05-6-1119-2014/2023

Priority:	1

Status: In-progress

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

Leaders: Gh. Adam
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Deputies: J. Busa
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Participating Countries and International organizations:

Armenia, Belarus, Brazil, Bulgaria, Canada, CERN, China, Czech Republic, France, Georgia, Germany, Hungary, Italy, 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 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 main results in the current year:

- Three-dimensional computer simulation of magnets for the NICA (JINR), NUCLOTRON (JINR) and CBM (GSI) projects. The magnetic field map construction for analysis of the field distribution quality in the working areas of the magnets.

  Optimization of a portable magnetic device designed to study the ROT-effects in the fission of heavy nuclei.

  Implementation of a hybrid FEM-BEM method for modeling complex magnetic accelerator systems in the COMSOL Multiphysics® environment and its use to multi-physical modeling of the magnetic system for the SC230 isochronous cyclotron. Development of methods for correcting the average magnetic field of an isochronous cyclotron based on the solution of the equations of motion. Development and implementation of the CORD (Closed ORbit Dynamics) program into the JINRLIB library for the analysis of field maps of the SC230 isochronous cyclotron.

  Molecular dynamics modeling of structural changes in metals and metal composites under irradiation with heavy ions and alpha particles, description of experimental data.

  Numerical simulation of phase transitions (melting, evaporation and ablation) in materials exposed to femtosecond laser pulses.

  Numerical study of the statistical properties of structures with extended nanosize defects.

  Computer modeling of spin dynamics in spintronic materials and development of methods governing spin reversal effects.

  Investigation of the spin filtering effect by the corrugation graphene.

Research and software implementation of methods for the numerical solution of stiff systems describing spintronic models.

Study of nucleus-nucleus and proton-nucleus interactions in a wide range of energies using microscopic models and various models of the density of colliding nuclei. Investigation of reactions involving the ^{17}F isotope on stable targets at medium energies.

Application of the dibaryon resonance model to study and calculate the characteristics of light nuclei with A = 6, including the two-proton decay of ^{6}Be.

Estimation of the drip-line for neutron-excess nuclei.

Study of spatially localized temporally periodic or quasiperiodic solutions of the phi-4 equation on the basis of new finite-mode approximations for the bound state of the wobbling kink and breather in one dimension and for the three-dimensional oscillon.

Analytical and numerical study of the role of the spinor field in the formation of black holes and the evolution of the Universe.

Development of algorithms for computing the primary atomic displacement cross sections by fast electrons in solids.

Modernization of software developed for the study of properties of new materials and nanosystems by modern neutron scattering methods.

Extension of the basic element method (BEM) to the solution of stiff problems and its use for solving applied problems, including processing and analysis of neutron noise of the IBR-2M reactor and approximating the dependence of the energy losses of charged particles in the ionization chamber (STAR experiment).

Development of Bayesian automatic adaptive quadrature algorithms of high fidelity.

Application to open systems of the developed methodology for the stochastization of dynamic one-step systems.

Modification of the Bayesian selection method of the best model parameters of nuclear matter in the analysis of the latest existing and planned discoveries of astrophysical phenomena of compact stars by multichannel astronomy.

Numerical study of the quark-hadron phase transition in the energy range of the NICA collider.

Numerical analysis of heavy ion fragmentation reactions in the framework of transport-statistical models, comparison with the experiment.

- Development of phenomenological models of hadron-hadron interactions of the Geant4 package for the energy range in which the perturbative QCD does not work, and their application for calculating the experimental conditions of JINR, GSI, CERN experiments with hadronic and nuclear beams.

  Creation of a combined generator of nucleus-nucleus collisions DCM-QGSM-SMM, with further modification by including the production of heavy resonances, dileptons and hyperphragments. Mass generation of nucleus-nucleus collisions for the BM@N and MPD experiments.

  Optimization, development and refactoring of the MPD detector software.

  Development of alignment algorithms for the time-projection camera TPC of the MPD detector, taking into account the accumulating space charge.

  Development of the structure, software and operating model of a quantum intelligent regulator of nitrogen and helium consumption for a superconducting magnet, taking into account possible operating modes, various emergency situations included.

  Development of an intelligent system for controlling the modes of the high-frequency stations of the Nuclotron of the NICA accelerating complex using quantum soft computations.

  Completion of the development and upgrade of information systems of geometric and configuration databases, as well as a database of metadata of physical events for the NICA experiments.

  Development of event reconstruction algorithms, realistic simulation of responses and detailed ROOT geometry for the configuration of the central track detectors of the BM@N experiment in 2022.

  Development and implementation of algorithms for modeling and data reconstruction in the track detectors of the BM@N experiment for the preparation and conduct of the physical session in 2022.

