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	Status: Extended

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

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Participating countries and international organizations:

Australia, Armenia, Azerbaijan, Belarus, Belgium, Brazil, Bulgaria, Canada, CERN, China, Czech Republic, France, Georgia, Germany, Italy, Israel, Japan, Kazakhstan, Moldova, Mongolia, Poland, Portugal, Romania, Russia, Slovakia, South Africa, Switzerland, Tajikistan, USA, Vietnam.

Issues addressed and main goals of research:

Carrying out paramount advanced research in computational mathematics and 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 physics studies. This subject area includes a wide spectrum of investigations approved for completion in JINR within the seven year period 2017–2023 in high energy physics, nuclear physics, physics of condensed matter and of nanostructures, biophysics, information technologies, the solution of which is inseparable from the use of computing. Such subject matters of the outmost importance in JINR are the NICA project, the neutrino program, the superheavy and exotic nuclei physics, the neutron based investigations. The needed numerical or symbolic-numerical computing will be done on the Multifunctional Information and Computing Complex (MICC), primarily the HybriLIT heterogeneous computing platform which involves the training and test cluster HybriLIT and the "Govorun" supercomputer and the emerging Big Data distributed infrastructure. The research teams include both experienced scientists with outstanding scientific achievements and enthusiastic young scientists and engineers. The requested financing will cover salaries, participations in scientific conferences, scientific visits and the acquisition of a minimal number of personal computers and licenses, within the approved resources for LIT-JINR. A distinctive feature of this research is the close cooperation of the Laboratory of Information Technologies (LIT) with research groups from all JINR laboratories and Member State institutions.

Expected results in the current year:

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

  Support for 3D multi-physical simulations using the COMSOL Multiphysics package for development of a superconducting proton therapy cyclotron in Dubna. Analysis of the measured magnetic field maps, calculations of the beam dynamics as well as of the influence of additional elements on the distribution of the magnetic field.

  Development of methods and algorithms for efficient highly accurate three-dimensional modeling of magnets and computations targeted to the creation of superconducting cyclotrons for proton therapy, in collaboration with DLNP.

  Generalization of Nambu – Jona-Lasinio – Polyakov model for the numerical description of properties of nuclear matter at NICA energies.

  Development of new molecular dynamics algorithms aimed at increasing accuracy and significantly reducing the computing time.

  Development of models for numerical studies of long-range structural changes of materials under heavy ion and nanocluster irradiation.

  Numerical modeling of ablation at material surfaces under the action of ultrashort laser pulses.

Development of numerical methods for describing equilibrium and nonequilibrium properties of mesoscopic systems of trapped atoms.

Numerical investigation of nuclear-physical processes within microscopic models, including reactions with light exotic nuclei.

Modeling neutrino-induced electromagnetic cascades at extremely high energies.

Development of methods for modeling the reflection of neutrons from layered nanostructures. Studies of magnetic films as structures consisting of vector micro-objects.

Study the role of spinor field in the evolution of the Universe (for minimal and non-minimal coupling) and in the formation of black holes and wormholes.

Maintenance of SAS primary processing program for YuMO spectrometer; development of a program for position sensitive detectors (isotropic and anisotropic scattering cases).

Step-by-step creation of an alert system for the BAIKAL project of DLNP.

Development of an extrapolation method of the sixth order with the aim at improving the algorithm efficiency for the numerical solution of a wide range of tasks.

Development of methods and algorithms for processing and analysis of the neutron noise of the IBR-2M reactor.

Multistage multiscale approach to the Bayesian automatic adaptive quadrature.

Development of algorithms for the numerical simulation of the evolution of a liquid crystal in a pulsed electric field, as well as under the influence of an orienting structured surface.

Simulation of peculiarities of the absorption-emission and photon density of states of a cholesterol liquid crystal with isotropic defect inside.

Transport approach based modeling of heavy-ion fragmentation reactions and comparison with experimental data.

