast proton impact in different kinematic regimes.

  Development and implementation of new parallel algorithms for computations on hybrid architectures, including Intel Xeon Phi (KNL) processors and NVIDIA graphics accelerators.

Development and support on the cluster HybriLIT of a program devoted to particle identification in the search for anomalous lepton.

Study of the efficiency of various parallelization techniques implemented in the ROOT package, when computing on the heterogeneous HybriLIT cluster.

Maintenance of the information site created to support the ROOT users at JINR.

Optimization of software developed for solving NICA project problems on multiprocessor computing systems.

Development of algorithms and program modules of optimal h-p discretization by discontinuous least-squares method for parallel solving nonlinear magnetostatic problems.

Conducting research with the aim of reconciling the continuous thermal spike and molecular dynamics models for the description of thermoelastic processes under sample irradiation with heavy ion beams.

Fast FEM algorithm for numerical solution of the 3D magnetostatic problems in COMSOL Multiphysics environment capable of yielding the high accuracy field maps for dipole magnets with superconducting coils.

Analysis of the 3D thermo-electric modelling of the quench initiating and propagating in the superconducting coils and its precise detection for various cooling conditions based on the COMSOL Multiphysics ®.

Development of methods and parallel algorithms for the reconstruction of the tracks of elementary particles based on neural networks with deep learning for the objectives of the project NICA.

Formulation of the optimization problem for the nonlinear heat equation and development of parallel algorithms for solving it in hybrid computing architectures.

Development of new effective algorithms for improving LDPC decoding performance.

- Development of an algebraic method for constructing quasi-probability distributions of composite finite-dimensional quantum systems.

Analysis of the interplay between the negativity of the Wigner functions quasi-probability and the entanglement for mixed quantum states of finite-dimensional quantum systems.

Development of algorithmic methods for constructing the first differential approximation (modified equations) of difference schemes for systems of quasilinear partial differential equations with polynomial nonlinearity.

Construction of data structures for systems of nonlinear algebraic equations which admit efficient parallelization and implementation on the heterogeneous cluster HybriLIT of algorithms for the transformation of such systems to canonical involutive forms.

Creation of algorithms and programs for the analysis of metastable and bound states of a Beryllium trimer with realistic pair interactions in a collinear configuration.

Creation of algorithms and programs for generating orthonormal Bargmann-Moshinsky basis for the evaluation of spectra of the collective nuclear model.

Development of an effective algorithm for irreducible component splitting of unitary group representations describing quantum systems.

New compact formulae for the one-loop 3, 4, 5 and 6-point Feynman integrals in arbitrary space -time dimension.

List of activities:

	Activity or experiment **Laboratory or other Division of JINR**	**Leaders** **Main researchers**
1.	**Mathematical and computation methods for simulation of complex physical systems**	**Gh. Adam** **I.V. Puzynin**