  Development of the data aquisition software for the Baikal-GVD project.

  Monte Carlo modeling of the OLVE-HERO prototype within the FAIRRoot and Geant4 framework. Study of the systematic errors and the influence of the geometry of the experiment on the results.

  Testing the developed algorithms for building the distributions of cosmic rays arrival directions for their correctness while processing the NUCLEON experiment data obtained in different modes of the cosmic apparatus flight.

Development of non-standard statistics analysis methods of rare events in experiments with superheavy nuclei.
Agreed support for the ATLAS experiment software: further development of the ATLAS Event Picking Service, maintenance of the ATLAS EventIndex monitoring system; development and upgrade of the CREST information system, software for the conversion of ATLAS ConditionDB data from COOL API to CREST; upgrade of operational monitoring of the ATLAS TDAQ system based on new versions of GRAFANA.
Improvement of methods for reconstructing the trajectories of charged particles and calculations of the efficiency and resolution of cathode-strip chambers with updated electronics in the CMS experiment.
Testing, debugging in accordance with user requirements and commissioning of the geometry database for the CBM experiment. Development of a database concept for selecting useful events.

- Solving the problem of image segmentation based on deep learning algorithms for morphological research in radiation biology. Application of the neural network approach and computer vision methods for the tasks of analyzing radiobiological research data.
  Creation of a computer package for calculating the QCD phase diagram on the HybriLIT platform.
  Further development of efficient scalable deep learning algorithms of the local and global types for the reconstruction of multiple tracks and vertices of events in high-energy physics experiments related to MPD, BM@N, BES-III, SPD and CBM.
  Application of machine learning methods for the recognition and analysis of the properties of fine structures in the mass distribution of nuclear reaction products in experiments with transuranium elements.
  Enhancement of the efficiency of the applied deep learning algorithms for the tasks of predicting the state of the environment and detecting plant diseases; development of new, time series based, statistical analysis methods for air pollution monitoring; expansion of forecasting areas to new regions of Russia, Europe and Asia.
  Utilization of the shared CPU-GPU memory of the HybriLIT computational platform for the COMSOL Multiphysics® environment to improve the speed of simulations.
  Investigation of the structure and properties of polydispersed vesicular systems in the framework of the separated form factors model: parallel optimization of the model parameter fitting to the experimental small-angle scattering data.
  Development of methods and software packages for high-performance numerical research of complex processes in multiparameter models of nuclear physics and condensed matter physics.
  Development, optimization and implementation of new parallel versions of algorithms and programs for molecular dynamics modeling on the HybriLIT platform.
  Simulation of the evolution of liquid crystals under the influence of orienting forces using molecular dynamics software packages on modern graphic systems.
  Development of a parallel version of the FITTER program designed to study the supramolecular structure and functional characteristics of biological nanosystems and polymer nanomaterials.
  Development of highly scalable parallel algorithms and programs for solving nonlinear magnetostatic problems by the finite element discontinuous hp-method.
  Development of parallel algorithms and programs for studying the properties of nuclear matter in heavy ion collisions and the cores of compact stars.
  Development and application of new computational methods for the treatment of basic problems of relativistic quantum chemistry and physics, in particular, in the study of the electronic structure and spectroscopic properties of heavy atoms and molecules.
  Development and numerical implementation of the method of Compton pulse spectroscopy of light atoms and molecules.
  Development of a software and hardware complex for collecting, storing and analyzing Big Data for solving service and applied problems (monitoring and security of computing systems, physical and engineering applications).
  Development of a prototype system for intelligent monitoring of the functioning and security of distributed computing systems based on Big Data technologies and machine learning methods.
  Application of Big Data methods, algorithms, and platforms to solving relevant applied tasks, including the analysis of JINR's performance indicators and automated intelligent text processing of scientific publications.

- Development of quantum algorithms for modeling the electron shells of atoms of superheavy elements. Development of algorithms based on quantum neural networks for solving equations of mathematical physics.
  Quantum information processing in artificial intelligence networks with long- and short-term memories of active nodes.

Development of quantum circuits, of quantum and classical algorithms, based on the tensor network method, for modeling phase transitions in quantum chromodynamics at nonzero temperature and finite baryon density.

Study of the relationship between the negativity of the Wigner function and the nonclassicality of states of finite-dimensional quantum systems.

Formulation of constructive models for the study of decomposition of quantum systems into subsystems and analysis of quantum correlations within multi-component systems.

Development and implementation of a grid version of the algorithm for computing Gröbner and involutive bases of algebraic nonlinear polynomial systems.

