# Computer Infrastructure and Scientific Computing at JINR Dubna

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The ***computer infrastructure*** and ***scientific computing*** are indelible parts of the modern research in **all natural sciences**.

An overview is provided of these two directions of LIT-JINR research and development. Their main goal is the design and implementation of ***adequate informational suppor***t of the multidisciplinary research environment of JINR and JINR Member States and particularly of the mega-science projects, such as NICA, ELI-NP, etc.

The emphasis on the ***computer infrastructure*** is on its backbone, the ***Multifunctional Information and Computing Complex*** (**MICC**), a **basic JINR facility**, with its main components: CMS Tier-1, CICC/Tier-2 (including NICA off-line and storage system), the cloud infrastructure, the two-stage heterogeneous high performance facility comprising the HybriLIT cluster and the new revolutionary “Govorun” supercomputer.

The large area of the ***scientific computing***, which supports a significant part of the JINR research, ***is illustrated by a few selected topics*** related to the computer simulation of physical installations and processes, the experimental data processing and analysis, the design and implementation of parallel computer codes, computer algebra and quantum computing.

# Outline

- Laboratory of Information Technologies in JINR
- The Multifunctional Information and Computing Complex (MICC) in LIT JINR
- Instances of computer physics challenges
- Miscellanea

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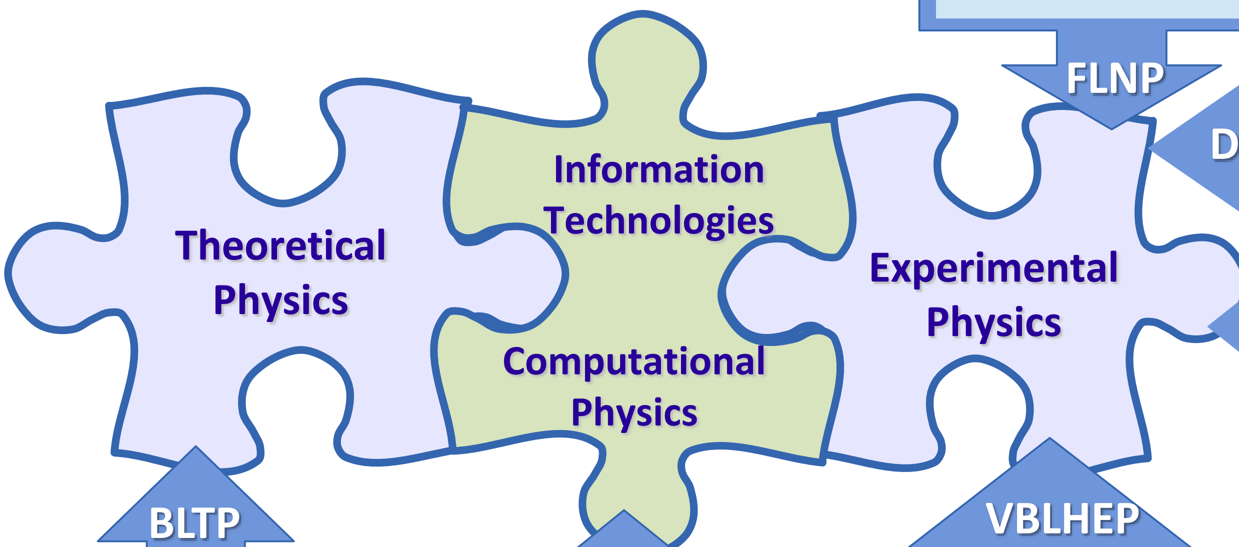
# The Laboratory of Information Technologies (LIT)

- The Joint Institute for Nuclear Research (JINR) has defined the ambitious 2017-2023 *Seven-Year-Plan for JINR development*, with specific tasks assigned to each of its **seven Laboratories**.
- The ***Laboratory of Information Technologies*** (LIT) of the JINR is a *forerunner at the worldwide scale* in two directions:
  - The *design* and *implementation* of a *dedicated computing infrastructure* of the *highest level worldwide* (and, at times, exceeding the performances got in the most advanced similar centers): *the Multifunctional Information and Computing Complex* (MICC)
  - The development of *efficient numerical* or *symbolic-numerical algorithms* and *software* for: the solution of mathematical models, the modeling of experimental installations, the validation of their built-up components, the processing and analysis of experimental data.

# LIT involvement in JINR research: 53 projects of 31 JINR topics of the 2018 Topical Plan of JINR




## FLNP

04-4-1122-2015/2020 [1]
*Leaders: S.A. Kulikov, V.I. Prikhodko*

03-4-1128-2017/2019 [1]
*Leader: V.N. Shvetsov,*
*Deputies: Yu.N. Kopatch, E.V. Lychagin, P.V. Sedyshev*

04-4-1121-2015/2020 [3]
*Leaders: D.P. Kozlenko, V.L. Aksenov , A.M. Balagurov*

## DLNP

02-0-1081-2009/2019 [1]
*Leader: V.A. Bednyakov*
*Deputies: E.V. Khramov, A.P. Cheplakov*

02-2-1099-2010/2018 [1]
*Leaders: D.V. Naumov, A.G. Olshevskiy*

02-2-1125-2015/2017 [2]
*Leader: L.G. Tkatchev, Deputy: V.M. Grebenyuk*

03-2-1101-2010/2017 [2]
*Leader: A.V. Kulikov, Deputy: Z.Tsamalaidze*

02-2-1124-2015/2017 [1]
*Leader: V.V. Glagolev, Scientific leader: J.A. Budagov*

03-2-1102-2010/2018 [2]
*Leaders: G.A. Karamysheva, S.L. Yakovenko, Scientific leader: L.M. Onischenko*

02-2-1123-2015/2019 [1]
*Leader: A.S. Zhemchugov*

02-2-1134-2018/2019 [1]
*Leader: Z. Tsamalaidze*

## FLNR

04-5-1131-2017/2021 [1]
*Leaders: S.N. Dmitriev, P.Yu. Apel*

03-0-1129-2017/2021 [1]
*Leaders: G.G. Gulbekyan, S.N. Dmitriev, M.G. Itkis*
*Scientific leader: Yu.Ts. Oganessian*

03-5-1130-2017/2021 [1]
*Leaders: M.G. Itkis*
*Scientific leader: Yu.Ts. Oganessian*

## BLTP

01-3-1113-2014/2018 [2]
*Leaders: D.I. Kazakov, O.V. Teryaev, A.B. Arbuzov*

01-3-1114-2014/2018 [2]
*Leaders: V.V. Voronov, A.I. Vdovin, N.V. Antonenko*

01-3-1115-2014/2018 [2]
*Leaders: V.A. Osipov, A.M. Povolotskii*

01-3-1116-2014/2018 [1]
*Leaders: A.P. Isaev, A.S. Sorin*
*Deputy: S.O. Krivonos*
*Scientific leader: A.T. Filippov*

01-3-1117-2014/2018 [1]
*Leaders: V.V. Voronov, A.S. Sorin*
*Scientific leader: A.T. Filippov*

## LIT

05-6-1118-2014/2019
Information and Computing Infrastructure of JINR

05-6-1119-2014/2019
Methods, Algorithms and Software for Modeling Physical Systems, Mathematical Processing and Analysis of Experimental Data

## VBLHEP

02-1-1097-2010/2018 [2]
*Leader: A.D. Kovalenko,*
*Deputies: N.M. Piskunov, V.P. Ladygin, M. Finger (Jr.), R.A. Shindin*

02-1-1088-2009/2019 [2]
*Leader: A.S. Vodopyanov*

02-1-1106-2011/2019 [2]
*Leader: A. Malakhov, V. Ivanov*

02-0-1066-2007/2020 [4]
*Leaders: R. Lednicky, Yu.A. Panebratsev*

02-0-1065-2007/2019 [5]
*Leaders: V.D. Kekelidze, A.S. Sorin*
*Deputies A.D. Kovalenko, I.N. Meshkov*

02-0-1085-2009/2019 [1]
*Leader: A.P. Nagaytsev, Scientific leader: I.A. Savin*

02-0-1083-2009/2019 [5]
*Leader: A. Zarubin, Scientific leader: I.A. Golutvin*

02-0-1108-2011/2017 [1]
*Leader: G.D. Alexeev*
*Deputies: A.N. Skachkova, A.S. Vodopyanov*

05-8-1037-2001/2019 [1]
*Leader: N.A. Russakovich*

06-0-1120-2014/2018 [1]
*Leaders: V.A. Matveev , S.Z. Pakuliak*

# Outline

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- **The Multifunctional Information and Computing Complex (MICC) in LIT JINR**
- Instances of computer physics challenges
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# MICC – the main LIT objective in the JINR 7-year plan (2017-2023)

***MICC* is a *basic JINR facility*** creating a ***unified information environment*** which integrates a large variety of tools, concepts, techniques, and software resulting in ***optimal approaches*** to the solution of a great many ***scientific*** and ***applied*** tasks needing the use of ***advanced information and computing techniques.***

**Unified environment Many components**

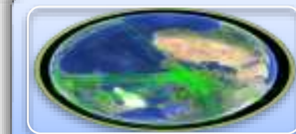
- Grid
- Supercomputer (heterogeneous)
- Cloud
- Local computing cluster
- ….

**Features**

- fault-tolerance
- scalability
- interoperability
- fitting new technical solutions
- operability 12 months a year in 24x7 mode

# MICC – at a glance

**Data Intensive Tasks**



JINR grid sites of WLCG/EGI: **Tier1 for CMS**
**Tier2** for ALICE, ATLAS, CMS, STAR, LHCb, BES, biomed, fermilab, COMPASS


**Cloud infrastructure**

NICA

**Off-line cluster and storage system for BM@N, MPD, SPD.** Storage and computing facilities for local users

**Computing Intensive Tasks**

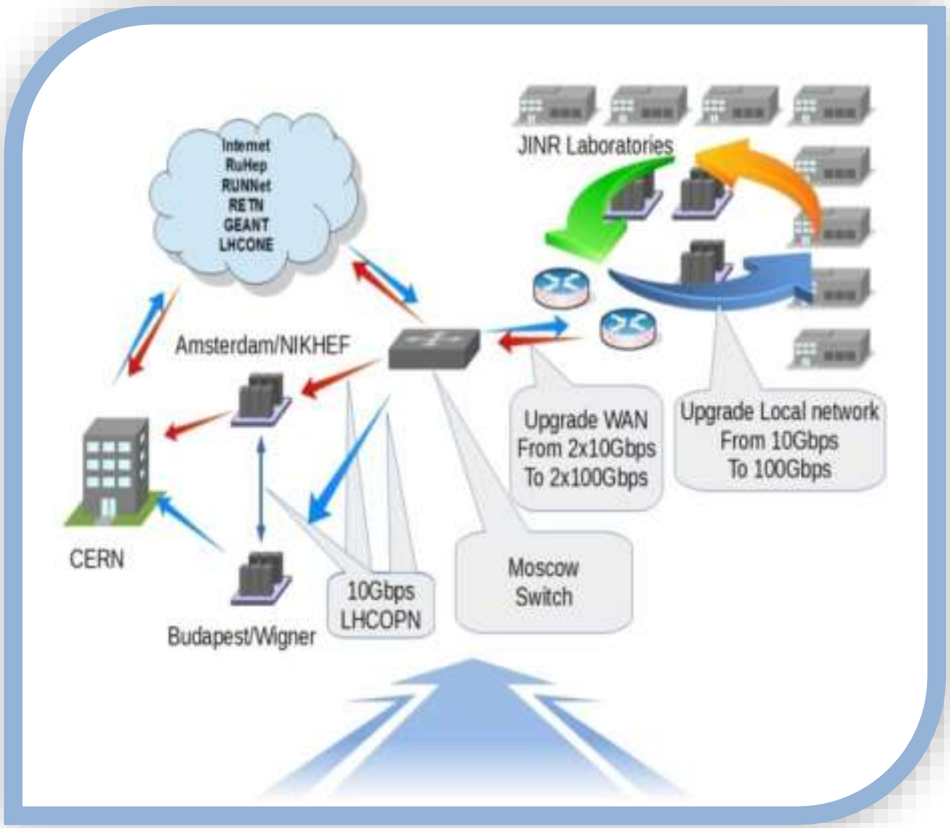
**Heterogeneous (CPU + GPU) computing platform: HybriLIT cluster + GOVORUN supercomputer**

**Communi-cation & Engineering**

**Telecommunication data links and local area network infrastructure**

**Underlying Engineering infrastructure**
(Power&Cooling)

# Network and Telecommunication Channels Essentials

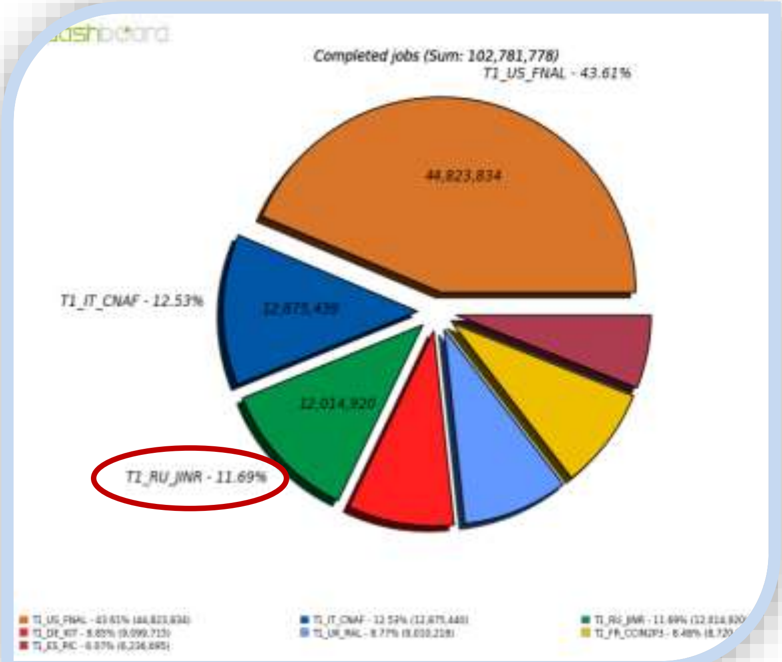


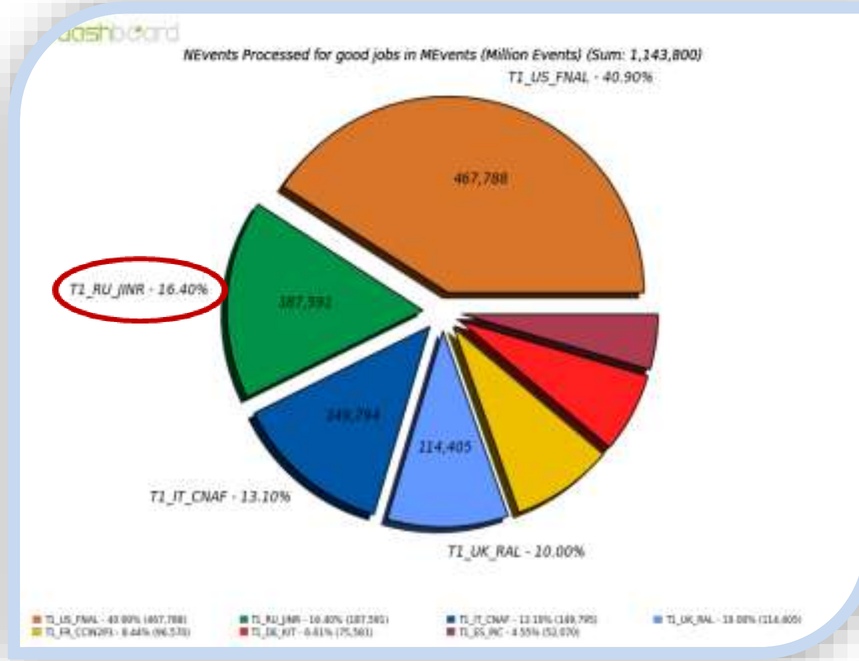

**Provide high throughput data flows in the today physics experiments**

**Local Area Network – 10Gbps,**
**LAN upgrade to 100Gbps underway**

**WorldWide Area Network –**
**100Gbps + 2x10Gbps**
**WAN planned upgrade to 2x100Gbps**

# MICC: CMS Tier1 – 2018 Features




**From 2017-01-01**
**To 2018-09-11**

**Completed jobs – 12 014 920 (11,6% of total CMS jobs)**
**Events processed – 187 592 Mevents (16,4 % of total CMS events)**