- Within the Geant4 package: modeling interactions and application in various experiments (PANDA, NICA/MPD, NICA/SPD).

  Development of software support, processing and analysis of data in NUCLEON experiment.

  Software support for the BM@N experiment: development and implementation of algorithms for modeling, processing and analysis of data for the BM@N track system consisting of gas and semiconductor detectors with microstrip information acquisition (GEM, SILICON, CSC) and their subsequent integration into the BMNRoot.

  Development and refinement of the DQGSM model by comparison with experimental data of the BM@N.

  The MPD experiment: participation in the realization of a laser calibration system for detector alignment, monitoring drift velocity and for taking electric field distortion into account inside the Time-Projection Chamber (TPC) of the MPD central barrel.

  Further development of statistical methods for the analysis of experimental data under small statistics and incomplete observation of the studied processes.

  Development of batch processing of neutron diffraction spectra measured in real-time in situ mode (HRFD at IBR-2, FLNP).

  Software support of ATLAS experiment: development and maintenance of configuration and management of ATLAS TDAQ and of the EventIndex project

  Software support of CMS experiment: development, testing and implementation into the official CMS release of algorithms for the separation of overlapping signals and for building track segments in cathode strip chambers (CSC).

  The CBM experiment: development of a method for signal event selection in the CBM experiment based on a $J/\psi \to \mu^+\mu^-$ trigger. Adaptation of the ω_n^k criterion for the selection of doubly charged particles using the STS detector. Development of methods for the selection of rare decays associated with the hypernuclei.

  Improvement of the geometry database for the problems of the CBM experiment and the NICA project.

Approximation of the Internet traffic measurements in the trunk channel with the sum of log-normal distributions.

Analysis of nanostructure and properties of vesicular systems of phospholipids using the small-angle scattering data in the framework of the separated form factors model.

Massive calculations of electrostatic potentials of Zn-transcription factors with the aim at determining the nature of their interaction with the operator DNA.

- Development of ML/DL-based algorithms, including algorithms based on recurrent and convolutional neural networks with deep learning, for the rapid recognition of multiple tracks in particle physics experiments, including the NICA megaproject and the neutrino program.

  Development of algorithms based on the neural network approach for analysis and classification of medical and biological data and for forecasting the status of the environment.

  Parallelization of the most time-consuming functions using OpenMP, MPI, CUDA/OpenCL tools for modeling and reconstructing events in NICA experiments.

  Development of mathematical methods based on deep learning neural network approach for the determination of fine structures in the distribution of nuclear reaction products by mass and energy.

  Development and implementation of FEM solution of complex nonlinear magnetostatic problems within the COMSOL Multiphysics package.

  Parallel software on heterogeneous computing platforms for high performance numerical simulation of complex physical processes (Josephson junctions, localized states in condensed media, gas-hydrodynamic processes in porous media).

  Numerical study of multidimensional models based on evolutionary equations.

  Parallel algorithms for solving equations of motion of the molecular dynamics and equations of continuous media.

  Study of the possibility of increasing the performance of data analysis in ROOT through the use of graphics processors, comparative analysis of parallelization using PROOF and OpenCL (for applications in NICA project).

  Parallel implementation of large scale random matrices diagonalization.

  Parallel algorithms and codes for the solution of non-standard problems of magnetostatics.

  Solving optimization problems aimed at getting best parameters of superdense nuclear matter models in the simulation of heavy ion collisions and in astrophysical applications.

  Development of LDPC-like efficient decoding algorithms based on a genetic approach.

  Development of finite element method based computational schemes for the description of the quadrupole oscillations of the collective model of the nucleus.

  Development of computational schemes for the triangular three-center Coulomb problem and application to the H_3^+ molecule ion and H_2O molecule.

  Rebuilding mathematical packages entering the JINRLIB and CERNLIB (MATHLIB) libraries using modern software development tools, including open source (Intel Parallel Studio, GNU Compiler Collection).