LIT	S. Adam, R. Akhat, P.G. Akishin, I.V. Amirkhanov, E.A. Ayrjan, I.V. Barashenkov, A.A. Bogolubskaya, I.L. Bogolubsky, N.D. Dikoussar, H. Grigorian, M. Kakenov, Yu.L. Kalinovsky, T.V. Karamysheva, N.A. Kutovskyi, K.V. Lukyanov, N.V. Makhaldiani, T.I. Mikhailova, G.J. Musulmanbekov, A.V. Nechaevsky, K. Oganesyan, G.A. Ososkov, R.V. Polyakova, B. Saha, I. Sarkhadov, N.Yu. Shirikova, A.G. Soloviev, T.M. Solovieva, L.A. Siurakshina, A.V. Uzhinsky, A.V. Volokhova, O.O. Voskresenskaya, A. Wojczechowski, R.M. Yamaleev, E.P. Yukalova, E.V. Zemlyanaya
VBLHEP	S. Gevorkyan, M.N. Kapishin, A.O. Kechechyan, H.G. Khodzhibagiyan, A.D. Kovalenko, E.E. Perepelkin, O.V. Rogachevski, V. Zhezher
BLTP	D. Blaschke, A.V. Friesen, M. Hnatic, E.-M. Ilgenfritz, R.V. Jolos, V.K. Lukyanov, A.V. Sushkov, V.D. Toneev, V.I. Yukalov, V.Yu. Yushankhai
FLNR	A.G. Artukh, B. Erdemchimeg, S.M. Lukyanov, Yu.E. Penionzhkevich, Yu.V. Pyatkov+1, Yu.M. Sereda, Yu.G. Sobolev
FLNP	M.V. Frontasyaeva, O.I. Ivankov, A.I. Kuklin, D.V. Soloviev, 3 pers.
DLNP	L.G. Afanasiev, S.N. Dolya, G.A. Karamysheva, I.N. Kiyan, V.A. Malinin, D.V. Popov
2. Software complexes and mathematical methods for processing and analysis of experimental data	**P.V. Zrelov** **V.V. Ivanov**
LIT	T.O. Ablyazimov, E.P. Akishina, E.I. Aleksandrov, I.N. Aleksandrov, D.A. Baranov, S. Belogurov, O.Yu. Derenovskaya, N.D. Dikoussar, I.A. Filozova, A.A. Kazakov, A.I. Kazymov, P.I. Kisel, B.F. Kostenko, G.E. Kozlov, L.Yu. Kruglova, A.A. Lebedev, M.A. Mineev, E.V. Ovcharenko, V.I. Palichik, R.V. Polozov, I. Satyshev, V.N. Shigaev, S.K. Slepnev, A.G. Soloviev, T.M. Solovieva, A.N. Sosnin, V.V. Uzhinsky, N.N. Voitishin, O.O. Voskresenskaya, A.V. Yakovlev, E.V. Zemlyanaya, E.I. Zhabitskaya, V.B. Zlokazov
VBLHEP	P.N. Batyuk, B.V. Batyunya, Yu.V. Ershov, A.S. Galoyan, K.V. Gertsenberger, A.O. Golunov, I.A. Golutvin, N.V. Gorbunov, A.Yu. Kamenev, M.N. Kapishin, V.Yu. Karzhavin, V.P. Ladygin, V.V. Lenivenko, A.M. Makan'kin, A.I. Malakhov, S.P. Merts, S.A. Movchan, A.N. Morozov, V.V. Perelygin, Yu.P. Petukhov, O.V. Rogachevsky, M.M. Rumyantsev, M.G. Sapozhnikov, V.N. Shchetinin, V.N. Spaskov, N.D. Topilin, S.E. Vasiliev, A.V. Zarubin
FLNR	A. Fomichev, S. Belogurov, V. Chudoba, Yu.S. Tsyganov, V.K. Utenkov

	FLNP	A.M. Balagurov, A.V. Belushkin, I.A. Bobrikov, M.A. Kiselev, D.P. Kozlenko, S.A. Manoshin, Yu.N. Pepelyshev
	DLNP	I.V. Bednyakov, V.A. Bednyakov, I.A. Belolaptikov, V.B. Brudanin, A.G. Olshevsky, D.B. Pontecorvo, B.A. Shaibonov, L.G. Tkachev, A.S. Zhemchugov
	UC	S. Pakuliak
3. **Numerical methods, algorithms and software computationally adapted to multicore and hybrid architectures**		**Gh. Adam** **P.V. Zrelov** **O.I. Streltsova**
	LIT	E.I. Aleksandrov, A.S. Ayriyan, D.A. Baranov, M.V. Bashashin, D.V. Belyakov, J. Busa, Yu.A. Butenko, A.M. Chervyakov, O. Chuluunbaatar, H. Grigorian, A.A. Gusev, M. Kirakosyan, D.V.A. Luu, M.A. Matveev, S.V. Mitsyn, G.A. Ososkov, D.V. Podgainy, T.P. Puzynina, V.S. Rikhvitsky, A.A. Sapozhnikov, T.F. Sapozhnikova, N.R. Sarkar, S.I. Serdyukova, Z.A. Sharipov, A.G. Soloviev, T.M. Solovieva, Sh. Torosyan, Z.K. Tukhliev, A.V. Volokhova, O.I. Yuldashev, M.B. Yuldasheva, T.N. Zaikina, E.V. Zemlyanaya, E.I. Zhabitskaya, M.I. Zuev
	LIT-MICC	V.V. Korenkov, V.V. Mitsyn, T.A. Strizh
	FLNR	N.Yu. Kazarinov, R.A. Rymzhanov, V.A. Skuratov
	BLTP	D.B. Blashke, S.N. Nedelko, Yu.V. Popov, Yu.M. Shukrinov, S.I. Vinitsky
	VBLHEP	A.V. Belyaev, A.Yu. Boytsov, E.E. Donets, I.V. Golutvin, V.A. Nikitin, O.V. Rogachevsky, 2 pers.
	DLNP	G.A. Karamysheva, G.D. Shirkov, Yu.Yu. Stepanenko
	FLNP	E.B. Askerov
4. **Methods, algorithms and software of computer algebra**		**V.P. Gerdt**
	LIT	V. Abgaryan, A.A. Bogolubskaya, O. Chuluunbaatar, A.A. Gusev, A.M. Khvedelidze, V.V. Kornyak, Yu. Palii, A.M. Raportirenko, I.A. Rogozhin, O.V. Tarasov, A.G. Torosyan, D.A. Yanovich
	BLTP	A.V. Czhizhov, P. Fiziev, D.I. Kazakov, V.S. Melezhik, A.I. Titov, S.I. Vinitsky
	FLNR	B.N. Gikal