**Resources:**

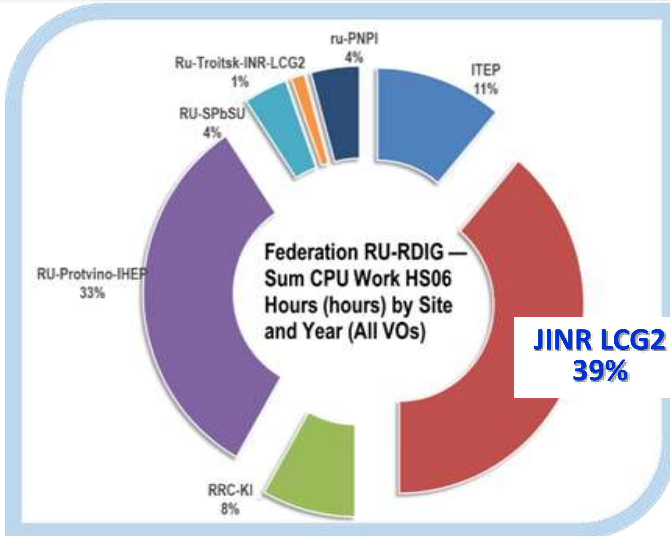
- **Computing power: 4720 cores/slots for batch**
- **Disk storage: 8.3 PB** • **Tape storage: 10.8 PB**
- **Reliability and availability: 100%**

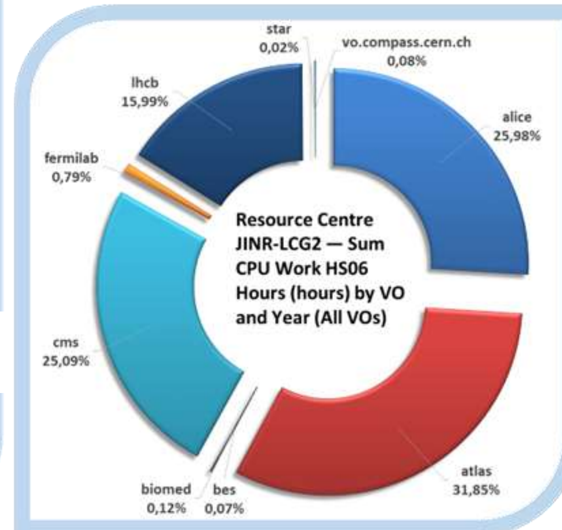
**Tasks:** ***safe-keeping*** of ***raw and reconstructed data***, ***large-scale reprocessing*** **and safe-keeping of corresponding output**, ***distribution of data*** to Tiers 2 and ***safe-keeping*** of a share of ***simulated data*** produced at these Tiers 2

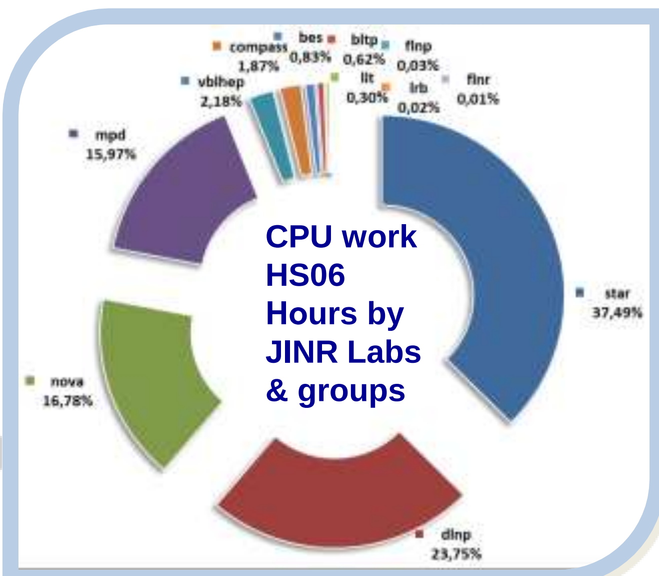
# MICC: Tier2 & CICC – 2017 Computing

## Experiments

BM@N
MPD
CMS
ATLAS
ALICE
LHCb
COMPASS
DIRAC
PANDA
CBM
STAR
NOvA
BESIII
OPERA
NEMO
Mu2e
NUCLON
HONE
FUSION
BIOMED




## Resources

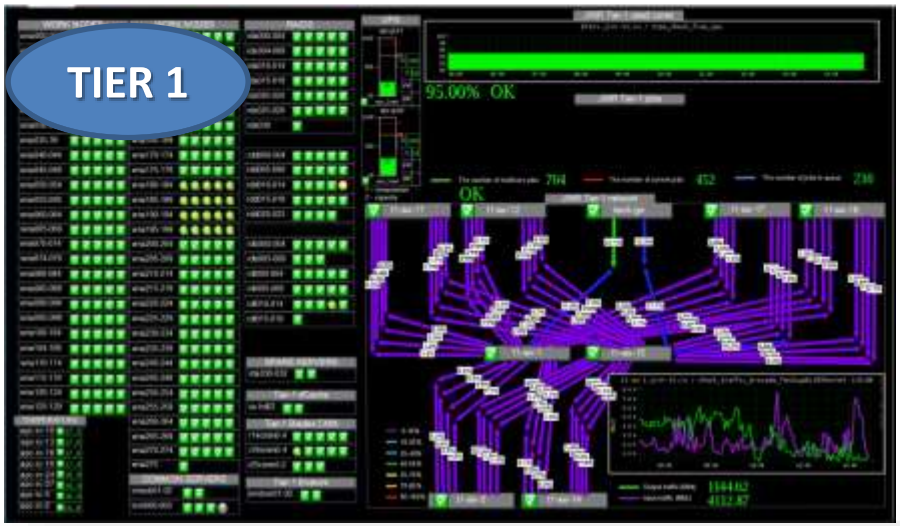
- Computing power: 4128cores/slots for batch
- Disk storage: 3.0 PB

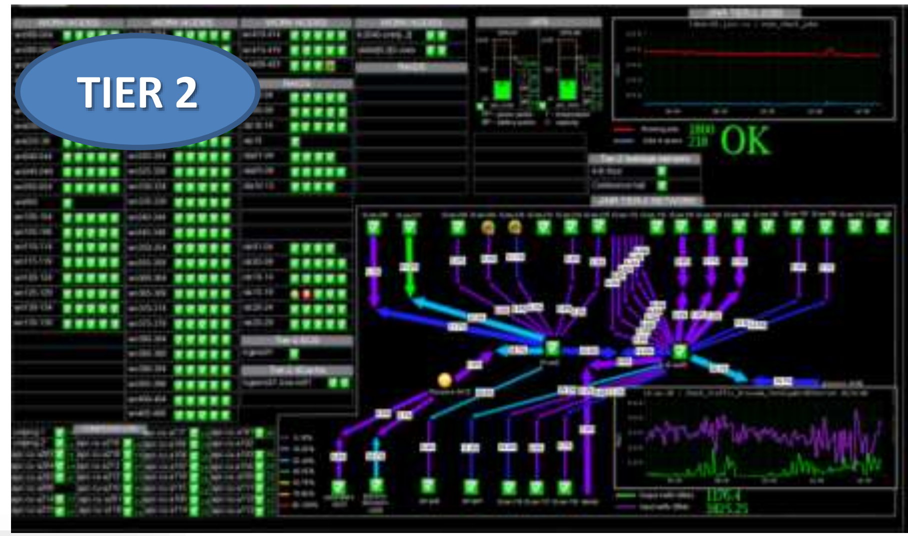
## Tasks

To ***store sufficient data*** and
To provide ***adequate computing power***
for specific analysis tasks

# MICC monitoring

For a robust performance of MICC it is necessary to monitor the state of all nodes and services - from the supply system to the robotized tape library.





Within MICC, ~ 850 elements are under observation
~ 8000 checks in real time
~ 100 scripts

The whole computing complex is kept under control. In case of emergency, alerts are sent to habilitated persons via e-mail, SMS, etc.

# From HybriLIT cluster to GOVORUN supercomputer

**The supercomputer "Govorun" is a joint project of the Bogolubov Laboratory of Theoretical Physics and the Laboratory of Information Technologies under support of JINR Directorate. The project is aimed to radically accelerate large scale theoretical and experimental studies underway at JINR, including the NICA facility**

***HybriLIT* cluster**

**GOVORUN (CPU + GPU)**

**2017**

**Total peak performance:**
**140 Tflops - single precision**
**50 TFlops - double precision**

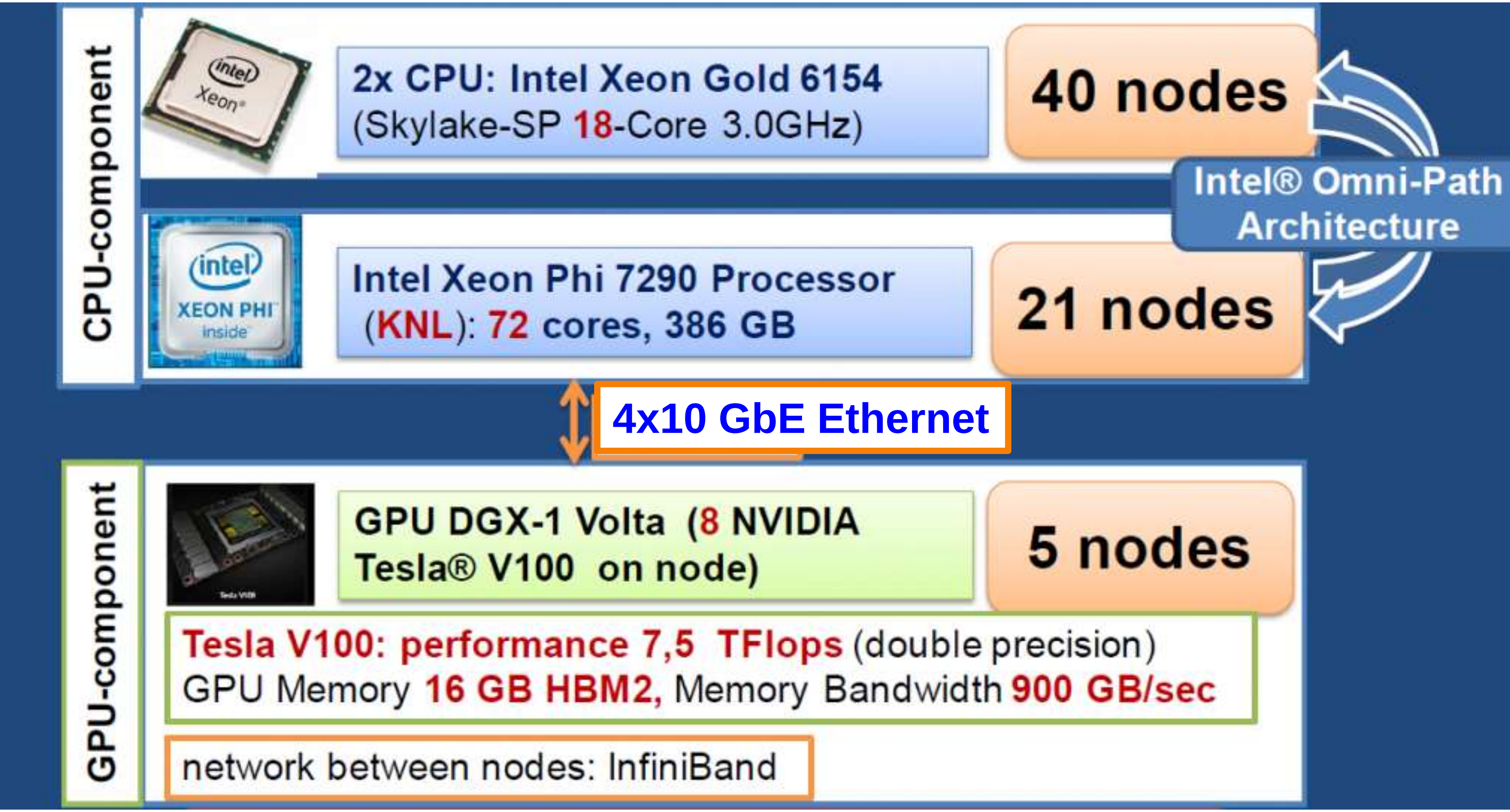
**2018**

**Total peak performance:**
**1000 TFlops - single precision**
**500 TFlops - double precision**

## *Basic features*

- The HybriLIT + GOVORUN are operated through a **unified software and information environment**
- **HybriLIT** serves as an **education and testing cluster**
- **GOVORUN supercomputer** serves to the solution of **large scale problems** which are best suited to its CPU and GPU components.

# Unique Features of Govorun Supercomputer (1)




- **The CPU component**: «RSC Tornado» based on **Intel® Xeon® Scalable** and **Intel® Xeon Phi™**
- **The GPU component**: uses the latest generation computing servers with **NVIDIA Volta** graphics accelerators. Each **NVIDIA Volta** combines both **CUDA cores** (5120) and the latest **Tensor Cores** (640) plus 16GB of RAM and is specifically designed for deep learning.

# Unique Features of Govorun Supercomputer (2)

- The **CPU-component** is a unique multipurpose heterogeneous, high performance, ***hyper-converged*** (Intel® Omni-Path interconnect) system with energy effective **direct hot water cooling**.
  - •• Its Power **Usage Effectiveness (PUE) =** 1.0277

    PUE = (Total Facility Energy)/IT Equipment Energy.

As a result up to **6% of total power will be spent to cooling subsystem**. The system may be **easily scaled** up to hundreds of PFLOPS and PBYTES in 50sq.m.

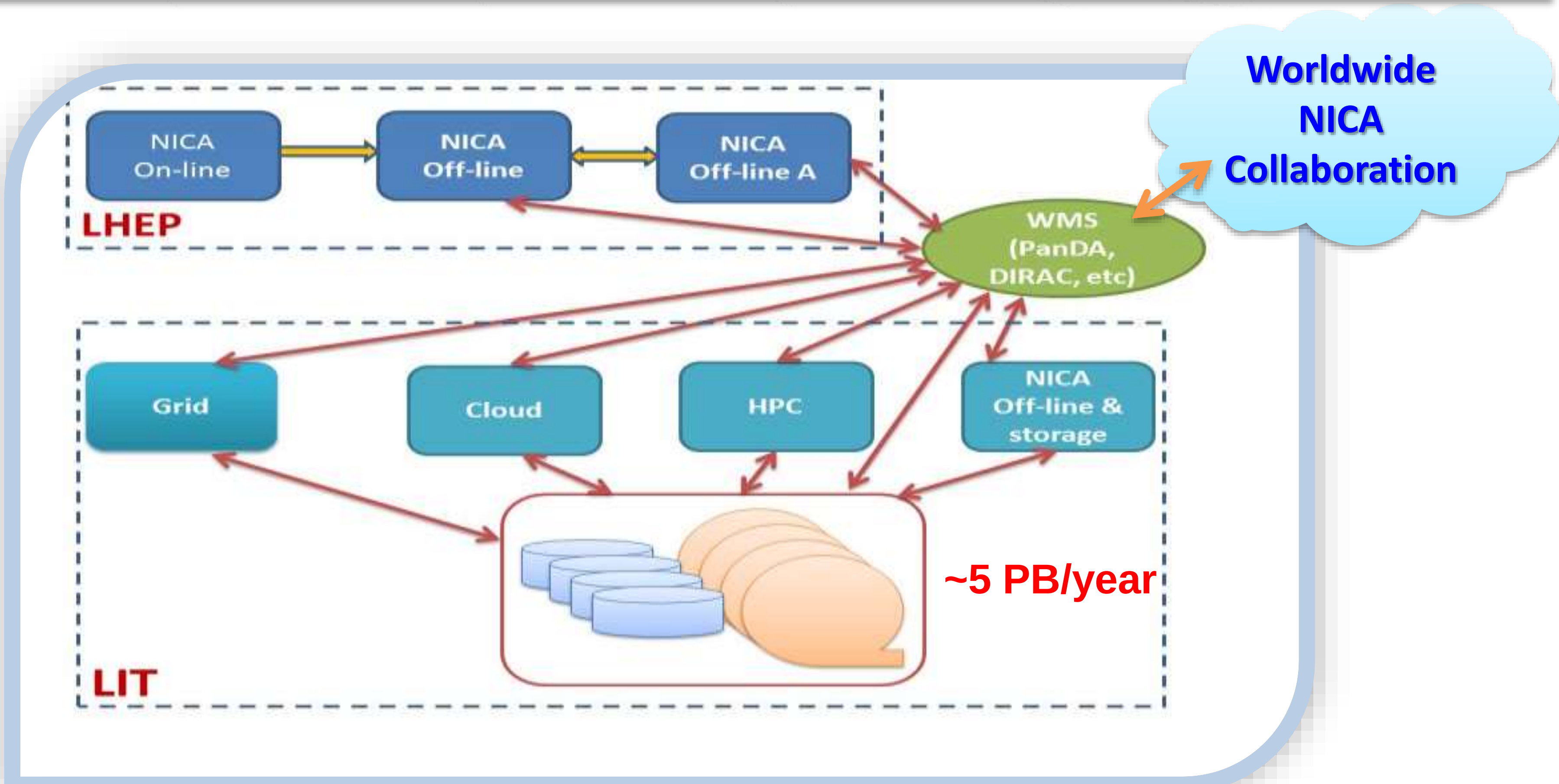
- •• Fast interconnect support up to **200 Gbit/s per node**

  ⇛ Intel® Omni-Path, IB EDR;   Ethernet 1/10/25/40Gb
- •• Datacenter Management Platform

- The **GPU-component DGX-1** uses the **NVLink bus for communication between the host system and Tesla cards**, which is 5 to 12 times faster than PCI-E.