Development of finite element schemes with interpolation Hermite polynomials for solving boundary value problems for systems of ordinary differential equations.

Creation of a package for high precision evaluation of 3- and 4-point one-loop Feynman integrals with the help of the method of functional reduction.

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	V. Abgaryan, 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, A.M. Chervyakov, N.D. Dikussar, H. Grigorian, M. Kakenov, Yu.L. Kalinovsky, T.V. Karamysheva, D.S. Kulyabov, K.V. Lukyanov, N.V. Makhaldiani, T.I. Mikhailova, G.J. Musulmanbekov, E.G. Nikonov, R.V. Polyakova, T.P. Puzynina, V.S. Rikhvitsky, B. Saha, I. Sarkhadov, S.I. Serdyukova, Z.A. Sharipov, N.Yu. Shirikova, A.G. Soloviev, T.M. Solovieva, 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, H.G. Khodzhibagiyan, V.P. Ladygin, E.E. Perepelkin, M.M. Shandov
	BLTP	D.E. Alvarez-Castillo, D. Blaschke, A.A. Donkov, A.V. Friesen, M. Hnatič, R.V. Jolos, A.S. Khvorostukhin, E.E. Kolomeitsev, S. Liebing, V.K. Lukyanov, L.A. Malov, K.A. Maslov, R.G. Nazmitdinov, I.R. Rakhmonov, L.A. Sevastyanov, Yu.M. Shukrinov, A.V. Sushkov, D.N. Voskresensky, V.I. Yukalov
	FLNR	A.G. Artukh, E. Batchuluun, M.N. Mirzaev, A. Oleinichak, Yu.M. Sereda, V.A. Skuratov
	FLNP	A.S. Doroshkevich, T.A. Lychagina, D.I. Nikolaev, V.V. Novitsky, E.P. Popov, Yu.N. Pepelyshev
	DLNP	G.A. Karamysheva, O.V. Karamyshev, I.N. Kiyan, I.D. Lyapin, V.A. Malinin, D.V. Popov, K. Semek, 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, A.S. Bondyakov, J. Buša Jr., O.Yu. Derenovskaya, I.A. Filozova,