  Development of the concept of a scalable software-analytical platform for the collection, storage and processing of results for the MPD experiment within the Big Data approach.

  Development of approaches for simulation, reconstruction and data processing of experiments on the basis of Big data Analytics for hybrid systems; use of new mathematical methods such as DQC (Dynamic Quantum Clustering), etc.

  Application of machine learning and artificial intelligence techniques for the optimization of the functioning of distributed computing for physical experiments; use of new mathematical methods such as Complex Networks, etc.

  Creation of a prototype system for intelligent monitoring of distributed computing systems based on the Big Data Analytics platform using streaming data and time series analysis methods.

- Modeling intelligence networks performing operations based on quantum decision theory; numerical analysis of models of artificial intelligence.

  Construction of an involutive monomial division providing compactness of the canonical involutive form.

  Development of an algorithm for reduction of systems of nonlinear algebraic equations to compact involutive form.

  HybriLIT GPU implementation of an algorithm for reduction of polynomial algebraic systems to canonical involutive form.

  Development of algorithms and programs to study multipartite quantum systems with spatial structure.

  Choice and analysis of a model of artificial neural network admitting implementation of the track reconstruction problem on existing adiabatic quantum computers.

  Definition of the basic elements for a quantum algorithm for the study of phase transitions in lattice QCD models at finite density.

  Computation of quasi-probability distributions for two qubit system.

  Computation of conditional probabilities of qubit state separability for non-negative Wigner distributions.

  Development of Lindblad equation for open relativistic systems based on the Bogolyubov equations for the state vector in relativistic quantum field theory.

  Embedding the FORM system module of field-theoretical calculations in high-energy physics into the Axiom system of computer algebra.

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** **J. Buša** **I.V. Puzynin**
LIT	S. Adam,R. Akhat, P.G. Akishin, I.V. Amirkhanov, E.A. Ayrjan, A.S. Ayriyan, I.V. Barashenkov, M.V. Bashashin, A.A. Bogolubskaya, I.L. Bogolubsky, A.M. Chervyakov, N.D. Dikusar, H. Grigorian, M. Kakenov, Yu.L. Kalinovsky, T.V. Karamysheva, M. Kakenov, D.S. Kulyabov, N.A. Kutovskyi, K.V. Lukyanov, N.V. Makhaldiani, T.I. Mikhailova, E.G. Nikonov, K. Oganesyan, T.P. Puzynina, B. Saha, N.R. Sarkar, I. Sarkhadov, Z.A. Sharipov, N.Yu. Shirikova, A.G. Soloviev, T.M. Solovieva, Yu.B. Starchenko, L.A. Siurakshina, Z.K. Tukhliev, A.V. Volokhova, O.O. Voskresenskaya, A. Wojczechowski, R.M. Yamaleev, E.P. Yukalova, E.V. Zemlyanaya, E.I. Zhabitskaya
VBLHEP	A.Yu. Boytsov, E.E. Donets, S. Gevorkyan, H.G. Khodzhibagiyan, V.A. Nikitin
BLTP	D.B. Blashke, V.V. Braguta, D.E. Castilio Alvares, A.V. Friesen, M. Hnatic, A.S. Hvorostuhin, E.-M. Ilgenfritz, V.K. Lukyanov, K.A. Maslov, L.A. Sevastianov, V.D. Toneev, V.V.Voronov, D.N. Voskresensky, V.I. Yukalov, V.Yu. Yushankhai
FLNR	M.K. Kochnev, S.M. Lukyanov, A. Oleinichak, Yu.E. Penionzhkevich, R.A. Rymzhanov, V.A. Skuratov
FLNP	E.B. Askerov, A.V. Belushkin, A.I. Kuklin, A.I. Ivankov, Yu.N. Pepelyshev