The combination of CUDA and Tensor cores is **specifically designed for deep learning**. The NVIDIA-dockers for DGX-1 provide Machine Learning frameworks optimized by NVIDIA through **HPC Apps Containerized**.

# Computing Infrastructure for MPD-BM&N/NICA




**Integration** of various resources from NICA VBLHEP and MICC LIT for the development of computer infrastructure of NICA project

**Requirements:** reliability, scalability, interoperability, adaptability to new technical solutions, year-round operation in 24x7 mode

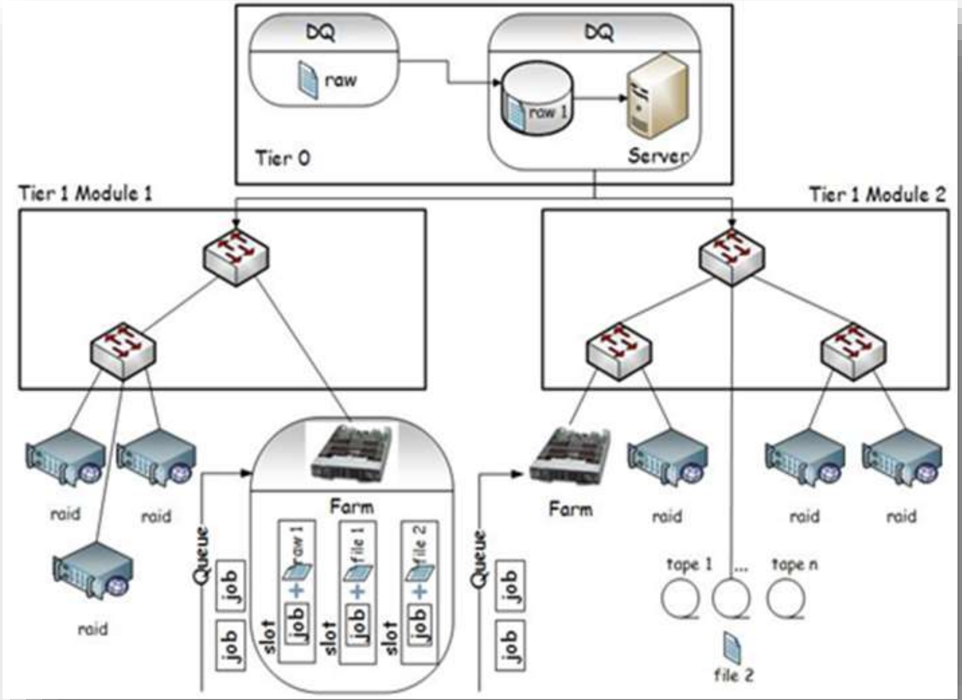
# SyMSim: LIT developed simulation of NICA computing facilities

**SyMSim** (**Sy**nthesis of **M**onitoring and **Sim**ulation) simulates grid-cloud structures by **combining a simulation program with a real monitoring system** of the grid/cloud service in frame of the same program. ***Three main parts***:

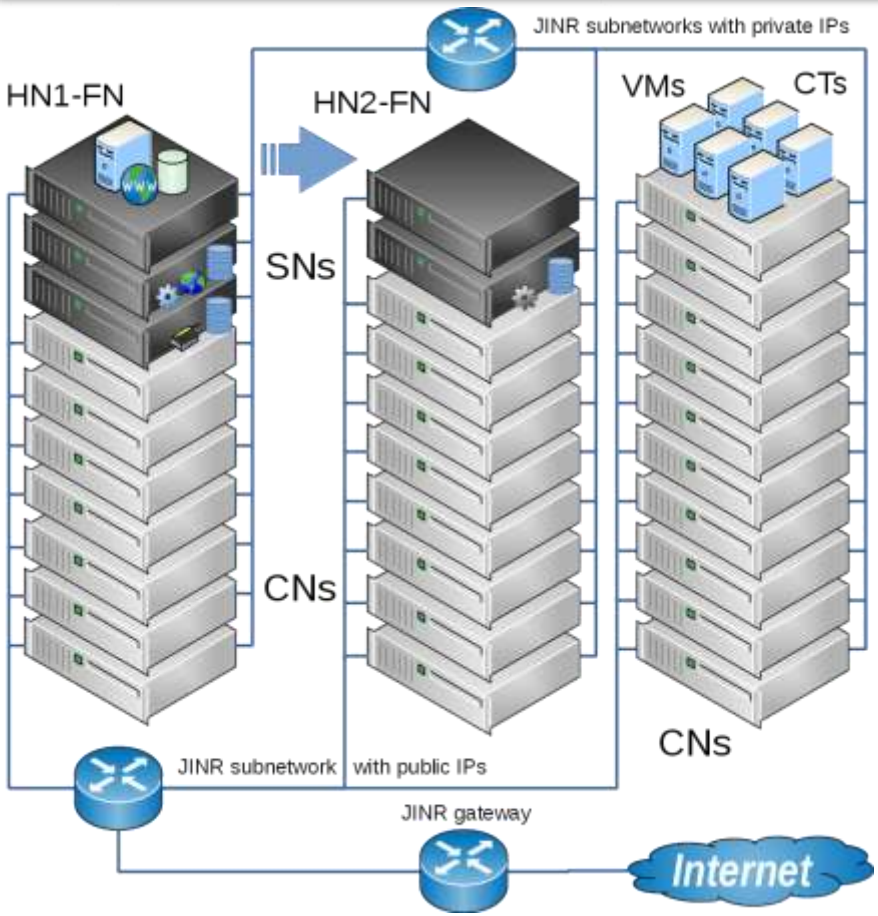
1. ***Data model*** – describes data generation processes, their volumes, storage conditions
2. ***Data processing model*** – rules for the use of resources such as CPU, memory and I/O between concurrently running tasks
3. ***Data traffic communication model***: different protocols in local & global networks

**SyMSim answers**: 1. optimization of architecture and equipment.
2. definition of main parameters and structures of data processing system.

**SyMSim provided outputs for**: (i) infrastructure modeling and optimization of the CMS JINR Tier1 center; (ii) NICA project predictions on future computing system infrastructure; (iii) choosing a proper architecture of the BM@N computing system infrastructure.



# MICC: Cloud Infrastructure




## Purpose

- Increase the efficiency of hardware and proprietary software utilization
- Improve IT-services management

## Implementation

- Cloud Platform: **OpenNebula (v4.12)**
  - core, scheduler, MySQL DB
  - Interfaces (web-GUI, CLI, API)
  - OneGate, OneFlow
  - ***Cloud bursting model***
- **High availability&reliability**

## Cloud – resources

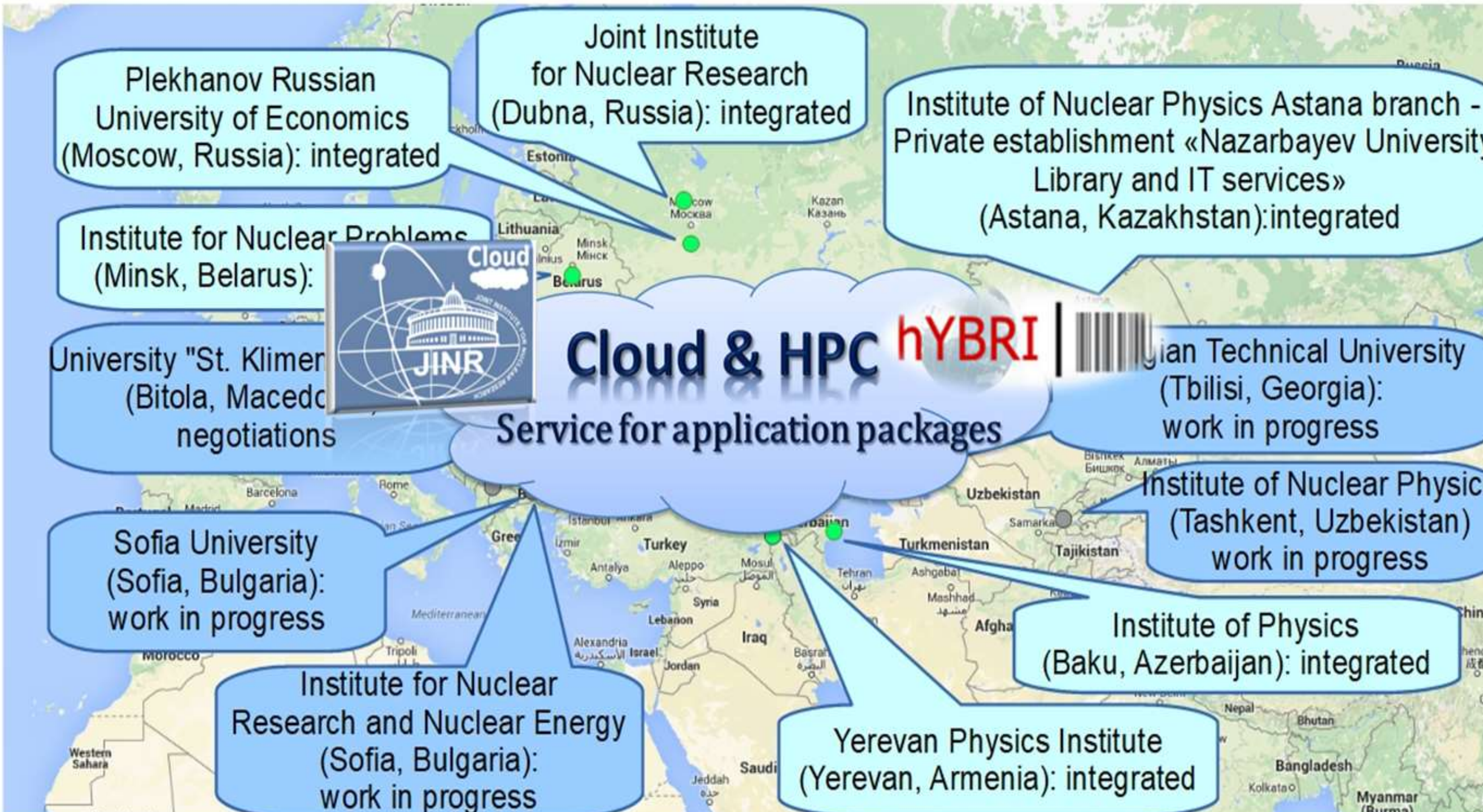
- **Computing power: 1100 cores**
- **RAM: 5.7 TB**
- **Disk storage: 896 TB**
- **220 VMs and CTs, 120 users**

## Utilization

- VMs&CTs for JINR users
- **Computational resources** for Baikal-GVD, BESIII, Daya Bay, JUNO, NOvA experiments
- Testbeds for development and R&D in IT

# JINR Cloud + HPC

**New challenge – integration of JINR Member States clouds and the Supercomputer into a unified distributed computational infrastructure**



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# Reliance on new mathematics

- **Hardware availability does not guarantee success**.

**Tough scientific problems** cannot be simply solved by the access to the most powerful computing facilities.

- **New approaches to solution** are as a rule needed to secure:

— **inheritance** of the **genuine algebraic properties of the model under discretization**;

— **reduction of the computational complexity**;

— **avoidance of artefacts** coming from the **finite precision** of the floating point representation of the machine numbers, which may result in **modifications of fundamental** well established features over the field of the real numbers.

# CHALLENGES: distributed data storage evolution: DATALAKES

**GOAL:**

- to provide a unified computing infrastructure to the experiments, the data storage and analysis
- to achieve storage consolidation where geographically distributed storage centers (potentially deploying different storage technologies) are operated and accessed as a single entity.

**EOS** - a CERN open-source storage software solution to manage multi PB storage.

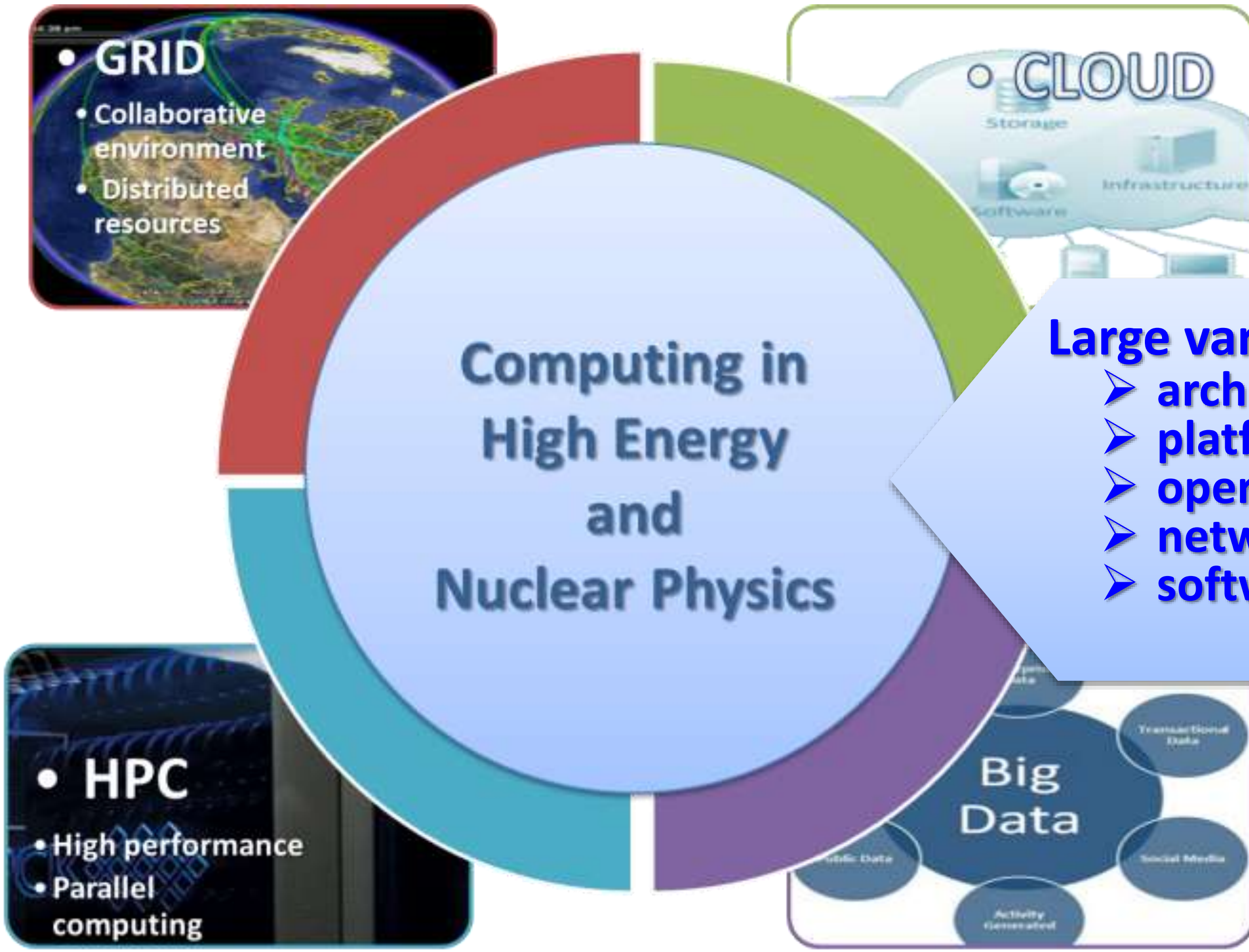
**XRootD** - core of implementation framework providing a feature-rich remote access protocol.

