05-6-1119-2014/2023			
		Priority:	1
		Status:	Being concluded

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

Theme leaders: Gh. Adam
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Participating Countries and International organizations:

Armenia, Belarus, Bulgaria, CERN, China, Egypt, France, Georgia, Germany, Israel, Italy, Kazakhstan, Mexico, Moldova, Mongolia, Poland, Romania, Russia, Serbia, Slovakia, South Africa, 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 MLIT-JINR. A distinctive feature of this research is the close cooperation of the Meshcheryakov Laboratory of Information Technologies (MLIT) with research groups from all JINR laboratories and Member State institutions.

Expected results in the current year:

1. Detailed three-dimensional numerical analysis of the main characteristics of superconducting magnets within the NICA and NEW NUCLOTRON projects. Simulation of the operating modes of the MSC230 future isochronous cyclotron.

   Development of methods and software packages for the symbolic-numerical research of: processes (expansion of matter, crater formation, ablation) in materials under the action of ultrashort laser pulses; nuclear interactions (calculation of their characteristics, comparison with experimental data and theoretical estimates); stochastic kinetic models; models of complex systems in condensed matter physics.

   Development of effective approximation, smoothing and numerical integration algorithms based on the basic element method (BEM).

   Simulation of 5CB and 8CB nematic liquid crystals under the influence of orienting forces.

   Development of techniques for modeling the irradiation of complex structure targets with high-energy particles on the basis of the complex optimization of parallel algorithms and programs of molecular dynamics and of the continuous-atomistic method.

   Adaptation and application of the separated formfactors method for the study of the vesicular structure of phospholipid-based nanodrugs from small-angle scattering data.

   Simulation of the temperature evolution of neutron stars with strong magnetic fields, taking into account additional heat sources. Application of the Bayesian inference method for constructing the mass spectra of isolated neutron stars from multichannel astronomy data.

Investigation of the properties of diquarks and baryons in dense and hot nuclear matter, their effect on the birth of strangeness. Theoretical description and numerical simulation of $gg \to \pi\pi$ gluon scattering processes in heavy-ion collisions.

2. Geant4 package-based analysis of the strange particle yield in hadron-hadron and nucleus-nucleus collisions within the BM@N and MPD experiments. Modeling of pp interactions in the SPD experiment within the hadronic programs QGS and FTF of the Geant4 package, in particular, the production of charmed particles.

   Development and support of the Monte-Carlo generator of heavy-ion collisions, DCM-QGSM-SMM, and its application to the analysis of physical effects measured at the BM@N, SRC and MPD facilities.

   Algorithmic and software support for the MPD experiment: automation of the indication and removal of obsolete packages and of their dependencies during automated builds of nicadist for mpdroot.

   Algorithmic and software support for the BM@N experiment: modeling of detector signal responses, restoration of spatial coordinates, data reconstruction in new configurations of track detectors (runs 2022-2023); geometric alignment of detectors.

   Testing and debugging, in line with user requirements, and commissioning of the configuration, geometric information systems, and the database of physical event metadata, for the NICA experiments.

   Software support for the ATLAS experiment: refinement of the ATLAS Event Picking Service and commissioning of the second version of the service; adaptation of the CREST information system for work in the ATHENA software environment, development of operational monitoring of the TDAQ system based on GRAFANA9.

   Development and improvement of the algorithms and methods for reconstructing the trajectories of charged particles in the cathode-strip chambers, assessment of the spatial resolution of cathode-strip chambers in the CMS experiment Run3 data (2022–2023).

   Development of data processing system software for the Baikal-GVD project.

   Monte-Carlo simulation of the background counting of the scintillation-tungsten component of the OLVE-HERO detector.

   Development of the SAS software package for the primary processing of data obtained on the small-angle neutron scattering spectrometer with the multidetector system (modernization before the start of the reactor).

