Computer physics challenges in LIT-JINR

Gheorghe ADAM
LIT JINR & IFIN-HH

ROLCG 2015, Cluj-Napoca, October 28-30, 2015

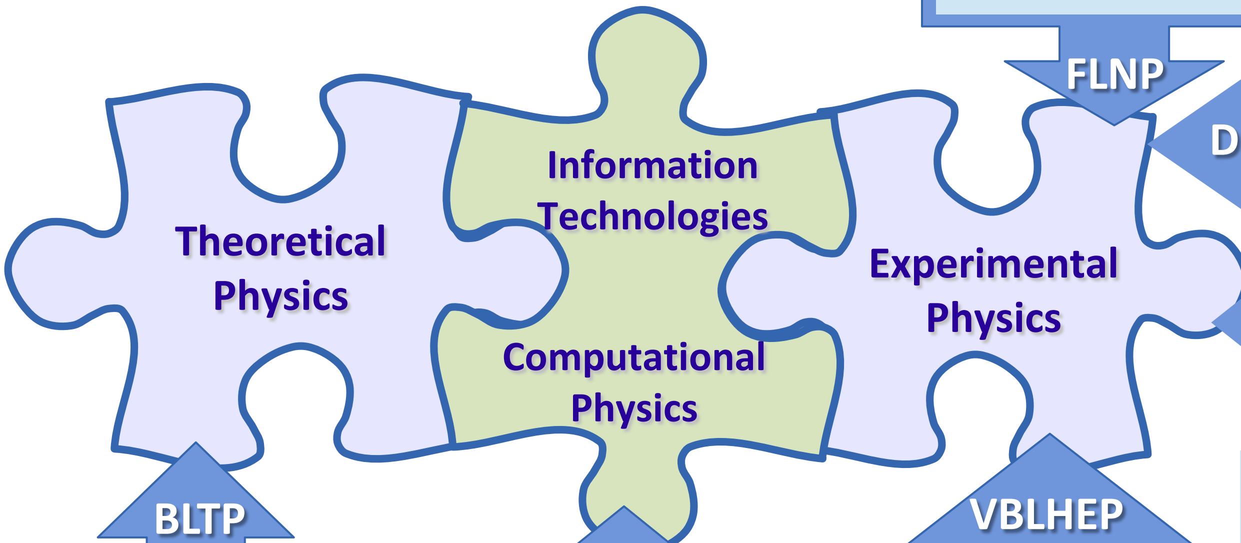
Outline

- Causes of changes in computer physics
- The Multifunctional Information and Computing Complex in LIT JINR
- Instances of computer physics challenges

Outline

- **Causes of changes in computer physics**
- The Multifunctional Information and Computing Complex in LIT JINR
- Instances of computer physics challenges

LIT participates in 48 projects of 30 JINR topics of the 2015 Topical Plan of JINR



FLNP

04-4-1122-2015/2017 [1]
Leaders: S.A. Kulikov, V.I. Prikhodko

03-4-1104-2011/2016 [1]
Leader: V.N. Shvetsov,
Deputies: Yu.N. Kopatch, E.V. Lychagin, P.V. Sedyshev

04-4-1121-2015/2017 [1]
Leaders: D.P. Kozlenko, V.L. Aksenov , A.M. Balagurov

04-4-1111-2013/2017 [1]
Leader: G.M. Arzumanyan

DLNP

02-2-1080-2009/2015 [1]
Leader: L.G. Afanasyev

02-2-1099-2010/2015 [3]
Leaders: D.V. Naumov, A.G. Olshevskiy

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

03-2-1101-2010/2015 [2]
Leaders: A.V. Kulikov

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

03-2-1102-2010/2015 [1]
Leaders: G.A. Karamysheva, S.L. Yakovenko,
Scientific leader: L.M. Onischenko

02-2-1123-2015/2016 [1]
Leader: A.S. Zhemchugov

FLNR

04-5-1076-2009/2016 [1]
Leaders: S.N. Dmitriev, P.Yu. Apel

03-0-1095-2010/2016 [1]
Leaders: G.G. Gulbekyan, S.N. Dmitriev, 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