EOS

Allow improvement of already existing production quality through Data Management Services.

**Scalable technologies for federating storage resources and managing data in highly distributed computing environments.**

# Computing in High Energy and Nuclear Physics




**Large variety of**

- architectures
- platforms
- operational systems
- network protocols
- software products

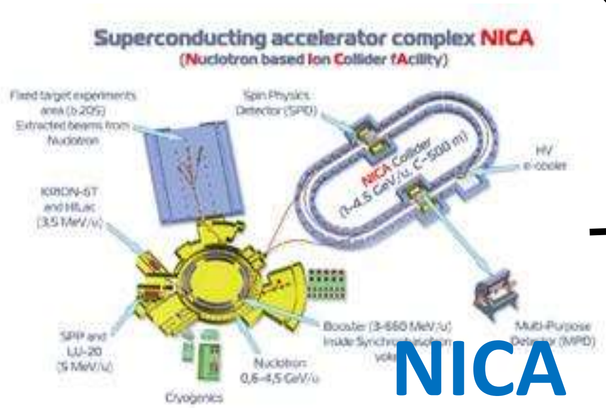
**The environment interface is to provide the organization of collective development, solution of problems of various complexity and subject matter, management and processing of data of various volumes and structures, training and organization of scientific and research processes**

# HEP Big science projects



FAIR

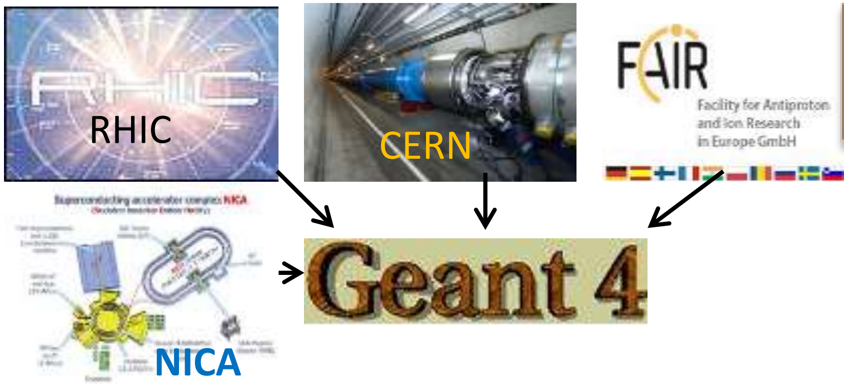
Facility for Antiproton and Ion Research in Europe GmbH




Geant 4

+

## Project driven software developments

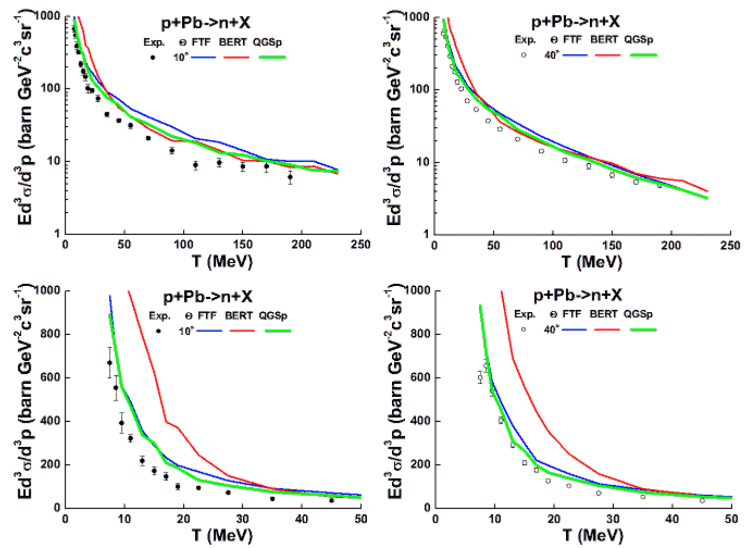



# Improvement of QGSp in Geant4

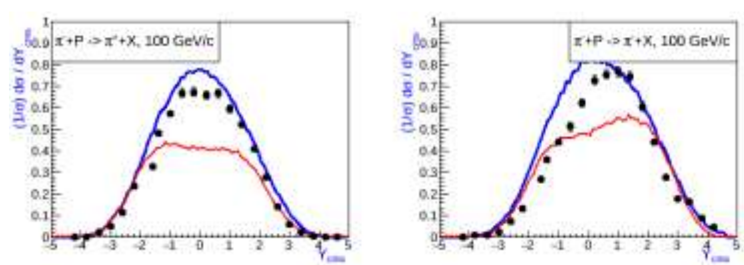
**Now FTFP_BERT Physics List is a favorite Physics List of Geant4**
**Physics List – QGSp_BERT used by ATLAS and CMS**

**Geant4** – toolkit for simulating particle passage through matter.
**Areas of application**: high energy, nuclear and accelerator physics, medical and space science.
**Main task –** Simulation of hadronic interactions and electromagnetic showers.
**Main yield of LIT**: Development of Fritiof (FTF) hadronic model; Simulation of interactions: (1) **π, K, p, n, Λ, Nucleus+Nucleus** (2) **Anti-proton, Anti-Nucleus+Nucleus**
**Specific tasks solved**: • Improvement of string fragmentation; • Improvements of processes cross sections; • Inclusion of the Reggeon cascading for correct description of nucleus breakups; • Improvement of parton momenta sampling
**Future tasks: •• Contribution to code parallelization within Geant 4 modules**

The [present status of Geant4] was defined with the important co-authorships of A. Galoyan (VBLHEP) and V.V. Uzhinsky (LIT). See, Nuclear Instruments and Methods, A835 (2016) 186–225, DOI: 10.1016/j.nima.2016.06.125




**Slow neutron production, ITEP experimental data (1983)**
[Shower shape improvement]




**πP interactions at 100 GeV/c**
**Red lines – old QGSp Blue lines – new QGSp**

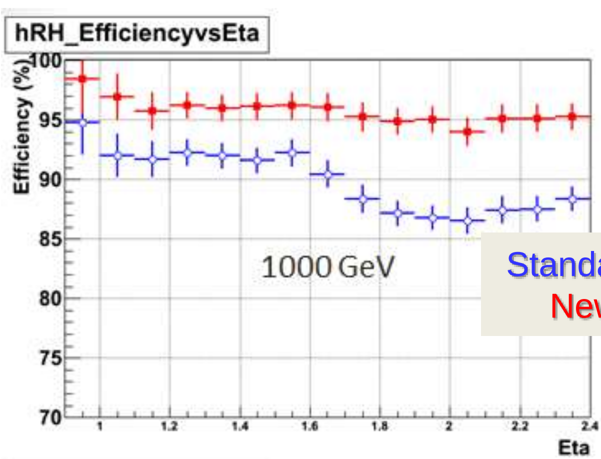
[Author of original code – N.S. Amelin (LIT, JINR)] **Developer – V.V. Uzhinsky (LIT, JINR)**

# New segment building algorithm for the Cathode Strip Chamber (CSC) of the CMS facility

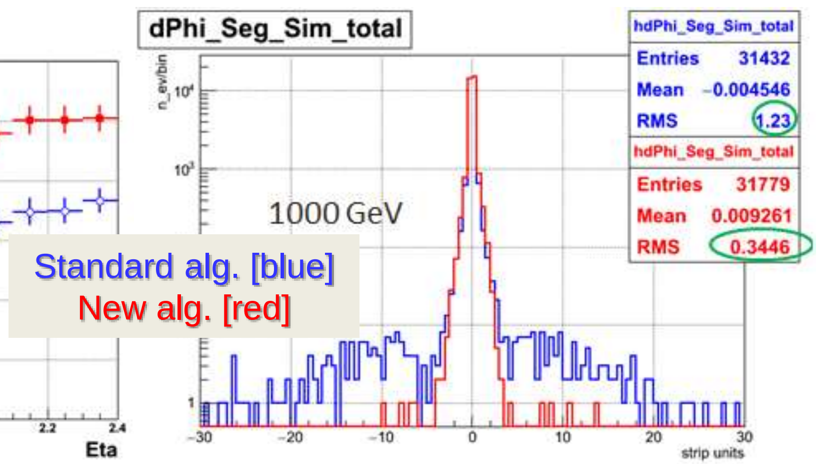
**Purpose**: to improve the reconstruction for high hit rate and big backgrounds due to luminosity increase

The **new algorithm** was implemented in the **official CMS software package in July, 2016, extensive testing period until end of January 2017**. It proved to be ***effective, stable and robust***.

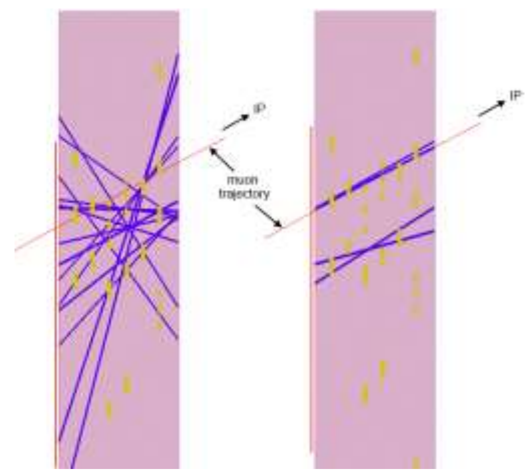
**Future**: **Further reconstruction procedure refinements**, **its use as** reconstruction algorithm **for the new GEM detectors** that will be included in the experimental setup for the next major upgrade.




Reconstruction efficiency vs. pseudorapidity (new alg. efficiency is **high** and **almost constant**, standard alg. eff. decreases with the increase of the pseudorapidity)



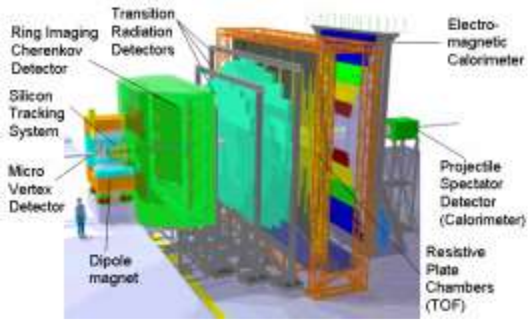

Distance in strip units between the reconstructed and the simulated segment (**3.5 times signal improvement**)

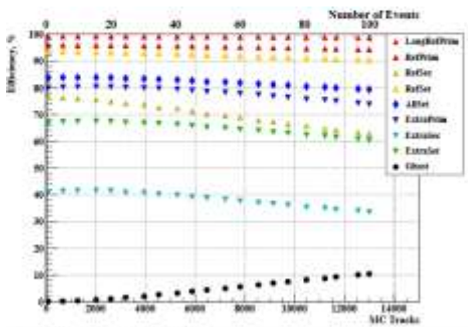


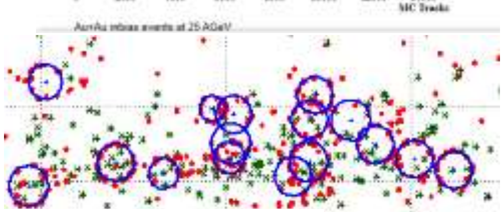

Example of a high hit multiplicity event reconstruction (standard alg. – left, new alg. – right) [# of fake segments: is considerably reduced]

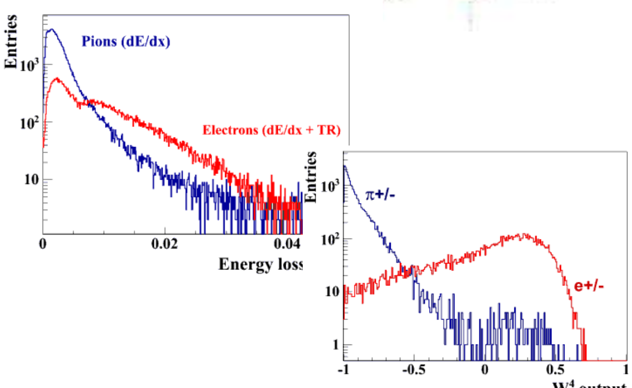

I. Golutvin, V. Karjavin, V. Palichik, N. Voytishin and A. Zarubin, EPJ WoC, vol. 108, 02023, 2016
DOI: http://dx.doi.org/10.1051/epjconf/201610802023

# CBM@GSI – Methods, Algorithms & Software for Fast Event Reconstruction



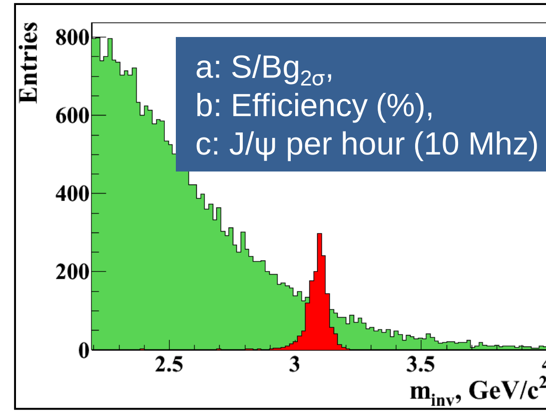






**Tasks under investigation:**

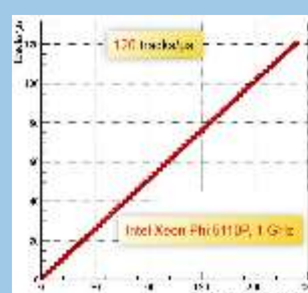
- global track reconstruction;
- event reconstruction in RICH;
- electron identification in TRD;
- clustering in MVD, STS and MUCH;
- participation in FLES (First Level Event Selection);
- development of the Concept of CBM Databases;
- magnetic field calculations;
- beam time data analysis of the RICH and TRD prototypes;
- contribution to the CBMROOT development;
- D0-, vector mesons, $J/\psi \rightarrow e^+e^-$ and $J/\psi \rightarrow \mu^+\mu^-$ reconstruction;




| | a | b | c |
|---|---|---|---|
| pC@30GeV | 14 | 22 | 11 |
| pAu@30GeV | 18 | 22 | 27 |
| AuAu@10AGeV | 0.18 | 18 | 64 |
| AuAu@25AGeV | 7.5 | 13.5 | 5250 |

**Modern parallelization involves multiplicative effects coming from:**

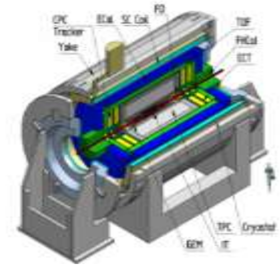
1) Vectorization (SIMD - Single Instruction Multiple Data) factor 2 to 4;
2) Multithreading – factor 4/3 ; 3) υ -Many core processor – factor υ. Total ≈ 4 υ



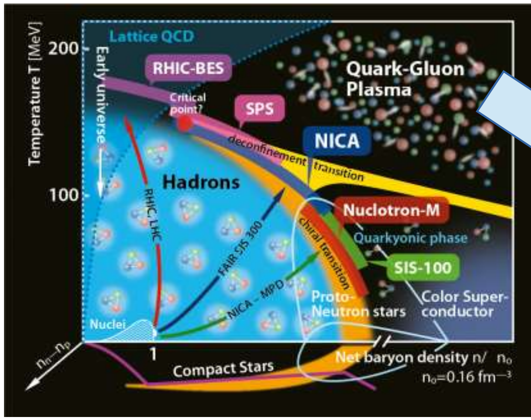

| STS: CA | STS: Kalman Filter | RICH: ring reconstruct. | TRD: track reconstruct. | TRD: el. id. ω(k,n) criterion | KFPar - ticle |
|---|---|---|---|---|---|
| 164.5 | 0.5 | 49.0 | 1390 | 0.5 | 2.5 |

Average time per core (μs/track or μs/ring) of SIMD-algorithms (besides track reconstruction in the TRD) for data processing. Global throughput increases linearly with the number of cores.