		S. Hnatič, A.I. Kazymov, A.O. Kondratyev, B.F. Kostenko, E.A.Kuznetsov, M.A. Mineev, G.J. Musulmanbekov, V.V. Palichik, D.I. Pryakhina, A.G. Reshetnikov, V.S. Rikhvitsky, T.F. Sapozhnikova, I. Satyshev, S.V. Semashko, G.V. Shestakova, S.K. Slepnev, A.G. Soloviev, A.N. Sosnin, S.V. Ulyanov, V.V. Uzhinsky, N.N. Voitishin, A.V. Yakovlev, V.B. Zlokazov
	VBLHEP	A.S. Andreev, P.N. Batyuk, B.V. Batyunya, O.I. Brovko, A.V. Butenko, A.V. Bychkov, I.R. Gabdrakhmanov, A.S. Galoyan, K.V. Gertsenberger, I.A. Golutvin, E.V. Gorbachev, N.V. Gorbunov, A.Yu. Kamenev, M.N. Kapishin, V.Yu. Karzhavin, S.A. Kostromin, V.V. Lenivenko, A.M. Makan'kin, S.P. Merts, D.V. Monakhov, A.N. Morozov, M. Patsyuk, V.V. Perelygin, Yu.P. Petukhov, G.P. Reshetnikov, O.V. Rogachevsky, M.M. Rumyantsev, S.V. Shmatov, V.N. Spaskov, A.V. Zarubin, V. Zhezher
	BLTP	V.D. Toneev
	FLNR	Yu.S. Tsyganov, V.K. Utenkov
	DLNP	V.A. Bednyakov, I.A. Belolaptikov, V.M. Grebenyuk, A.G. Olshevsky, A.E. Pan, D.B. Pontecorvo, 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** **O.I. Streltsova**
	MLIT	P.Kh. Atanasova, A.S. Ayriyan, D.R. Badreeva, D.A. Baranov, M.V. Bashashin, S.D. Belov, D.V. Belyakov, J. Buša Jr., Yu.A. Butenko, A.M. Chervyakov, G. Chuluunbaatar, I.A. Filozova, P.V. Goncharov, H. Grigorian, A.A. Gusev, A.V. Ilina, J.N. ogly Javazade, I.S. Kadochnikov, M. Kakenov, Yu.L. Kalinosky, M.A. Matveev, A.V. Nechaevsky, D.A. Oleinik, G.A. Ososkov, V.V. Papoyan, I.S. Pelevanyuk, A.Sh. Petrosyan, D.V. Podgainy, D.I. Pryakhina, I.V. Puzynin, T.P. Puzynina, R.N. Semenov, Z.A. Sharipov, A.G. Soloviev, T.M. Solovieva, A.V. Stadnik, V. Svozilik, L.A. Syurakshina, Z.K. Tukhliev, A.V. Uzhinsky, A.V. Volokhova, O.I. Yuldashev, M.B. Yuldasheva, E.V. Zemlyanaya, E.I. Zhabitskaya
	MLIT-MICC	V.V. Mitsyn, T.A. Strizh
	FLNR	R. Kabytayeva, S.V. Mitrofanov, Yu.Ts. Oganesyan, Yu.V. Pyatkov
	BLTP	D. Blaschke, A.A. Donkov, A.V. Friesen, A.S. Hvorostuhin, Yu.V. Popov, S.I. Vinitsky, D.N. Voskresensky, V.Yu. Yushankhai
	VBLHEP	A.Yu. Boytsov, E.E. Donets, K.V. Gertsenberger
	DLNP	G.A. Karamysheva, A.S. Zhemchugov
	FLNP	M. Balasoiu, W. Badavy, M.V. Frontaseva, M.F. Kiselev, N. Kucherka, A.I. Kukli, I. Pavlikova, I. Zinicovscaia
	LRB	I.A. Kolesnikova, M.G. Lalkovicova, 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**	
MLIT	V. Abgaryan, M. Bures, O. Chuluunbaatar, A.A. Gusev, V.V. Kornyak, E.A. Kotkova, Yu. Palii, A.M. Raportirenko, I.A. Rogozhin, N. Saktaganov, A.V. Stadnik, O.I. Streltsova, O.V. Tarasov, A.G. Torosyan, D.A. Yanovich, E.P. Yukalova, M.I. Zuev	
BLTP	R.G. Nazmitdinov, V.V. Braguta, A. I. Titov, N.A. Tyurin, 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
		RAU
		YSU
Belarus	Brest	BrSU
	Minsk	IM NASB
Brazil	Sao Carlos, SP	IFSC USP
Bulgaria	Plovdiv	PU
	Sofia	IMI BAS
		INRNE BAS
		SU
Canada	Toronto	IBM Lab
CERN	Geneva	CERN
China	Beijing	CIAE
		IHEP CAS
Czech Republic	Ostrava	VSB-TUO
	Prague	CTU
France	Nancy	UL
	Saclay	IRFU
Georgia	Tbilisi	GTU
		TSU
		UG
Germany	Darmstadt	GSI
	Frankfurt/Main	Univ.
	Hamburg	Univ.
	Karlsruhe	KIT
	Kassel	Uni Kassel
	Munich	LMU
	Rostock	Univ.
Hungary	Budapest	Wigner RCP
Italy	Genoa	INFN
Kazakhstan	Almaty	INP
		KazNU
Lithuania	Kaunas	VMU
Moldova	Chisinau	IAP
		MSU
Mongolia	Ulaanbaatar	IMDT MAS

Poland	Krakow	INP PAS
		JU
		UEK
	Lublin	UMCS
	Warsaw	IMGW-PIB
	Wroclaw	UW
Romania	Bucharest	IFIN-HH
		UB
	Cluj-Napoca	INCDTIM
	Magurele	IFA
		ISS
	Timisoara	UVT
Russia	Dolgoprudny	MIPT
	Dubna	Dubna State Univ.
	Gatchina	NRC KI PNPI
	Irkutsk	ISU
	Moscow	GPI RAS
		ITEP
		MRSU
		MSU
		NNRU "MEPhI"
		PFUR
		PRUE
		RCC MSU
		SINP MSU
	Moscow, Troitsk	INR RAS
	Novosibirsk	SKIF
	Perm	PSNRU
	Puschino	IMPB RAS
	Saratov	SSU
	St. Petersburg	NIIEFA
		SPbSU
	Vladikavkaz	NOSU
Slovakia	Banska Bistrica	UMB
	Kosice	IEP SAS
		TUKE
		UPJS
	Zilina	UZ
South Africa	Cape Town	UCT
	Port Elizabeth	NMU
	Stellenbosch	SU
Switzerland	Zurich	ETH
Tajikistan	Dushanbe	PHTI NAST
	Khujand	KSU
United Kingdom	London	Imperial College
	Plymouth	Univ.
USA	Cambridge, MA	MIT
	Davis, CA	UCDavis
	Los Angeles, CA	UCLA
	Louisville, KY	U of L
	San Diego, CA	SDSU
	Upton, NY	BNL
Vietnam	Hanoi	VNU
	Ho Chi Minh City	CNT VINATOM