   Development of a web application designed to fit data obtained in the study of the crystallographic texture of various objects using neutron diffraction and other state-of-the-art methods of neutronography.

   Application of artificial neural networks and cellular automata in tasks of experimental data processing.

3. Development of neural network algorithms for the recognition, segmentation and classification of brain cells and behavioral patterns of laboratory animals.

   Development of machine and deep learning methods for: event reconstruction in the MPD, BM@N and SPD experiments; analysis of fine structures in the mass distribution of nuclear reaction products in experiments with transuranic elements; study of nanocomposite thin films using neutron and X-ray reflectometry methods; plant disease detection tasks; environmental monitoring.

   Further development of hp-adaptive high-precision methods for solving elliptic problems on multicore computers and development of highly scalable parallel algorithms for spatial problems of magnetostatics.

   Development of methods and programs for integrating multidimensional functions using neural networks in the case of functional limits.

   Calculation of the adsorption characteristics of superheavy atoms at the surface of gold by density functional theory methods using the AMS computing software package on the "Govorun"supercomputer.

   Development of algorithms to calculate sub-barrier fusion reactions of heavy nuclei within the channel coupling method.

   Development of digital methods to assess the growth rate of rounding errors in a uniform metric using the REDUCE system on the "Govorun" supercomputer.

   Development of methods and software tools to solve service and applied tasks using the technologies of Big Data processing and data mining.

Elaboration and development of methods for storage, processing and physical analysis of data for the experiments of the NICA megaproject within the Big Data approach.

4. Development of quantum algorithms and their implementation in the environment of quantum computing simulators for the investigation of the electron shells of superheavy element atoms, for experimental data processing and analysis, as well as for the intelligent control of different systems.

   Development of embedded quantum intelligent regulators for use as control modules of different robotic devices. Development of a prototype of a quantum intelligent regulator for the coordinated control of the pressure and consumption of nitrogen and helium during the automated cooling of a superconducting magnet (different emergency situations included).

   Development and testing of an intelligent system for controlling the modes of the high-frequency stations of the Nuclotron of the NICA accelerator complex on the basis of the principles of quantum software engineering.

   Modeling of quantum algorithms on simulators using classical computing architectures (CPU, GPU) to solve the problem of calculating the structure of the electronic spectrum of simple molecules.

   Numerical study of the role of collective information in networks of quantum agents.

   Development of algorithms for the constructive decomposition of quantum systems into subsystems using computer algebra methods and computational group theory.

   Derivation of criteria for the reducibility of polynomials to zero based on machine learning methods.

   Development of a software package for analytical computations of one-loop Feynman integrals entering the light-by-light scattering processes, gg→WW, hh→ZZ, hh→ZH, gg→hh.

   Simulation of the real time non-equilibrium evolution and quantum phase transitions in the two-dimensional quantum Ising model on a quantum computer.

   Creation of a software package for the fast generation of arbitrary rank random qudit density matrices.

   Modeling of quantum registers and quantum logic gates based on quantum dots of complex geometry.

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. Busa** **I.V. Puzynin**
	MLIT	S. Adam, P.G. Akishin, I.V. Amirkhanov, A.S. Ayriyan, E.A. Ayrjan, D.R. Badreeva, I.V. Barashenkov, M.V. Bashashin, A.A. Bogolubskaya, A.M. Chervyakov, N.D. Dikussar, H. Grigorian, Yu.L. Kalinovsky, T.V. Karamysheva, D.S. Kulyabov, K.V. Lukyanov, N.V. Makhaldiani, T.I. Mikhailova, E.G. Nikonov, R.V. Polyakova, T.P. Puzynina, V.S. Rikhvitsky, B. Saha, I. Sarkhadov, Z.A. Sharipov, Shirikova, Z.K. Tukhliev, A.V. Volokhova, O.O. Voskresenskaya, R.M. Yamaleev, N. Yu, E.P. Yukalova, E.V. Zemlyanaya, E.I. Zhabitskaya
	VBLHEP	G.N. Agakishiev, H.G. Khodzhibagiyan
	BLTP	A.A. Donkov, A.V. Friesen, M. Hnatič, E.E. Kolomeitsev, A.S. Khvorostukhin, V.K. Lukyanov, A.B. Pestov, L.A. Sevastyanov, D.N. Voskresensky, V.I. Yukalov
	FLNR	E. Batchuluun, M.N. Mirzaev, Yu.M. Sereda, V.A. Skuratov
	FLNP	A.S. Doroshkevich, N. Kučherka, E.E. Perepelkin, E.P. Popov, Yu.N. Pepelyshev, E.P. Shabalin