# NICA computing challenges asking for HPC

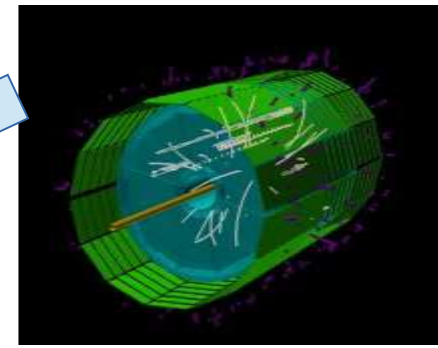


MPD experiment

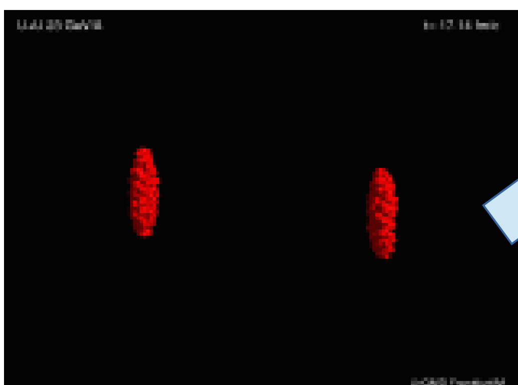



QCD phase diagram

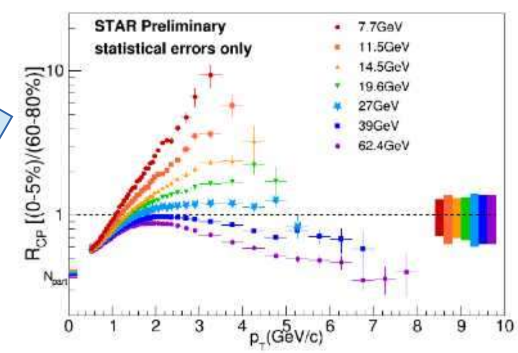
GOVORUN



Events reconstruction



Simulations




Physics analysis

# Hot theoretical physics topics for HPC

## THEORY OF HADRONIC MATTER UNDER EXTREME CONDITIONS

## Wide international cooperation on parallel and sequential computing at LIT for HMEC-TH

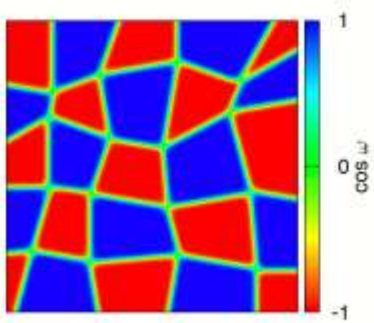
IMP CAS (Lanzhou, China),
Helsinki Univ. (Helsinki, Finland),
ITP Univ. Graz (Graz, Austria),
ITP Heidelberg Univ. (Germany), Jena Univ. (Jena, Germany),
ITP Giessen Univ. (Giessen, Germany), Technische Univ. Dresden (Dresden, Germany),
ITP Goethe-Univ. (Frankfurt, Germany), GSI (Darmstadt, Germany),
ITP Leipzig Univ. (Leipzig, Germany), ZOQ Hamburg Univ. (Hamburg, Germany),
Tokyo Institute of Technology (Tokyo, Japan), RCNP Osaka Univ. (Osaka, Japan),
RIKEN (Wako, Japan),
IOP Bhubaneswar (Bhubaneswar, India),
INFN Frascati (Rome, Italy), INFN ( Pisa, Italy),
Univ. of Wroclaw (Wroclaw, Poland),
FEFU (Vladivostok, Russia),
NRC Kurchatov Institute (Moscow, Russia), ITEP NRC KI (Moscow, Russia),
IHEP NRC KI (Protvino, Russia), MEPhI (Moscow, Russia),
IDSTU SB RAS (Irkutsk, Russia), Saratov Univ. (Saratov, Russia),
SINP MSU (Moscow, Russia), St. Petersburg Univ. (St. Petersburg, Russia),
P.J. Safarik University (Kosice, Slovakia), Matej Bel Univ. (Banska Bystrica, Slovakia),
Valencia Univ. IFIC (Valencia, Spain),
BITP (Kiev, Ukraine)

# Hot theoretical physics topics for HPC

## THEORY OF HADRONIC MATTER UNDER EXTREME CONDITIONS

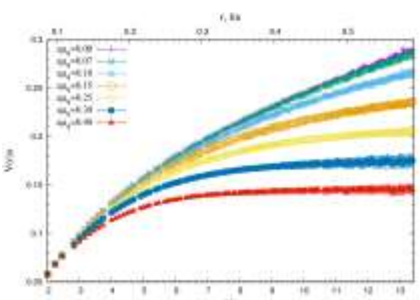
and other relativistic heavy-ion physics topics

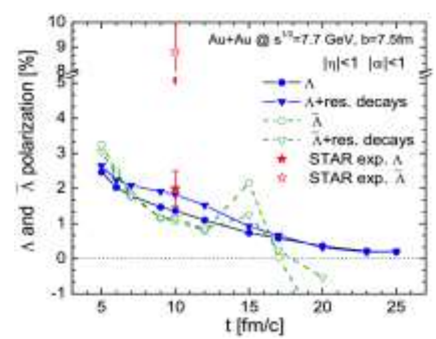
Parallel computing for Lattice QCD, functional RG,
statistical and hydrodynamical models of HIC,
sophisticated models of QCD vacuum



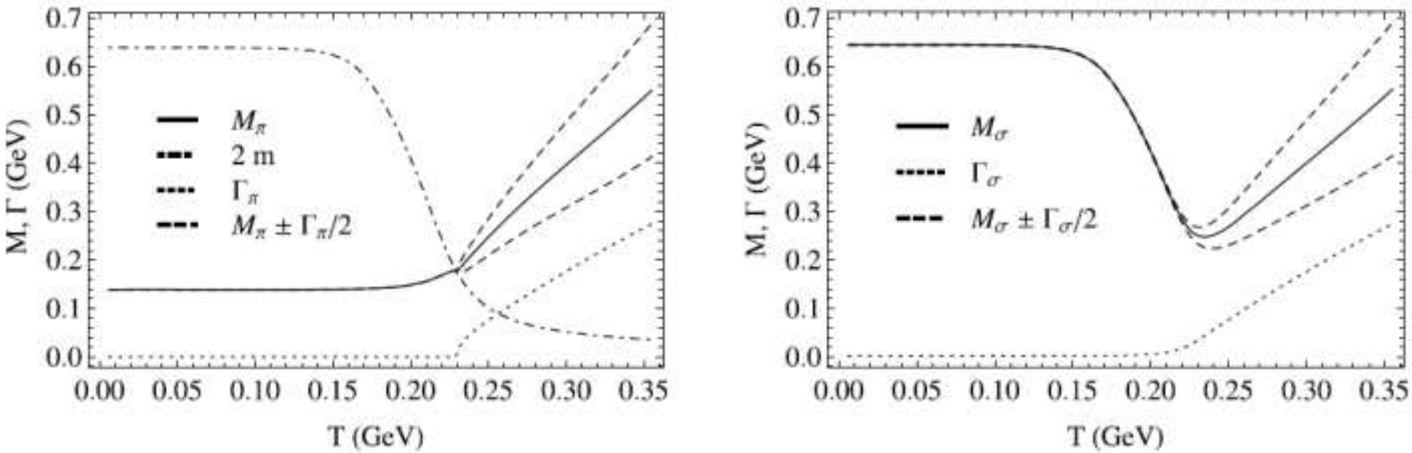

Critical phenomena in hot dense hadronic matter
in the presence of strong electromagnetic fields,
deconfinement and chiral symmetry restoration:

QCD Phase diagram
Thermodynamics of $N_f$=2+1+1 QCD
Real-time spectral properties of thermal QCD
Transport properties of hadronic matter
Properties of cold dense SU(2) QCD through lattice calculations
Anderson transition in the $N_f$=2+1+1 QCD
Z(N) symmetry & meta-stable states



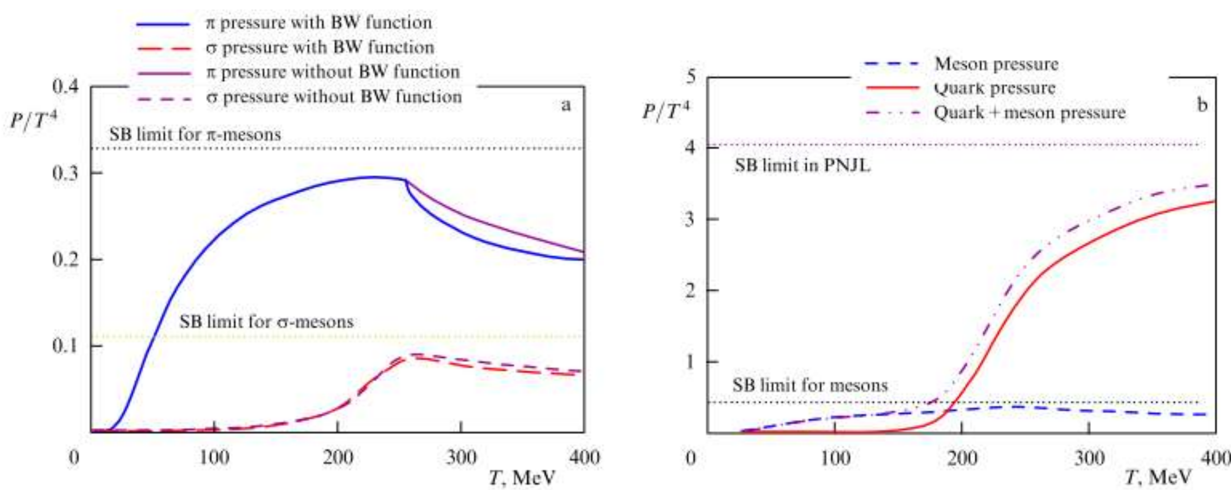


# **Modeling and prediction of meson properties at finite temperature and density** (PNJL: Polyakov-Nambu-Jona-Lasinio model)




Calculations within the two-flavor Polyakov-loop-extended Nambu–Jona-Lasinio model: Meson masses $M_{\pi/\sigma} \pm \Gamma_{\pi/\sigma}/2$, the double quark mass and meson width $\Gamma_{\pi/\sigma}$

A.V. Friesen, Yu.L. Kalinovsky, V.D. Toneev, Nuclear Physics A 923 (2014) 1–18

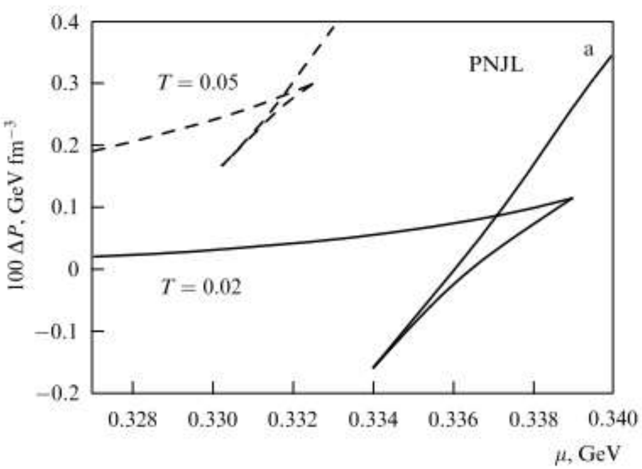


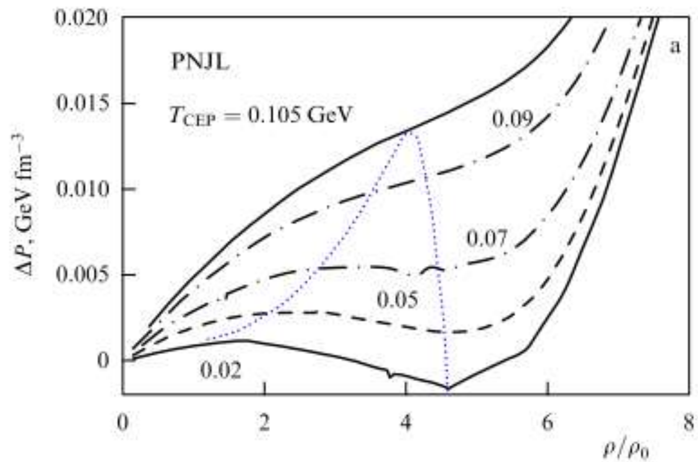

Effect of **meson correlations** on the hadron matter equation of state. Mesons bring noticeable contribution to the system pressure in the **mixed phase**. The spectral broadening and scattering **modify** the meson contribution to the system pressure.

Yu.L. Kalinovsky, V.D. Toneev, A.V. Friesen, Phys.Usp. 59 (2016) no.4, 367-382, Usp.Fiz.Nauk 186 (2016) no.4, 387-403

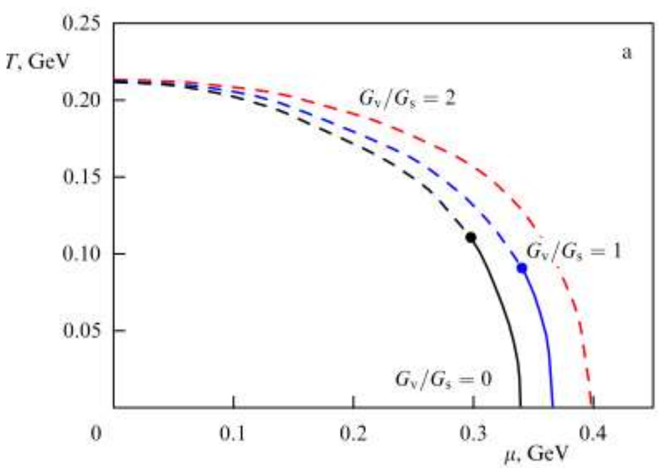
# QCD equation of state and phase diagram

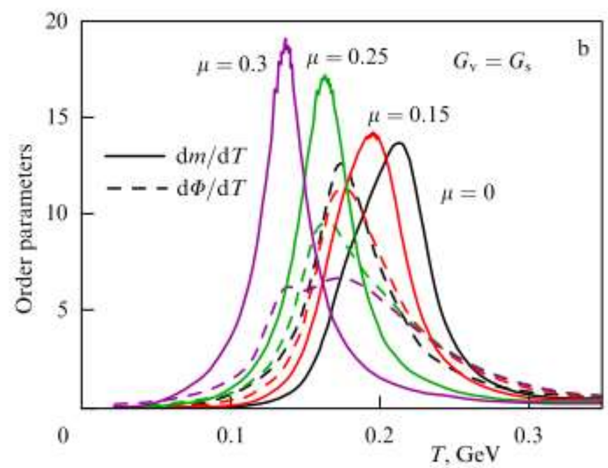
(PNJL: Polyakov-Nambu-Jona-Lasinio model)




**Left**: Pressure vs. chemical potential at different T. Mixed phase corresponds to straight lines.
**Right**: Pressure variation in terms of quark density.
1-st order phase transition corresponds to sign change from + to – of the variations (dotted spinodal boundary).




**Left**: Phase diagram of PNJL model: dependence of 1-st order phase transition point under addition of a vector interaction.
**Right**: Order parameters of PNJL model under $G_v = G_s$.
Solid lines correspond to chiral phase transition.
Interrupted lines define the order parameter of the confinement-deconefinement phase transition.

