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		Priority:	1
		Status:	In-progress

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

Leaders: Gh. Adam
P.V. Zrelov

Deputies: J. Busa
O. Chuluunbaatar

Participating Countries and International organizations:

Armenia, Belarus, Brazil, Bulgaria, Canada, CERN, China, Czech Republic, France, Georgia, Germany, Hungary, Israel, Italy, Japan, Kazakhstan, Lithuania, Moldova, Mongolia, Poland, Romania, Russia, Slovakia, South Africa, Switzerland, Tajikistan, United Kingdom, 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 main results in the current year:

- Three-dimensional computer simulation of superconducting magnets for the NICA (JINR) and FAIR (GSI) projects. Construction of maps of the magnetic field distributions in the working areas of the magnets with a view to their further application to simulate physical processes.

  Solution of non-standard magnetostatics problems arising due to ROT asymmetry in the fission of heavy nuclei.

  COMSOL Multiphysics based development of a comprehensive model of an isochronous cyclotron.

  Development of a mathematical model and calculation of beam dynamics in isochronous cyclotrons based on the use of equations of motion.

  Mathematical modeling of magnetic fields in the study of polarization phenomena and spin effects.

  Generalization of the Nambu–Jona-Lasinio model with Polyakov loop enabling analysis of available experimental data on the collision of heavy ions at the NICA energy range.

  Modeling radiation induced changes in structures with defects in the framework of the molecular dynamics method.

  Numerical simulation of effects produced by double femtosecond laser pulses on targets of various compositions.

  Numerical modeling of magnetization reversal in nanomagnetic materials using the chirping effect.

  Computer modeling of quantum solids with dislocations exhibiting superfluid properties.

Investigation of nuclear physics processes within the hybrid microscopic potential using various density models of colliding nuclei.

Numerical study of the structure of phospholipid membranes in vesicular systems based on small-angle neutron and x-ray scattering data.

Development of robust numerical methods for the study of complex processes in layered Josephson structures and systems of superconducting spintronics.

Numerical study of particle-like solutions in multidimensional models of field theory; investigation of solitary waves in condensed matter systems.

Numerical investigation of the essential characteristics of electromagnetic cascade showers in the energy range $E \geq 10^{15}$ eV.

Search for black-hole-, wormhole- and soliton-like solutions from a self-consistent system of Einstein-Maxwell-Dirac equations.

Upgrade of the SAS primary processing program for the YuMO spectrometer to include anisotropic pattern scattering samples at the position-sensitive detector.

Extension of the FITTER program by increasing the number of theoretical models, improving its performance and GPU interface for experimental data processing.

Development of an extrapolation method within the basic element method (BEM) on non-uniform three-point grids for data processing and the numerical solution of ordinary differential equation problems.

Further BEM application for the processing and analysis of neutron noise of the IBR-2M reactor.

BEM use for the approximation of the dependence of the energy losses of charged particles in the ionization chamber (STAR experiment).

Implementation of Bayesian automatic adaptive quadrature with two interpolatory rules.

Modeling the interaction of electrons with a grating in a free-electron laser of Smith-Purcell type.

Development of methods of extracting the mass spectrum of neutron stars from the comparison of the observations of surface temperature of pulsars with the simulation results of their cooling evolution.

Modeling heavy-ion fragmentation within the combined transport – statistical approach.

Numerical analysis of crystal fields in magnetic rare-earth systems using quantum chemistry methods.

Numerical study of electron scattering through a multiple corrugated graphene structure.

- Tuning of FTF and QGS models of Geant4 for charmed particle production.

Simulation and analysis of nucleus-nucleus interactions at the NICA energy range in the Geant4 FTF and QGS hadronic models.

Further extension of the Monte-Carlo generator of heavy-ion collisions, DCM-SMM, with features asked by the NICA projects.

Use of DCM-SMM for the mass simulation of events for BM@N, SRC and MPD and participation in data analysis within the experiments conducted at these facilities.

Development of detector alignment algorithms for the Time-Projection Chamber of the MPD central barrel.

Further contribution to the development of the complex of databases for the CBM, BM@N and MPD experiments.

Development and implementation of algorithms for data modeling and reconstruction at the BM@N track detectors.

FAIRRoot and Geant4 Monte-Carlo simulation of the experiments with the OLVE-HERO detector prototype during its testing at the SPS accelerator at CERN.

Development of methods and algorithms for identifying the distribution of events with hadronic and electromagnetic showers from arrival directions of cosmic rays recorded by the NUCLEON satellite experiment.