Collaboration

Country or International Organization	City	Institute or Laboratory
Armenia	Yerevan	Foundation ANSL IIAP NAS RA

		RAU
		YSU
Belarus	Minsk	IM NASB
	Gomel	GSTU
Brazil	Sao Carlos, SP	IFSC USP
Bulgaria	Sofia	IMI BAS
		INRNE BAS
		SU
	Plovdiv	PU
Canada	Toronto	IBM Lab
	Edmonton	U of A
CERN	Geneva	CERN
China	Nanning	GUFN
Czech Republic	Prague	CTU
France	Metz	UPV-M
Georgia	Tbilisi	GTU
		TSU
		UG
Germany	Bonn	UniBonn
	Darmstadt	GSI
	Dresden	IFW
	Frankfurt/Main	Univ.
	Hamburg	Univ.
	Kassel	Uni Kassel
	Munich	LMU
India	Kolkata	JU
Italy	Bari	UniBa
Japan	Osaka	Kansai Univ.
	Saitama	SU
Kazakhstan	Almaty	INP
Lithuania	Kaunas	VMU
Moldova	Chişinău	MSU
Mongolia	Ulaanbaatar	IPT MAS
		NUM
		MUST
Poland	Krakow	NINP PAS
	Lublin	UMCS
	Otwock-Swierk	NCBJ
	Warsaw	WUT
	Wroclaw	UW
Romania	Bucharest	IFA
		IFIN-HH
		ISS
		UB
	Cluj-Napoca	INCDTIM

	Timişoara	UVT
Russia	Moscow	GPI RAS
		ITEP
		JIHT RAS
		KIAM RAS
		MIET
		NIFHI
		NNRU "MEPhI"
		NRC KI
		PFUR
		RCC MSU
		SINP MSU
	Dolgoprudny	MIPT
	Dubna	Dubna State Univ.
	Gatchina	NRC KI PNPI
	Perm	PSNRU
	Protvino	IHEP
	Puschino	IMPB RAS
		IPR RAS
	Saratov	SSU
	St. Petersburg	NIIEFA
	Tomsk	TSU
Saudi Arabia	Tuval	KAUST
Slovakia	Košice	IEP SAS
		PJSU
		TUKE
	Banska Bistrica	UMB
South Africa	Cape Town	UCT
	Stellenbosch	SU
Switzerland	Zurich	ETH
Tajikistan	Dushanbe	PHTI ASRT
		TNU
	Khujent	KSU
United Kingdom	Bath	UB
	London	Imperial College
USA	Cambridge, MA	MIT
	Davis, CA	UCDavis
	Durham, NC	NCCU
	Los Alamos, NM	LANL
Vietnam	Hanoi	VNU