Yu.L. Kalinovsky, V.D. Toneev, A.V. Friesen, Phys.Usp. 59 (2016) no.4, 367-382, Usp.Fiz.Nauk 186 (2016) no.4, 387-403

# Symbolic-numeric simulation of slender structures (rods, fibers, cilia, flagella, etc.)

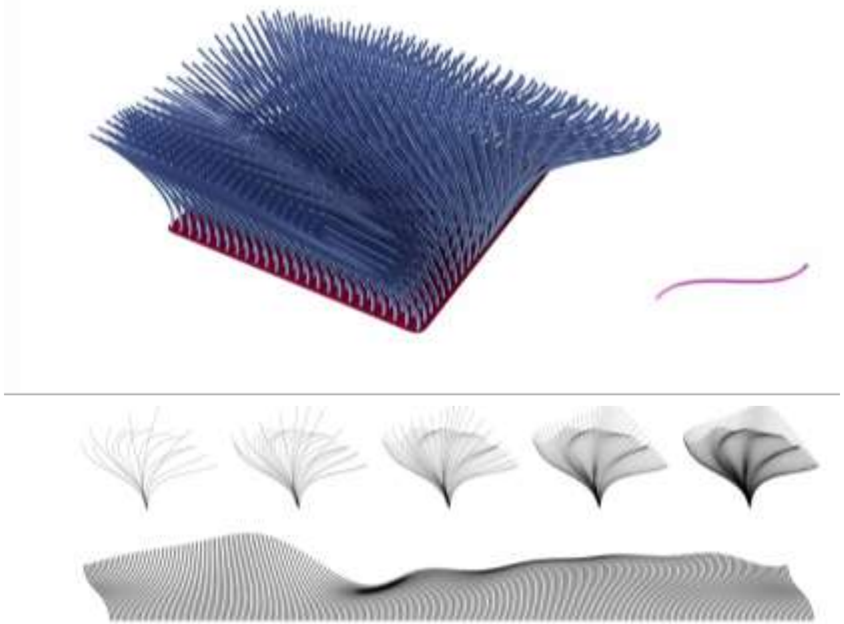
**Governing system of 12 nonlinear very stiff partial differential-algebraic equations:**

$$\rho A \partial_t \vec{v} = \partial_s \vec{n} + \vec{f}, \quad \rho I \partial_t \vec{\omega} = \partial_s \vec{m} + \mathrm{adiag}(1,-1)\,\vec{n} + \vec{l}, \quad \partial_t \vec{\kappa} = \partial_s \vec{\omega}, \quad \partial_s \vec{v} = \mathrm{adiag}(1,-1)\,\vec{\omega}, \quad \vec{\omega}\ \mathrm{adiag}(1,-1)\,\vec{\kappa}^T = 0, \quad \vec{v}\ \mathrm{adiag}(1,-1)\,\vec{\kappa}^T = 0$$

**To obviate stiffness, the solution derived by the authors from LIT JINR and HMTI-BAS (Minsk) combined computer algebra and numerical methods: analytical solution of the parameter-free part of the system and numerical for the remaining**

**Demonstration: simulation of the beating pattern of a cilium (of interest in the context of simulations in biology and biophysics, e.g., cilia carpets in the interior of the lung are responsible for the mucus transport).**

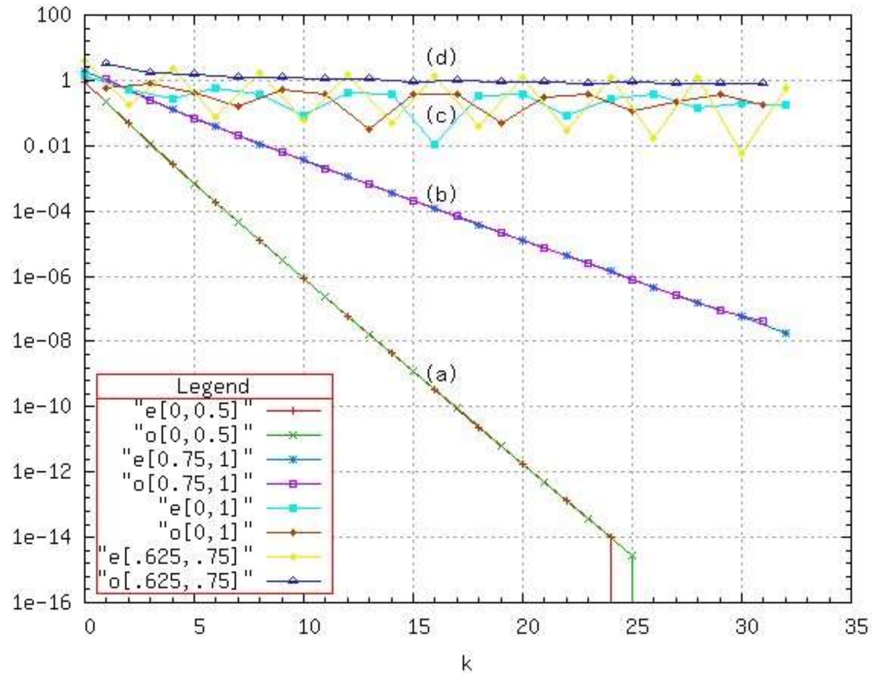
**As compared to a pure numerical solution, the step size can be increased by three orders of magnitude, which leads to two orders of magnitude decrease of CPU time.**

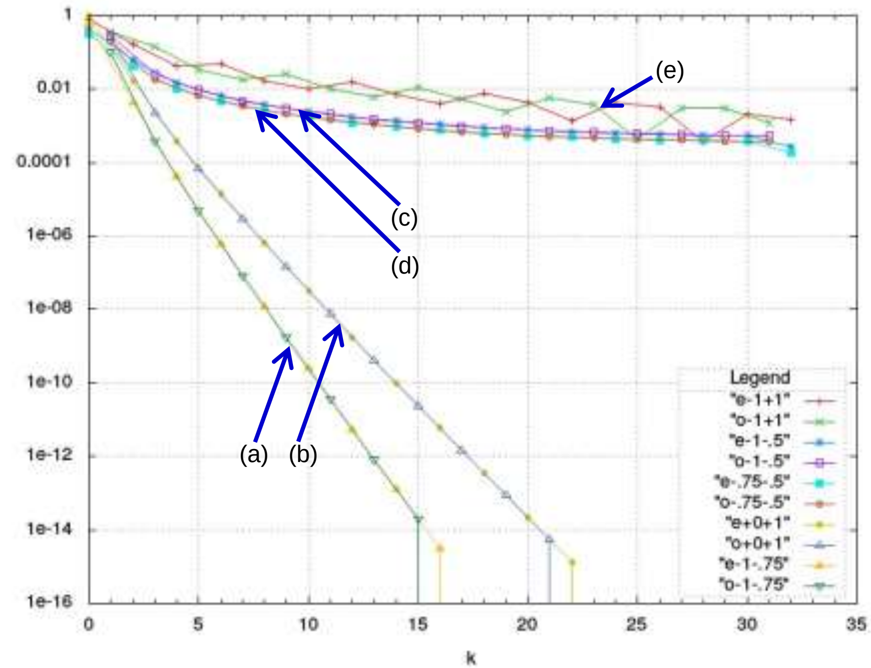


Simulation of a cilia carpet (top) composed of multiple cilia beating in a meta-chronal rhythm (middle) produces the appearance of a wave.

D.Michels (Stanford U), D.Lyakhov (HMTI, Minsk), V.Gerdt (LIT), G.Sobottka, A.Weber (Univ. Bonn), LNCS 9301, 2015, pp.320–331

# Bayesian Inference from Chebyshev Expansion Coefficients




## Singular integrand

(a) far outer singularity: ***fast convergence***

(b) nearby outer singularity: ***moderate convergence***

(c) – (d) inner singularity, various range lengths: – ***irregular behavior***

## Singular derivative

(a) – (b) Outer singularity: ***fast convergence***

Endpoint singularity – ***monotonic behavior***:
(c) larger intervals – smaller range of variation,
(d) smaller intervals – larger range of variation

(e) Inner singularity – ***irregular behavior***

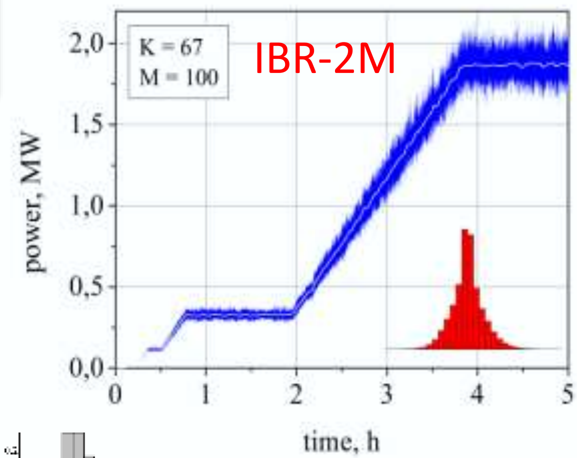
Gh. Adam, S. Adam, Disentangling complexity in Bayesian automatic adaptive quadrature, MMCP 2017 Conference, LIT-JINR, July 3-7, 2017, EPJ-WoC Vol.173, paper 01001, p1-p8 (2018)

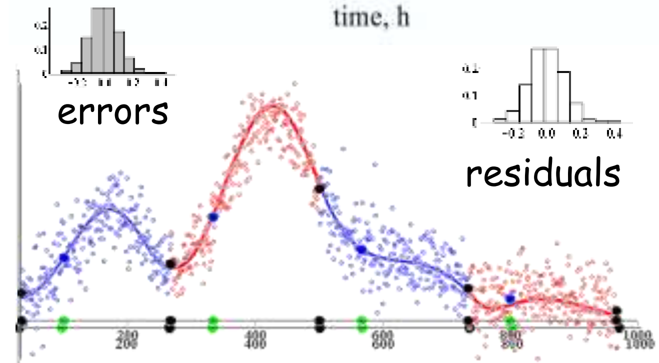
# **Basic Element Method** (BEM) **Applications**

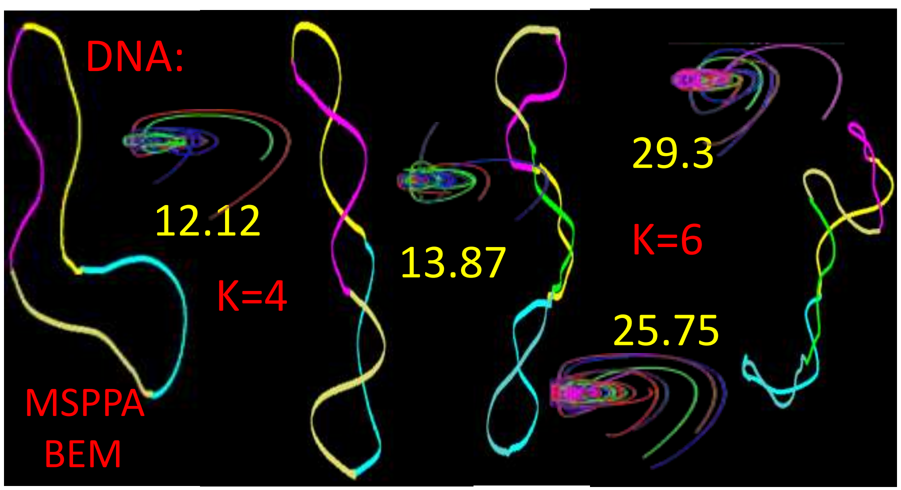
**A new approach to the BEM-polynomial basis definition has been developed [1], [2].**

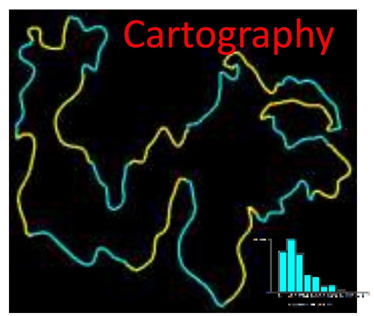
**The BEM polynomials allow the optimization of the piecewise polynomial approximation and smoothing of the 2D curves [3].**

**BEM may be used for solving IT problems such as contour analysis, digital processing of signals and images, pattern recognition, etc. :**

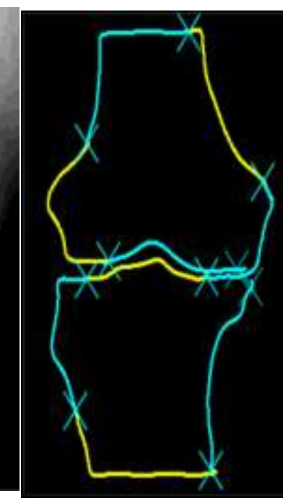




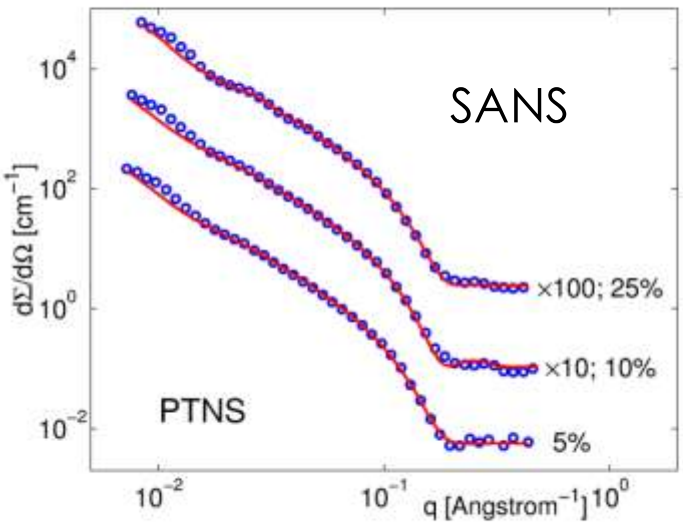


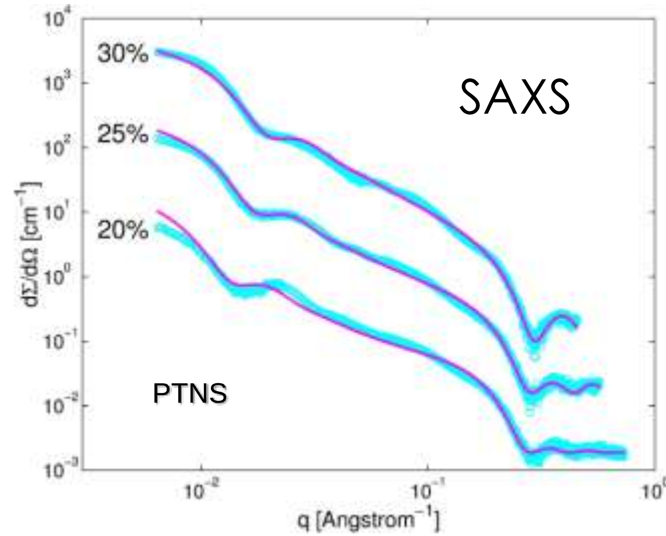

[1] Dikusar N.D. *ISSN 2070_0482,* **MMCS**, 2011, Vol. **3**, No**. 4**, pp. 492–507.
© *Pleiades Publishing, Ltd., 2011. – Springer*

[2] Dikusar N.D. ISSN 2070 0482**, MMCS**, 2016, Vol**. 8**, No**. 2**, pp,183–200.
© *Pleiades Publishing, Ltd., 2016. – Springer*

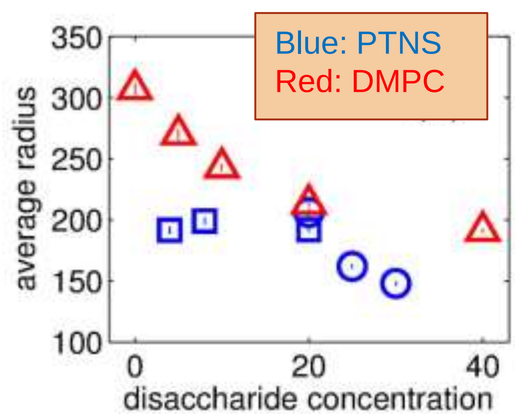
[3] Nikolay Dikusar. Shape Approximation Based on Higher-Degree Polynomials, **MMCP2017** (accepted for publication)