	DLNP	L.G. Afanasiev, I.A. Belolaptikov, G.A. Karamysheva, O. Karamyshev, I.N. Kiyan, B.A. Shaibonov, G.D. Shirkov
2. **Software complexes and mathematical methods for processing and analysis of experimental data**		**P.V. Zrelov** **V.V. Ivanov**
	LIT	E.P. Akishina, E.I. Aleksandrov, I.N. Aleksandrov, D.A. Baranov, M.V. Bashashin, S. Belogurov, O.Yu. Derenovskaya, I.A. Filozova, A.A. Kazakov, A.I. Kazymov, B.F. Kostenko, P.I. Kisel, G.E. Kozlov, L.Yu. Kruglova, M.A. Mineev, G.J. Musulmanbekov, A.V. Nechaevsky, G.A. Ososkov, E.V. Ovcharenko, V.V. Palichik, D.I. Pryakhina, V.S. Rikhvitsky, I. Satyshev, T.F. Sapozhnikova, V.N. Shigaev, S.K.Slepnyov, A.N. Sosnin, A.V. Uzhinsky, V.V. Uzhinsky, N.N. Voitishin, A.V. Volokhova, A.V. Yakovlev, E.V. Zemlyanaya, E.I. Zhabitskaya, V.B. Zlokazov
	VBLHEP	B.V. Batyunya, A.V. Bychkov, A.S. Galoyan, S.R. Gevorkyan, K.V. Gertsenberger, M.N. Kapishin, A.O. Kechechyan, V.P. Ladygin, V. Lenivenko, A.I. Malakhov, S.P. Merts, S.A. Movchan, S.V. Razin, O.V. Rogachevsky, V.N. Zhezher, M.A. Patsyuk
	BLTP	V.D. Toneev
	FLNR	A.G. Artukh, B. Erdemchimeg, A.S. Fomichev, Yu.E. Penionzhkevich, Yu.V. Pyatkov, Yu.M. Sereda, Yu.G. Sobolev, Yu.S. Tsyganov, V.K. Utenkov
	FLNP	A.M. Balagurov, I.A. Bobrikov, M.A. Kiselev, D.P. Kozlenko, M.V. Frontasyeva
	DLNP	I.V. Bednyakov, V.A. Bednyakov, A.G. Olshevsky, L.G. Tkachev, A.S. Zhemchugov
3. **Numerical methods, algorithms and software for multicore and hybrid architectures and Big Data analytics**		**Gh. Adam** **O. Chuluunbaatar** **P.V. Zrelov** **V.V. Korenkov** **O.I. Streltsova**
	LIT	E.I. Aleksandrov, A.S. Ayriyan, E.A. Ayrjan, M.V. Bashashin, S.D. Belov, D.V. Belyakov, J. Busa, Jr., A.M. Chervyakov, I.A. Filozova, A.A. Gusev, I.S. Kadochnikov, M.A. Matveev, I.S. Pelevanyuk, D.V. Podgainy, R.V. Polyakova, L.V. Popkova, T.P. Puzynina, A.A. Sapozhnikov, T.F. Sapozhnikova, N.R. Sarkar, I. Sarkhadov, R.N. Semyonov, S.I. Serdyukova, Z.A. Sharipov, A.G. Soloviev, T.M. Solovieva, Z.K. Tukhliev, N.N. Voytishin, A.V. Volokhova, O.I. Yuldashev, M.B. Yuldasheva, E.V. Zemlyanaya, E.I. Zhabitskaya, M.I. Zuev
	LIT-MICC	V.V. Mitsyn, T.A. Strizh
	FLNR	P.Yu. Apel, S.V. Mitrofanov, V.A. Skuratov
	BLTP	P.M. Krassovitskiy, R.G. Nazmitdinov, Yu.V. Popov, Yu.M. Shukrinov, S.I. Vinitsky

VBLHEP	K.V. Gertsenberger, A.D. Kovalenko, A.A. Moshkin, E.E. Perepelkin, O.V. Rogachevsky, V.V. Voronyuk
DLNP	V.A. Bednyakov, D.V. Naumov, A.G. Olshevskiy, O. Samoilov, E.A. Yakushev
FLNP	V.V. Novitsky + 3 pers