DLNP	G.A. Karamysheva, O.V. Karamyshev, I.N. Kiyan, I.D. Lyapin, V.A. Malinin, D.V. Popov, K. G.D. Shirkov
2. Software complexes and mathematical methods for processing and analysis of experimental data	**P.V. Zrelov** **V.V. Ivanov**
MLIT	E.P. Akishina, E.I. Aleksandrov, I.N. Aleksandrov, D.A. Baranov, J. Buša Jr., O.Yu. Derenovskaya, I.A. Filozova, S. Hnatič, A.I. Kazymov, B.F. Kostenko, M.A. Mineev, G.J. Musulmanbekov, V.V. Palichik, D.I. Pryakhina, V.S. Rikhvitsky, T.F. Sapozhnikova, I. Satyshev, G.V. Shestakova, Z.A. Sharipov,S.K. Slepnev, A.G. Soloviev, T.M. Solovieva, A.N. Sosnin, Z.K. Tukhliev, V.V. Uzhinsky, N.N. Voitishin, A.V. Yakovlev, V.B. Zlokazov
VBLHEP	Yu. V. Bespalov, D. K. Dryablov, I.R. Gabdrakhmanov, A.S. Galoyan, K.V. Gertsenberger, I.A. Golutvin, N.V. Gorbunov, A.V. Gus'kov, A.Yu. Kamenev, M.N. Kapishin, V.Yu. Karzhavin, V.V. Lenivenko, A.M. Makan'kin, S.P. Merts, A.N. Morozov, D. N. Nikiforov, M. Patsyuk, V.V. Perelygin, Yu.P. Petukhov, O.V. Rogachevsky, M.M. Rumyantsev, S.V. Shmatov, S.S. Shimansky, V.N. Spaskov, A.V. Zarubin, V. Zhezher
BLTP	V.D. Toneev
FLNR	Yu.S. Tsyganov, V.K. Utenkov
FLNP	M. Balasoiu, A.I. Ivan'kov, A.H. Islamov, Yu.S. Kovalev, A.I. Kuklin, Yu.L. Rizhikov, A.V. Rogachov, V.V. Skoy
DLNP	I.A. Belolaptikov, A.E. Pan, B.A. Shaibonov, L.G. Tkatchev
UC	A.Yu. Verkheev
3. Numerical methods, algorithms and software for multicore and hybrid architectures and Big Data analytics	**Gh. Adam** **O. Chuluunbaatar** **P.V. Zrelov** **O.I. Streltsova**
MLIT	A.I. Anikina, A.S. Ayriyan, D.A. Baranov, S.D. Belov, D.V. Belyakov, J. Buša Jr., Yu.A. Butenko, G. Chuluunbaatar, P.V. Goncharov, H. Grigorian, A.A. Gusev, A.V. Ilina, J.N. ogly Javazade, I.S. Kadochnikov, Yu.L. Kalinosky, M.A. Matveev, A.V. Nechaevsky, D.A. Oleinik, G.A. Ososkov, V.V. Papoyan, I.S. Pelevanyuk, A.Sh. Petrosyan, R.N. Semenov, S.I. Serdyukova, A.V. Stadnik, A.V. Uzhinsky, O.I. Yuldashev, M.B. Yuldasheva
MLIT-MICC	V.V. Korenkov, V.V. Mitsyn, T.A. Strizh
FLNR	N.V. Aksenov, A.A. Astahov, A.V. Karpov, Yu.Ts. Oganesyan, Yu.V. Pyatkov, V.V. Samarin
BLTP	Yu.B. Ivanov, S. Libing, Yu.V. Popov, I.R. Rahmonov, Yu.M. Shukrinov, S.I. Vinitsky, D.N. Voskresensky
VBLHEP	K.V. Gertsenberger
DLNP	A.S. Zhemchugov
FLNP	M.V. Avdeev, W. Badavy, M.V. Frontaseva, M.F. Kiselev, T.V. Tropin
LRB	I.A. Kolesnikova, K.N. Lyakhova, Yu.S. Severiukhin, D.M. Utina