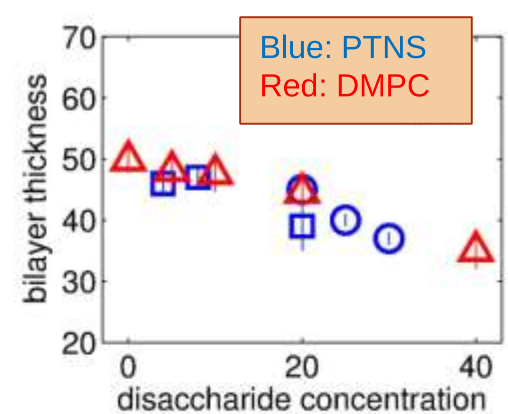
# ADE-SFF Data Analysis for Vesicular Systems




- Phospholipid unilamellar vesicles (ULVs, liposomes) are important in medicine.
- Data collected by SAXS and SANS methods on ULVs are analyzed within the Separated form factors model (SFF), using ADE minimization & parallel MPI programming
- Online interface was developed
  http://sff-sans.jinr.ru/

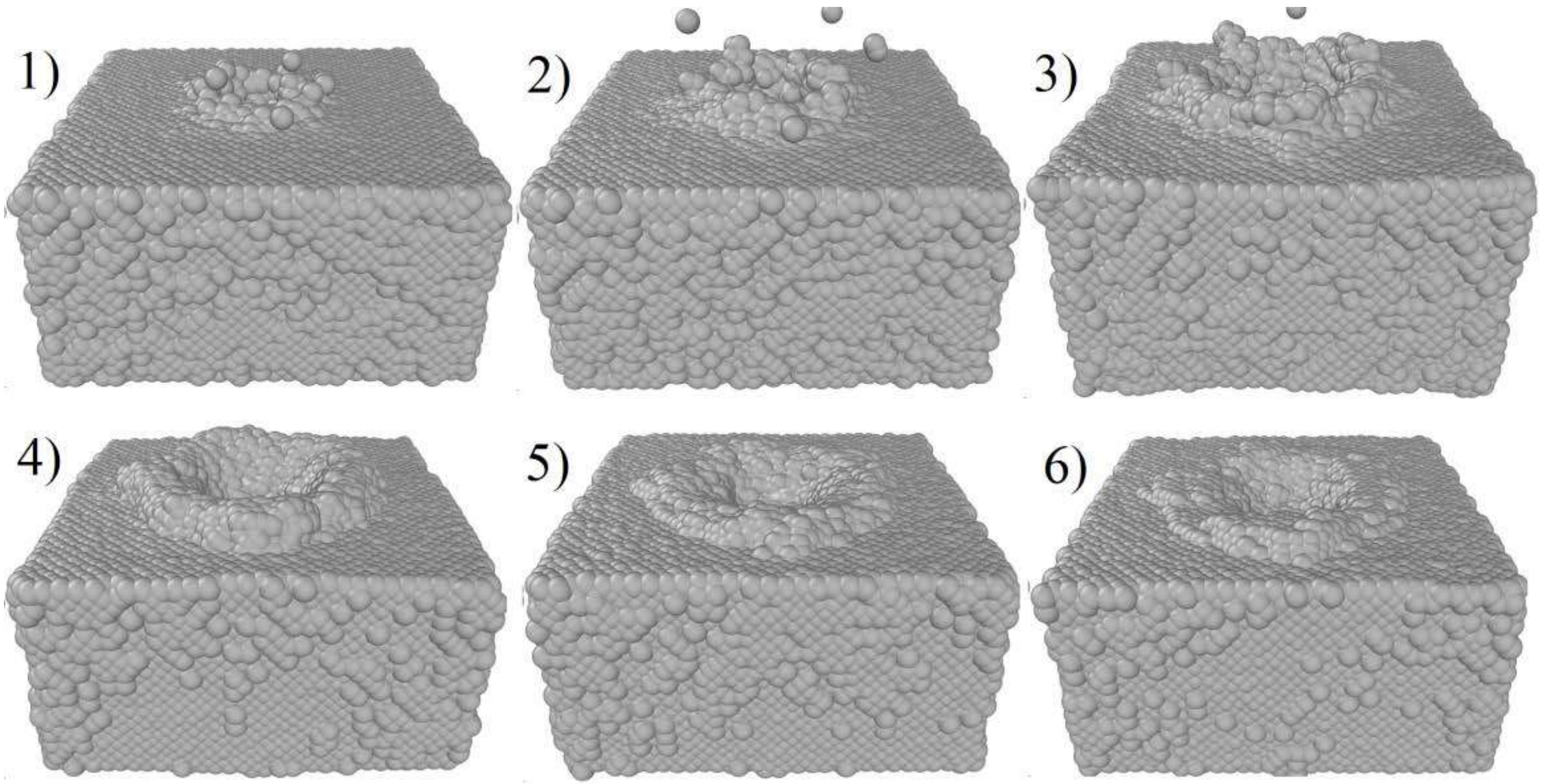



- Basic parameters of the Phospholipid transport nanosystem (PTNS) in water solutions of maltose were estimated from joint analysis of SANS and SAXS data in terms of the maltose concentration.


- M.Kiselev, E.Zemlyanaya, A.Gruzinov, E.Zhabitskaya, O.Ipatova, V.Aksenov. JINR Preprint P3-2017-32, “Crystallography Reports”, accepted
- E.Zemlyanaya, M.Kiselev, K.Lukyanov, I.Popov, K.Turapbay. Method. Journal of System Analysis in science and education, 2017, No.4
- M.Bashashin, E.Zemlyanaya, E.Zhabitskaya, M.Kiselev, T.Sapozhnikova, EPJ – WoC, Vol. 173 (2018)
- E.Zemlyanaya, M.Kiselev, E.Zhabitskaya, V.Aksenov, O.Ipatova, O.Ivankov. Journal of Physics CS,2018, accepted

# Modeling Structural Changes in Metals Irradiated by Copper Nanoclusters



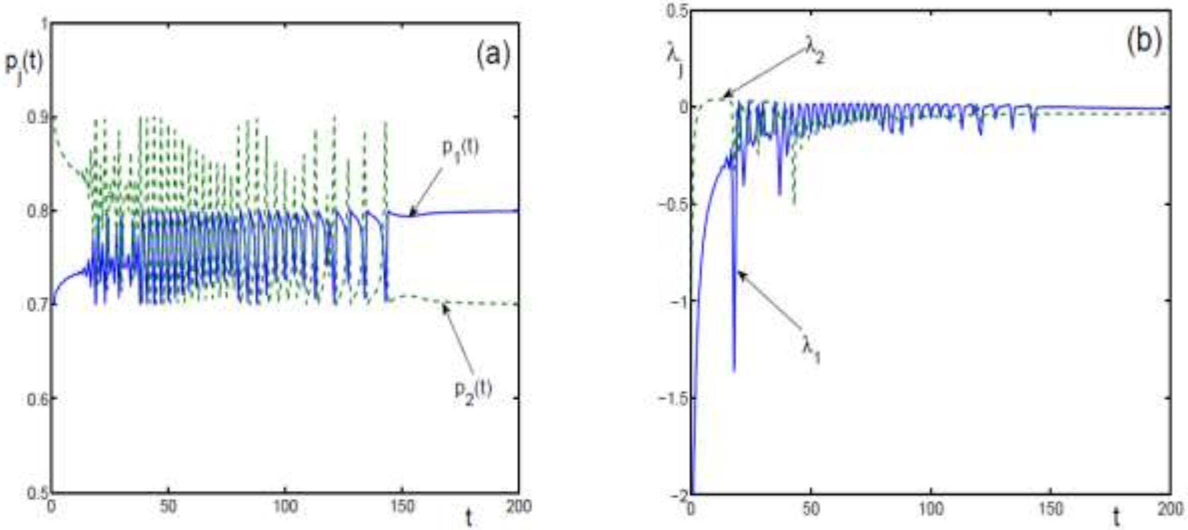

**Dynamics of *crater formation* in a target under irradiation with a 50-eV/atom nanoclusters at instants of time: 1) 0.5ps; 2)1ps; 3) 2ps; 4) 5ps; 5)10ps; 6) 20ps.**

B. Batgerel, S.N.Dimova, T.N.Kupenova, I.V. Puzynin, T.P. Puzynina, I.G.Hristov, R.D.Hristova, Z.K. Tukhliev, Z.A.Sharipov,
Communication at MMCP 2017, Dubna, July 3-7,
Bulletin of the Russian Academy of Sciences: Physics, Vol. 81, № 11, 1546-1550 (2017)

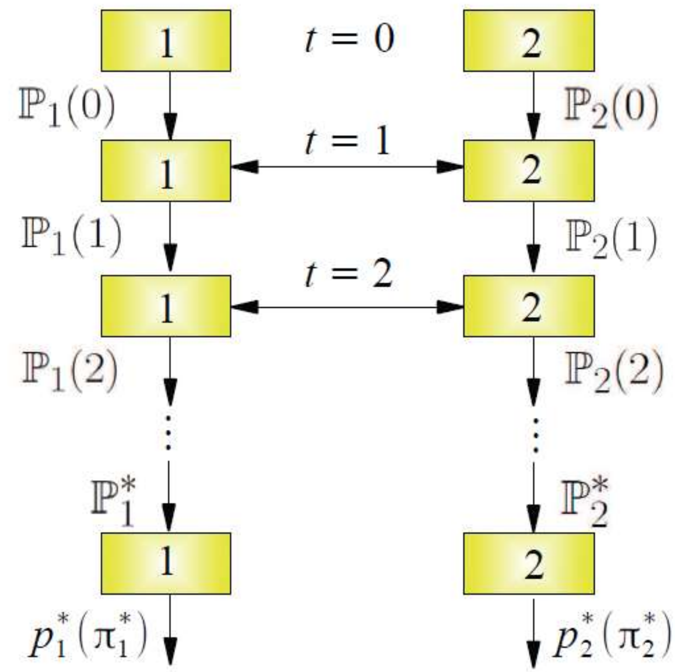
# Information Processing by Networks of Quantum Decision Makers

**A new model describing the artificial intelligence processing presents an intelligence network of decision makers exchanging information and forming their judgment, with collective decisions developed in time as a result of information exchange.**

**Such networks can describe dynamical processes occurring in artificial quantum intelligence composed of several parts or clusters of quantum computers.**




Two-partner reconstructive memory under conflict.
Dynamics of the probabilities (a) and local Lyapunov exponents (b)

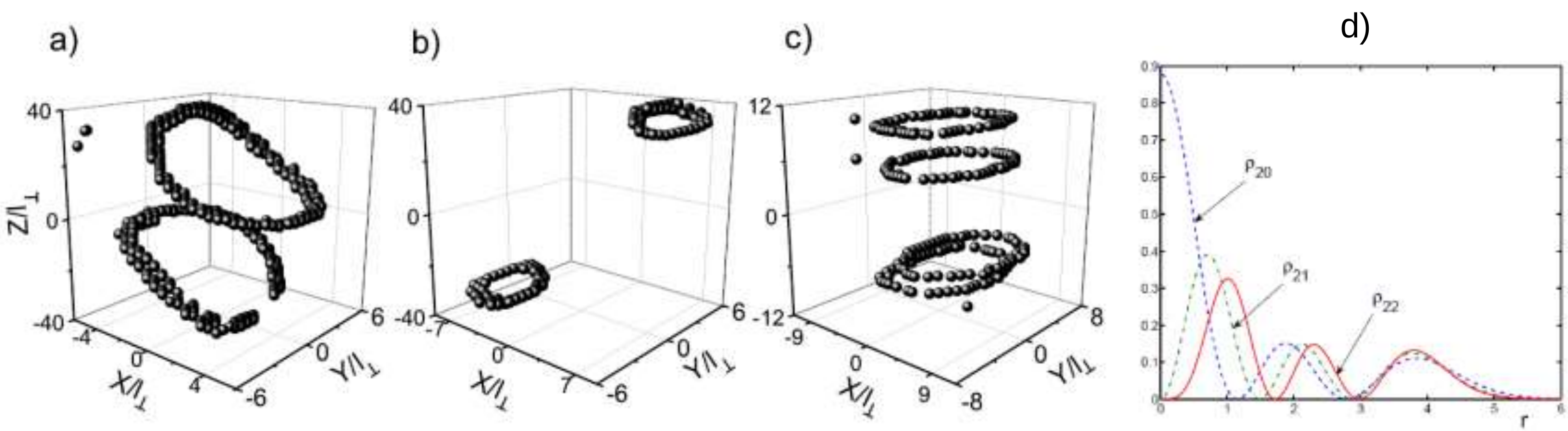



Dynamics of multistep decision making governed by information exchange between two agents

V.I. Yukalov, E.P. Yukalova, and D. Sornette, *Physica A 492 (2018) 747-766*

# Vortex rings and vortex ring solitons in a shaken Bose-Einstein condensate

In a **shaking Bose-Einstein condensate** confined in a **vibrating trap**, there can appear different **nonlinear coherent modes** such as vortex ring solitons and vortex rings. The energy required for creating vortex ring solitons is larger than that needed for forming vortex rings. The generation of vortex rings at moderate excitation energies is illustrated by numerical simulations for trapped rubidium $^{87}Rb$ atoms.



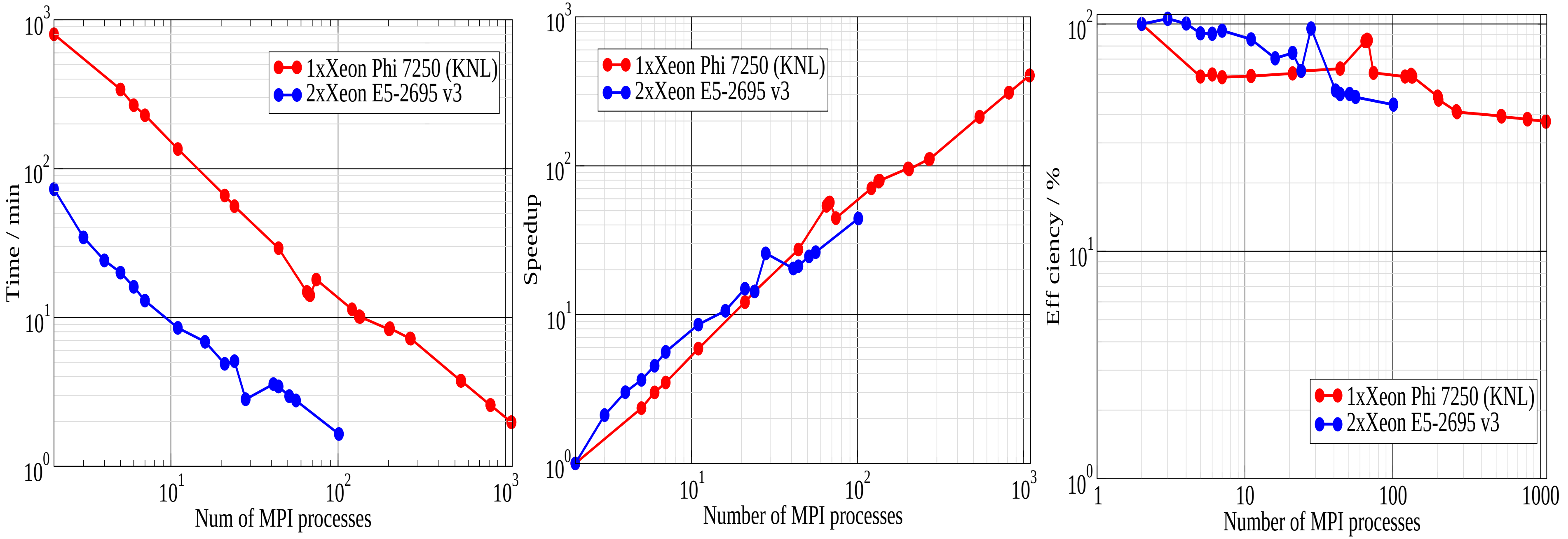

Spatial location of vortex rings after different shaking times:

a) t = 10.5 ms; b) t = 11ms; c) t = 14.4 ms;

d) Radial density of the **double ring state** (dashed line), composite **vortex state + double ring states** (dashed dotted line) and **vortex state** with the winding number m = 2 (solid line)

V.I. Yukalov, , A.N. Novikov, E.P. Yukalova, V.S. Bagnato, J. Phys. Conf. Ser. 691, 012019-10 (2016)

# Comparison of Parallel CPU Govorun Solutions of Compact Star Configurations for Sequence of Dense Nuclear Matter Models




**An MPI algorithm was developed for the simulation of neutron star configurations described by equation of state models of dense nuclear matter. The performance of the parallel algorithm has been investigated for testing set of EoS models on two different types of computational nodes: 1xXeon Phi (KNL) 7250 and 2xXeon E5-2695v3, the presented computations have been obtained with use of Advanced Vector Extensions SIMD: AVX512 and AVX2 correspondingly.**

A. Ayriyan, J. Busa Jr., H. Grigorian, and G. Poghosyan. Parallel Algorithm for Solving TOV Equations for Sequence of Cold and Dense Nuclear Matter Models // European Physics Journal WoC, vol. 177, 07001 (2018)

# Computer Linearization of Differential Equations

**Solving nonlinear ordinary differential equations is one of the fundamental and practically important research challenges in mathematics. However, the problem of linearizability for the equation**

$$y^{(n)} = f\left(x, y, y', \ldots, y^{(n-1)}\right) \xrightarrow[?]{u=\varphi(x,y),\ t=\psi(x,y)} u^{(n)}(t) = \sum_{k=0}^{n-1} a_k(t) u^{(k)}(t)$$

Sophus Lie
1842-1899

**set up in** "Sophus Lie. Vorlesungen über kontinuierliche Gruppen mit geometrischen und anderen Anwendungen. Teubner, Leipzig, 1883" **so far remained algorithmically unsolved**.