4. **Methods, algorithms and software of computer algebra and quantum computing** — **V.P. Gerdt**

LIT	N. Abbasly, V. Abgaryan, A.A. Bogolubskaya, A.M. Khvedelidze, V.V. Kornyak, E.A. Kotkova, A.M. Raportirenko, I.A. Rogozhin, K.K. Sharma, O.V. Tarasov, A.G. Torosyan, D.A. Yanovich, E.P. Yukalova
BLTP	A.V. Czhizhov, P. Fiziev, A.I. Titov, V.I. Yukalov
VBLHEP	O.V. Rogachevsky
FLNR	B.N. Gikal

Collaboration

Country or International Organization	City	Institute or Laboratory
Armenia	Yerevan	Foundation ANSL
		IIAP NAS RA
		RAU
		YSU
Australia	Sydney	Univ.
Azerbaijan	Baku	IP ANAS
Belarus	Minsk	IM NASB
		BSTU
Belgium	Brussels	ULB
	Louvain-la-Neuve	UCL
	Liege	ULg
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	Hangzhou	ZJU
	Hefei	IPP CAS
Czech Republic	Prague	CTU
France	Nancy	UL
	Nantes	SUBATECH
Georgia	Tbilisi	GTU

		TSU
		UG
		RMI TSU
Germany	Bonn	UniBonn
	Darmstadt	GSI
	Dresden	HZDR
		IFW
	Frankfurt/Main	Univ.
	Freiberg	TUBAF
	Giessen	JLU
	Hamburg	Univ.
	Jena	Univ.
	Kassel	Uni Kassel
	Karlsruhe	KIT
	Marburg	Univ.
	Munich	LMU
	Rostock	Univ.
	Wuppertal	UW
Greece	Thessaloniki	AUTH
Italy	Bari	UniBa
	Turin	INFN
	Catania	INFN LNS
	Frascati	INFN LNF
Israel	Tel Aviv	TAU
Japan	Osaka	Kansai Univ.
	Saitama	SU
Kazakhstan	Almaty	INP
Moldova	Chişinău	IAP
Mongolia	Ulaanbaatar	IPT MAS
		NUM
Poland	Krakow	NINP PAS
	Lublin	UMCS
	Otwock (Swierk)	NCBJ
	Warsaw	WUT
	Wroclaw	UW
Portugal	Lisbon	UL
Romania	Bucharest	IFIN-HH
		UB
	Cluj-Napoca	INCDTIM
	Magurele	ELI-NP
		IFA
		ISS
	Timişoara	UVT
Russia	Moscow	GPI RAS
		KIAM RAS

		IPMech RAS
		ICS RAS
		ITEP
		MRSU
		MSU
		RCC MSU
		NNRU "MEPhI"
		PFUR
		VIGG RAS
	Moscow, Troitsk	INR RAS
	Dubna	Dubna State Univ.
	Gatchina	NRC KI PNPI
	Novosibirsk	BINP SB RAS
	Perm	PSNRU
	Protvino	IHEP
	Puschino	IMPB RAS
		ITEB RAS
		IPR RAS
	Saratov	SSU
	St. Petersburg	NIIEFA
	Tomsk	TSU
	Tver	TvSU
Slovakia	Košice	IEP SAS
		UPJS
		TUKE
	Prešov	PU
	Banska Bistrica	UMB
South Africa	Cape Town	UCT
	Pretoria	UP
	Stellenbosch	SU
Switzerland	Zurich	ETH
Tajikistan	Dushanbe	PHTI ASRT
		TNU
	Khujand	KSU
USA	Davis, CA	UCDavis
	Los Angeles, CA	UCLA
	Madison, WI	UW-Madison
	La Jolla, CA	UCSD
	Lemont, IL	ANL
	Stanford, CA	SU
Vietnam	Hanoi	VNU