Support for the ATLAS experiment software: development and maintenance of the configuration and management of ATLAS TDAQ, EventIndex for future RUN3, the CREST data format and the CREST client library.

Development of methods for evaluating the characteristics of the Cathode Strip Chambers with updated electronics in the CMS experiment.

Development of models, methods, algorithms and software for the selection of rare processes in the CBM experiment.

- Development of methods and algorithms for machine and deep learning, as well as algorithms based on computer vision for automating the analysis of data from radiobiological studies of laboratory animals and radiobiological experiments.

Development of efficient scalable algorithms based on the neural network approach for reconstructing multiple tracks in high-energy physics experiments, including for the NICA megaproject.

Optimization of the most time-consuming parts of the algorithms used for event modeling and reconstruction in the NICA experiments using high-performance computing techniques such as OpenMP, MPI, CUDA/OpenCL.

Application of machine learning methods for the simulation and analysis of the properties of linear structures in the mass distribution of nuclear reaction products.

Further development of machine and deep learning methods and algorithms for predicting the state of the environment and detecting plant diseases.

Development and implementation of hybrid FEM-BEM algorithms for solving complex nonlinear magnetostatic problems with high-aspect ratio geometries within the COMSOL Multiphysics package.

Development and application of the parallel method of asynchronous differential evolution and other minimization algorithms for the study of multi-parameter models of nuclear physics and condensed matter physics.

Development of methods and software for the high-performance solution of multi-parameter physical models described by systems of nonlinear differential equations (including superconducting processes in Josephson structures and gas-hydrodynamic processes in porous media).

Development and implementation of parallel algorithms and programs for the molecular dynamics modeling of structures with defects on the HybriLIT platform.

Adaptation of the ROOT toolkit designed for the most plausible fitting and modeling of the expected distribution of events in physical analysis for the GPU component of the HybriLIT platform.

Completion of the implementation of the parallel package for heavy-ion collisions on the HybriLIT platform and its inclusion in the JINRLIB library.

Development of parallel algorithms on large-scale random matrices.

Solution of multi-physical problems in the accelerator design, dosimetry and radiation safety.

Development of parallel algorithms and program modules for the high-accuracy solution of nonlinear magnetostatics problems by means of higher-order discontinuous and two-level domain decomposition methods.

Optimization of the parameterization of superdense nuclear matter models in the simulation of heavy-ion collisions and in astrophysical applications.

Use of minimal information entropy as a criterion for selecting a code for an iterative process of decoding low-density parity-check (LDPC) codes.

Development of minimax optimization computational schemes for calculating the relativistic energies of the ground and excited states of single-electron homonuclear superheavy dimers and trimmers.

Numerical simulation of Compton double ionization of helium atoms near the threshold.

Study of the possibility of using Fortran library programs (from JINRLIB, CERNLIB) by modern programming languages (Python, C#).

Development of a prototype of an intelligent monitoring system for distributed computing systems for streaming data (computer infrastructure, data transmission networks, information security).

Application of methods and techniques of machine learning and artificial intelligence for the optimization of the functioning and security of distributed computing for physical experiments.

Development of algorithms for modeling, reconstruction and classification/identification of events, as well as of approaches and methods for the intelligent monitoring of detectors of physical experiments on hybrid systems.

Selection and implementation of a business analytics solution for a heterogeneous computing environment that allows solving the problems of analysis and visualization of the results of physical experiments, monitoring systems and other applications.

Application of the created methods and algorithms of Big Data Analytics for the solution of relevant applied problems from other fields of science, socio-economic research included.

- Analysis of errors caused by the hardware of 5-qubit IBM quantum computers on examples of quantum teleportation of the Bell states.

Development of quantum algorithms for Tensor Networks contractions with the aim at modeling phase transitions in Lattice QCD.

Calculation of non-classicality indicators of low-dimensional quantum systems based on the negativity of the Wigner functions.

Comparative analysis of the separability/entanglement probability with non-classicality indicators for low-dimensional quantum systems.

Application of the method of evolutionary Bogolyubov equations in quantum field theory to the description of open low-dimensional quantum systems.

Development and implementation of algorithms for studying entanglement in models of quantum systems based on unitary representations of wreath products of finite groups.

Development and implementation of new efficient algorithms for investigating and solving systems of nonlinear algebraic equations based on the use of GRID environment resources and on the construction of a new involutive division of monomials.

Development of new finite element schemes enabling collective nuclear spectra estimates.

Derivation of functional equations for 5- and 6-point one-loop Feynman integrals with massive particles.