4. Methods, algorithms and software of computer algebra and quantum computing	**D.V. Podgainy** **A.M. Khvedelidze** **P.V. Zrelov**
MLIT	V. Abgaryan, A.S. Bondyakov, M. Bures, O. Chuluunbaatar, A.A. Gusev, O.V. Ivancova, V.V. Kornyak, E.A. Kuznetsov, Yu. Palii, A.M. Raportirenko, A.G. Reshetnikov, A.R. Ryabov, N.V. Ryabov, I.A. Rogozhin, N. Saktaganov, S.V. Semashko, A.V. Stadnik, O.I. Streltsova, L.A. Syurakshina, O.V. Tarasov, A.G. Torosyan, S.V. Ulyanov, D.A. Yanovich, E.P. Yukalova, D.P. Zrelova, M.I. Zuev
BLTP	N.A. Tyurin, S.I. Vinitsky, V.I. Yukalov, V.Yu. Yushankhai
DLNP	M.S. Katulin
VBLHEP	O.I. Brovko, A.V. Butenko, G.P. Reshetnikov, O.V. Rogachevsky, E.V. Sedykh
LRB	A.V. Czhizhov

Collaboration

Country or International Organization	City	Institute or Laboratory
Armenia	Yerevan	Foundation ANSL
		RAU
		YSU
Belarus	Minsk	IM NASB
Bulgaria	Sofia	IMI BAS
		INRNE BAS
		SU
CERN	Geneva	CERN
China	Beijing	CIAE
Egypt	Giza	CU
France	Nancy	UL
	Saclay	IRFU
Georgia	Tbilisi	GTU
		TSU
		UG
Germany	Darmstadt	GSI
	Hamburg	Univ.
	Kassel	Uni Kassel
Israel	Tel Aviv	TAU
Italy	Genoa	INFN
Kazakhstan	Almaty	INP
		KazNU
Mexico	Mexico City	UNAM
Moldova	Chisinau	MSU
Mongolia	Ulaanbaatar	IMDT MAS
Poland	Krakow	INP PAS
		JU
		UEK
	Wroclaw	UW
Romania	Bucharest	IFIN-HH

Russia	Dolgoprudny	MIPT
	Dubna	Dubna State Univ.
	Irkutsk	ISU
	Moscow	ITEP
		MSU
		NNRU "MEPhI"
		PFUR
		PRUE
		RCC MSU
		RSTSREC
		SINP MSU
	Moscow, Troitsk	INR RAS
	Puschino	IMPB RAS
	Saratov	SSU
	St. Petersburg	NIIEFA
		SPbSU
	Tomsk	TSU
	Vladikavkaz	NOSU
Serbia	Belgrade	Univ.
Slovakia	Kosice	UPJS
South Africa	Cape Town	UCT
Tajikistan	Dushanbe	PHTI NAST
	Khujand	KSU
United Kingdom	Plymouth	Univ.
USA	Cambridge, MA	MIT
	Los Angeles, CA	UCLA
Vietnam	Hanoi	VNU
	Ho Chi Minh City	HCMUE