**The algorithmic solution of this problem, i.e. the verification of the existence of linearizable transformation and its construction, if such transformation exists, together with implementation in the computer algebra system Maple, was given in the paper**

**V.P.Gerdt (LIT JINR)**, D.A. Lyakhov, D.L. Michels (both KAUST, Thuwal, Saudi Arabia), Proceedings of ISSAC 2017, ACM Press, 2017, pp.285--292. *arXiv:1702.03829[math.CA]*

**ISSAC Distinguished Paper Award by ACM SIGSAM** ( http://www.issac-conference.org/2017/awards.php )

**for *n* ≥ 2 and for any rational function *f*.**

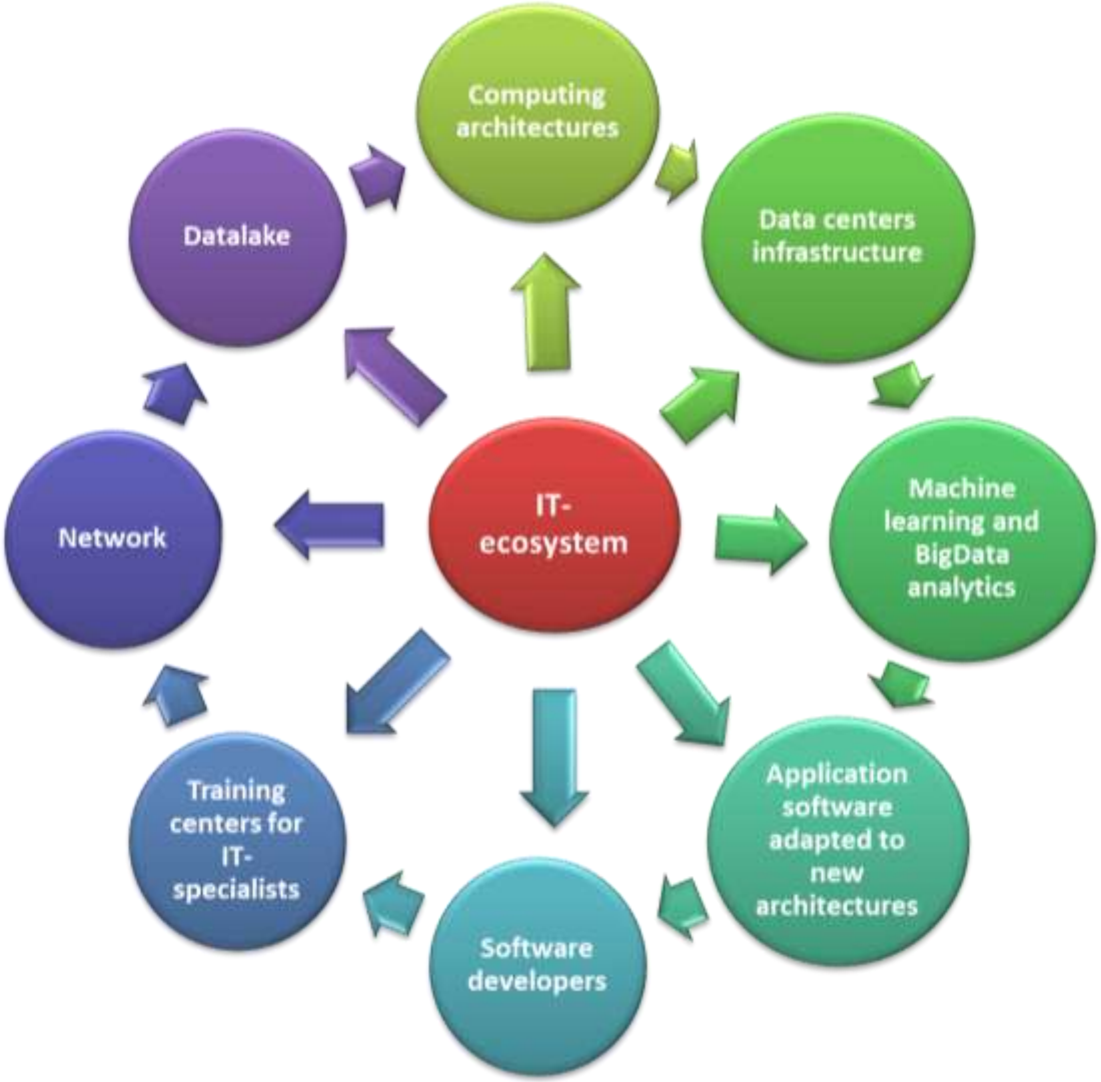
**Example:** Tremblay-Turbiner-Winternitz equation (G.Gubbiotti, M.C.Nucci. J.Math.Phys. 58, 2017, 012902)

$$yy''' + y'\left(16\omega^2 y + 3y''\right) = 0, \quad \omega > 0 \xrightarrow{u=\frac{\omega^2}{\sin^2(2\omega x)},\ t=\frac{1}{\tan(2\omega x)}} u'''(t) = 0 \ \rightarrow\ u = c_2 t^2 + c_1 t + c_0,\ c_i = const$$

# Strategy of Information Technologies and Scientific Computing in JINR

## Unity in Diversity

Covers the development of IT-technologies and scientific computing aimed at solving strategic tasks of JINR through the imagination and development of a great many advanced IT solutions, integrated into a unified computing environment – **a scientific IT ecosystem that combines a variety of technological solutions, concepts and methodologies**.



# Outline

- Laboratory of Information Technologies in JINR
- The Multifunctional Information and Computing Complex (MICC) in LIT JINR
- Instances of computer physics challenges
- **Miscellanea**

# International Cooperation & Education

Armenia, Azerbaijan, Australia, Belarus, Belgium, Brazil, Bulgaria, Canada, CERN, Czech Rep., Egypt, France, Georgia, Germany, Greece, India, Italy, Japan, Kazakhstan, Moldova, Mongolia, Poland, Portugal, Romania, Russia, Slovakia, South Africa, Sweden, Switzerland, Taiwan, Tajikistan, Ukraine, USA, Uzbekistan, Vietnam

Currently,
20 JINR Member States and Associated
15 Other Countries
comprising over 100 Institutes and International Organizations

- ***In 2017, JINR was habilitated to confer PhD and Dsc titles in Russian Federation***
- ***Young Specialists' Education***:
  - Creation of dedicated & distributed Grid and Cloud infrastructures;
  - Tutorials on Grid both at LIT and at connected Member State Centers;
  - Tutorials on the new heterogeneous cluster HybriLIT;
  - Dedicated Conferences for young scientists and specialists;
  - Individual or group periodic seminars/meetings on selected topics
- ***Users' Education and Training***:
  - Group and individual consultations
  - Tutorials upon request
- ***General Educational Activities***:
  - Specialized scientific Conferences with international participation
  - Scientific seminars, etc.
- ***LIT Staff involvement in Educational Processes at Dubna Univ. and other Univs. and at JINR UC***

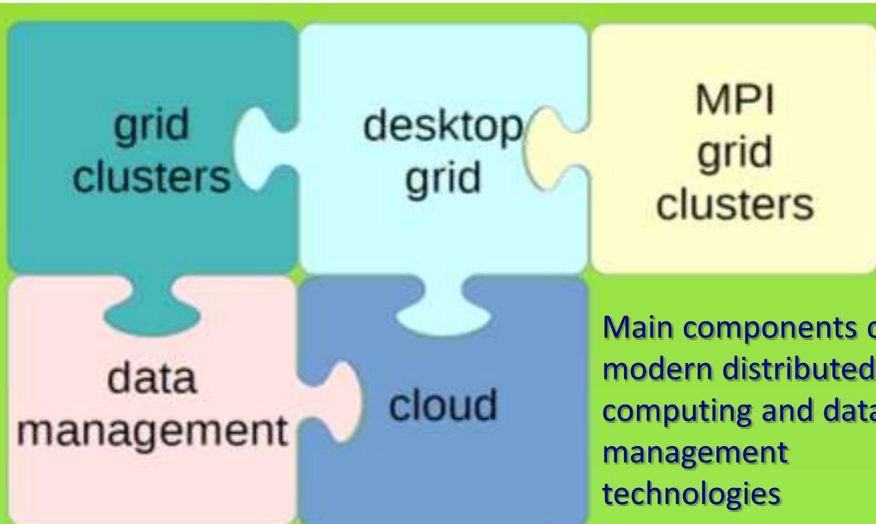
# HybriLIT: User training

**Tutorials** on the **HybriLIT** use:

- Regular tutorials on parallel programming techniques for the institute staff and, under JINR-UC organization, for students and young scientists from JINR Member-States;
- Specialized courses from leading software developers.

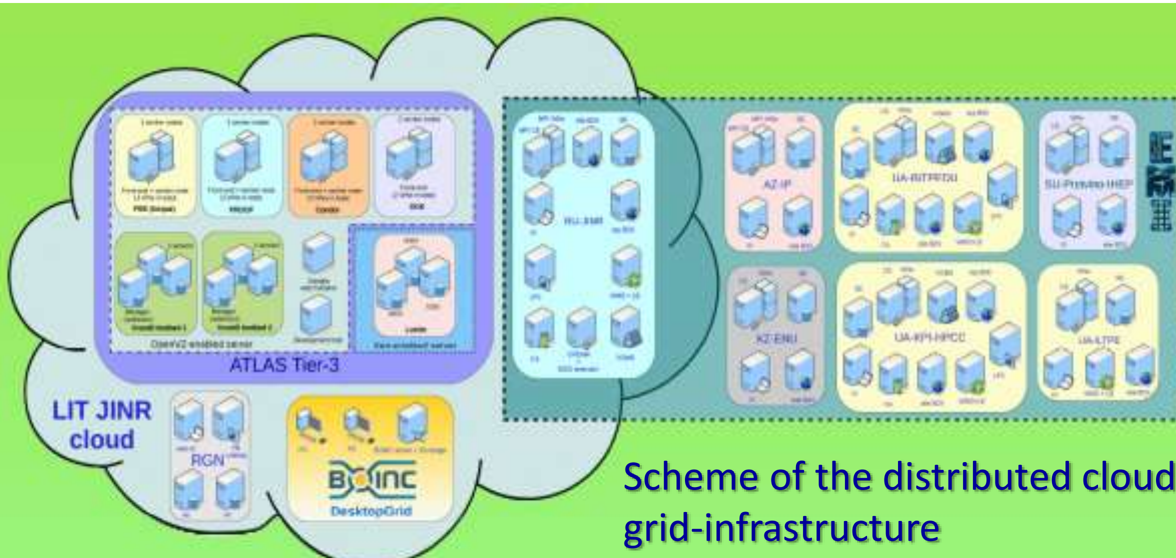
**Specialized courses** and **seminars** within JINR-organized conferences and schools. Instances: GRID’2014, International youth conference MPAMCS’2014, The Helmholtz International Summer School "Lattice QCD, Hadron Structure and Hadronic Matter" 2014; **MMCP 2015**, **NEC 2015**, **AIS-GRID 2015**, MMCP 2017.

# Grid: User training and research




Main components of modern distributed computing and data management technologies

A **production grid infrastructure** cannot be used for **training, research, development and testing in the grid environment**.
The efficient solution of such tasks uses **dedicated facilities**. At LIT, this integrates the **JINR cloud and educational grid infrastructures**.
More and more organizations from Russia and the JINR Member States showed interest in it and expressed their wish to set up and integrate their own grid sites into it as efficient means to use the modern grid technologies.

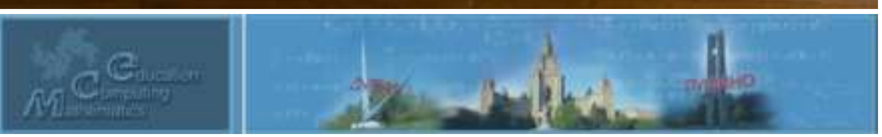



Scheme of the distributed cloud grid-infrastructure

- Institute of High-Energy Physics (Protvino, Moscow region),
- Bogolyubov Institute for Theoretical Physics (Kiev, Ukraine),
- National Technical University of Ukraine "Kyiv Polytechnic Institute" (Kiev, Ukraine),
- L.N. Gumilyov Eurasian National University (Astana, Kazakhstan),
- B.Verkin Institute for Low Temperature Physics and Engineering of the National Academy of Sciences of Ukraine (Kharkov,Ukraine),
- Institute of Physics of Azerbaijan National Academy of Sciences (Baku, Azerbaijan)

# LIT traditional conferences and schools


Distributed Computing and Grid-technologies in Science and Education



Mathematics. Computing. Education

DIGITAL LIBRARIES: ADVANCED METHODS AND TECHNOLOGIES, DIGITAL COLLECTIONS


## LIT schools

JINR / CERN

GRID AND ADVANCED INFORMATION SYSTEMS


***Left***: With over 37,600 downloads of the 41 papers, at a pace of over 500 monthly, the **LNCS 7125** volume was annually quoted by Springer ***in 2013-2017 as one of its top 50% most downloaded eBooks in this collection***:
http://www.bookmetrix.com/detail_full/book/8717d9eb-2653-4a3c-a8d9-adf82bdcd1d5#downloads

***Centre***: EPJ-WoC, Vol.108, with 58 accepted papers:
http://www.epj-conferences.org/articles/epjconf/abs/2016/03/contents/contents.html

***Right***: EPJ-WoC, Vol.173, with 100 accepted papers:
https://www.epj-conferences.org/articles/epjconf/abs/2018/08/contents/contents.html

# Conclusions

- *Creation of the Multifunctional Information and Computing Complex as basic JINR facility allowing to face up the future scientific research challenges in the JINR and the JINR Member States is a key development in the field of information technologies and computing*
- *The development of large scale high-performance computing at JINR required for the acceleration of the extensive theoretical research in hadron matter physics underway at the Bogolubov Laboratory of Theoretical Physics (BLTP) and the creation of possibility for using the latest computing platforms for the NICA computing is a significant step forward for JINR research*
- *In addition to the high energy physics, other investigations are also seeking novel computing models. Computing is essential to R&D, science and technology, corporative management*
- *The development of numerical methods and algorithms for parallel and hybrid calculations in scientific research will become pervasive*
- *The active participation of BLTP as a user community in the justification of Supercomputer parameters and future research program on it is a good example of new principles of the organization of computations leading to innovative changes in the research strategy*

*Thank you for your attention !*

# Addendum:
# Dubna is more than science