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** LIT	**Gh. Adam** **J. Busa** **I.V. Puzynin** S. Adam, P.G. Akishin, I.V. Amirkhanov, P.Kh. Atanasova, A.S. Ayriyan, E.A. Ayrjan, I.V. Barashenkov, M.V. Bashashin, A.A. Bogolubskaya, I.L. Bogolubsky, A.M. Chervyakov, N.D. Dikoussar, H. Grigorian, M. Kakenov, Yu.L. Kalinovsky, T.V. Karamysheva, D.S. Kulyabov, K.V. Lukyanov, N.V. Makhaldiani, T.I. Mikhailova, E.G. Nikonov, K. Oganesyan, D.V. Podgainy, R.V. Polyakova, T.P. Puzynina, V.S. Rikhvitsky,

		B. Saha, N.R. Sarkar, I. Sarkhadov, S.I. Serdyukova, Z.A. Sharipov, N.Yu. Shirikova, A.G. Soloviev, T.M. Solovieva, O.I. Streltsova, L.A. Syurakshina, Z.K. Tukhliev, O.O. Voskresenskaya, R.M. Yamaleev, E.P. Yukalova, O.I. Yuldashev, M.B. Yuldasheva, E.V. Zemlyanaya
	VBLHEP	G.N. Agakishiev, A.Yu. Boytsov, E.E. Donets, H.G. Khodzhibagiyan, A.D. Kovalenko, V.P.Ladygin, E.E. Perepelkin
	BLTP	D.E. Alvarez-Castillo, D. Blaschke, A.V. Friesen, M. Hnatič, R.V. olos, A.S. Khvorostukhin, E.E. Kolomeitsev, V.K. Lukyanov, R.G. Nazmitdinov, V.V. Papoyan, A.B. Pestov, L.A. Sevastyanov, V.D. Toneev, V.V. Voronov, D.N. Voskresensky, V.I. Yukalov, V.Yu. Yushankhai
	FLNR	A.G. Artukh, B. Erdemchimeg, R.A. Rymzhanov, Yu.M. Sereda, V.A. Skuratov
	FLNP	E.B. Askerov, O.I. Ivankov, A.I. Kuklin, V.V. Novitsky, Yu.N. Pepelyshev
	DLNP	G.A. Karamysheva, O.V. Karamyshev, I.N. Kiyan, V.A. Malinin, D.V. Popov, G.T. Torosyan
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, O.Yu. Derenovskaya, I.A. Filozova, Val.V. Ivanov, A.I. Kazymov, B.F. Kostenko, M.A. Mineev, G.J. Musulmanbekov, V.V. Palichik, R.V. Polozov, V.S. Rikhvitsky, T.F. Sapozhnikova, I. Satyshev, V.N. Shigaev, S.K. Slepnev, A.N. Sosnin, V.V. Uzhinsky, N.N. Voitishin, A.V. Yakovlev, V.B. Zlokazov
	VBLHEP	P.N. Batyuk, B.V. Batyunya, A.V. Bychkov, D.K. Dryablov, A.S. Galoyan, K.V. Gertsenberger, I.A. Golutvin, N.V. Gorbunov, A.Yu. Kamenev, M.N. Kapishin, V.Yu. Karzhavin, V.V. Lenivenko, A.M. Makan'kin, S.P. Merts, A.N. Morozov, M. Patsyuk, V.V. Perelygin, Yu.P. Petukhov, S.V. Razin, O.V. Rogachevsky, M.M. Rumyantsev, S.S. Shimansky, S.V. Shmatov, V.N. Spaskov, A.V. Zarubin, V. Zhezher
	BLTP	R.G. Nazmitdinov, V.D. Toneev
	FLNR	Yu.S. Tsyganov, V.K. Utenkov
	FLNP	A.M. Balagurov, A.V. Belushkin, D.P. Kozlenko, S.A. Manoshin
	DLNP	I.V. Bednyakov, V.A. Bednyakov, I.A. Belolaptikov, V.B. Brudanin, V.M. Grebenyuk, A.G. Olshevsky, A.E. Pan, D.B. Pontecorvo, B.A., F.V. Prokoshin, B.A. Shaibonov, L.G. Tkatchev
	UC	S.Z. Pakulyak
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	P.Kh. Atanasova, A.S. Ayriyan, D.R. Badreeva, D.A. Baranov, M.V. Bashashin, S.D. Belov, D.V. Belyakov, J.Busa, J. Buša Jr., Yu.A. Butenko, A.M. Chervyakov, G. Chuluunbaatar, O. Chuluunbaatar, P.V. Goncharov, H. Grigorian, A.A. Gusev, J.N. ogly Javazade, I.S. Kadochnikov, M. Kakenov, Yu.L. Kalinosky, M.A. Matveev, A.V. Nechaevsky, G.A. Ososkov, V.V. Papoyan, D.V. Podgainy, L.V. Popkova, T.P. Puzynina, A.A. Sapozhnikov, T.F. Sapozhnikova, R.N. Semenov, Z.A. Sharipov, T.M. Solovieva, A.V. Stadnik, Z.K. Tukhliev, A.V. Uzhinsky, 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	R. Kabytayeva, S.V. Mitrofanov, Yu.Ts. Oganesyan, Yu.V. Pyatkov
BLTP	Yu. B. Ivanov, S. Liebing, K.A. Maslov, R.G. Nazmitdinov, Yu.V. Popov, I.R. Rakhmonov, Yu.M. Shukrinov, S.I. Vinitsky
VBLHEP	A.Yu. Boytsov, E.E. Donets, O.V. Rogachevsky
DLNP	G.A. Karamysheva, G.D. Shirkov, A.S. Zhemchugov
FLNP	M.V. Frontaseva, M.F. Kiselev, N. Kucherka
LRB	I.M. Enyagina, I.A. Kolesnikova
4. Methods, algorithms and software of computer algebra and quantum computing	**V.P. Gerdt**
LIT	N. Abbasly, V. Abgaryan, M. Bures, 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	P. Fiziev, S.N. Nedelko, A. I. Titov, S.I. Vinitsky, V.I. Yukalov
VBLHEP	O.V. Rogachevsky
LRB	A.V. Czhizhov

Collaboration

Country or International Organization	City	Institute or laboratory
Armenia	Yerevan	Foundation ANSL
		IIAP NAS RA
		RAU
		YSU
Belarus	Brest	BrSU
	Gomel	GSTU
	Minsk	IM NASB
Brazil	Sao Carlos, SP	IFSC USP
Bulgaria	Plovdiv	PU
	Sofia	IMI BAS
		INRNE BAS
		SU
Canada	Toronto	IBM Lab
	Vancouver	UBC

CERN	Geneva	CERN
China	Beijing	IHEP CAS
Czech Republic	Prague	CTU
France	Marseille	UPC
	Nancy	UL
	Saclay	IRFU
Georgia	Tbilisi	GTU
		TSU
		UG
Germany	Berlin	MBI
	Bonn	UniBonn
	Darmstadt	GSI
	Dresden	IFW
	Frankfurt/Main	Univ.
	Giessen	JLU
	Hamburg	Univ.
	Heidelberg	MPIK
	Karlsruhe	KIT
	Kassel	Uni Kassel
	Munich	LMU
	Rostock	Univ.
Hungary	Budapest	Wigner RCP
Israel	Rehovot	WIS
	Tel Aviv	TAU
Italy	Bari	UniBa
	Catania	INFN LNS
	Genova	INFN
Japan	Saitama	SU
Kazakhstan	Almaty	INP
Lithuania	Kaunas	VMU
Moldova	Chisinau	IAP
Mongolia	Ulaanbaatar	IMDT MAS
Poland	Krakow	INP PAS
	Lublin	UMCS
	Otwock (Swierk)	NCBJ
	Wroclaw	UW
Romania	Bucharest	IFIN-HH
		UB
	Cluj-Napoca	INCDTIM
	Magurele	IFA
		ISS
	Timisoara	UVT
Russia	Dubna	Dubna State Univ.
	Gatchina	NRC KI PNPI
	Irkutsk	ISU
	Moscow	GPI RAS
		ITEP
		JIHT RAS
		MRSU
		MSU
		NNRU "MEPhI"
		PFUR
		RCC MSU
		SINP MSU

	Moscow, Troitsk	INR RAS
	Perm	PSNRU
	Puschino	IMPB RAS
	Saratov	SSU
	St. Petersburg	NIIEFA
		SPbSU
	Tomsk	TSU
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	Kosice	IEP SAS
		TUKE
		UPJS
South Africa	Cape Town	UCT
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	Stellenbosch	SU
Switzerland	Zurich	ETH
Tajikistan	Dushanbe	PHTI NAST
		TNU
	Khujand	KSU
United Kingdom	London	Imperial College
	Oxford	Univ.
	Plymouth	Univ.
USA	Arlington, TX	UTA
	Cambridge, MA	MIT
	College Station, TX	Texas A&M
	Davis, CA	UCDavis
	Denton, TX	UNT
	Los Angeles, CA	UCLA
	Newport News, VA	JLab
	San Diego, CA	SDSU
	Upton, NY	BNL
Vietnam	Hanoi	VNU