05-6-1118-2014/2016
Information and Computing Infrastructure of JINR

05-6-1119-2014/2016
Methods, Algorithms and Software for Modeling Physical Systems, Mathematical Processing and Analysis of Experimental Data

VBLHEP

02-1-1097-2010/2015 [2]
Leader: A.D. Kovalenko,
Deputies: N.M. Piskunov, V.P. Ladygin, M. Finger (Jr.), R.A. Shindin

02-1-1088-2009/2016 [2]
Leader: A.S. Vodopyanov

02-1-1106-2011/2016 [1]
Leader: A. Malakhov, V. Ivanov

02-1-1107-2011/2016 [1]
Leader: S.I. Tyutyunnikov

02-0-1066-2007/2015 [2]
Leaders: R. Lednicky, Yu.A. Panebratsev

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

02-0-1085-2009/2016 [1]
Leader: A.P. Nagaytsev, Scientific leader: I.A. Savin

02-0-1083-2009/2016 [4]
Leader: A. Zarubin, Scientific leader: I.A. Golutvin

02-0-1081-2009/2016 [1]
Leader: V.A. Bednyakov
Deputies: E.V. Khramov, A.P. Cheplakov

02-0-1108-2011/2016 [1]
Leader: A.G. Olshevskiy,
Deputies: G.D. Alexeev, A.S. Vodopyanov

05-8-1037-2001/2019 [2]
Leader: N.A. Russakovich

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

The Hardware-Software Environment

The activity done in LIT-JINR has resulted in a ***robust significant hardware and software environment*** (HSE) which allows the derivation of successful numerical or symbolic-numerical solutions to the mathematical problems raised by the approved scientific projects.

Long lasting HSE performances were obtained in spite of the existence of *fundamental external factors* causing *fragility and ephemerality*

Fundamental External Factors

• **The rapid change occurring in the offers of the hardware vendors.** During the last decade we have seen the appearance of multi-core chips, then of many-core ones, and of GPU accelerators.

• **Buying decisions within a tight budget.**

• **Ways of alleviating constraints.**

- **Modularity** of the implementation;
- **Careful study** of the **world environment** [hints following from solutions adopted elsewhere for similar development (**Grid** clusters or **parallel computing** clusters);
- **In-house studies** enabling tailor-made **customized parameters** of the acquired modules

The First Success: JINR-LCG2 Tier-2 site

- **In-house investigation of performance:**

1. Parallelization of the information transfer between the different blade-blade and blade-disk pairs,

2. Implementation of the fundamental set of primary software services making available the computing cluster to the **whole community of the JINR users**, working both inside and outside the Grid,

3. Development of a preventive exhaustive monitoring, enabled the site functioning at top performance (***availability and reliability*** > **99%**) within the LHC Grid.

Consequences of the substantial hardware changes

- **Need of fundamentally different software implementations able to fully exploit the new possibilities opened by the new hardware parallelism.**

1. New mathematical methods and algorithms enabling efficient information flow inside the new hardware.

2. Grasp of alternative programming paradigms and programming languages.

3. The evolving HSE allows the solution of **more sophisticated theoretical models**, characterized by newly added features which make them more realistic.

4. The reliable numerical or symbolic-numerical solution of such models asks, in its turn, for the **development of new approaches to their solutions**.

Intricacies coming from the mathematical side

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

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

2. Need of new approaches characterized by inventiveness **enabling the reduction of the computational complexity**.

3. Example 1: the **discretization** of partial differential equations (PDE) describing nonlinear mathematical models may **change** the basic algebraic properties of the starting continuous PDEs resulting thus in loss of significance, in numbers, not in insight.

4. Example 2: the **finite set** of the finite precision floating point machine numbers may result in **modifications of fundamental** well established features over the field of the real numbers. **Bayesian decision branches** are needed to define correctly the way to reliable solution and the significance of output status.

Outline

- Causes of changes in computer physics
- The Multifunctional Information and Computing Complex in LIT JINR
- Instances of computer physics challenges

A **Multifunctional Information and Computing Complex** (MICC) is in train to be implemented, with four main pillars: the JINR-LCG2 Tier-2 site, the JINR CMS Tier-1 site, the heterogeneous computing cluster for parallel and hybrid computations – HybriLIT, the cloud infrastructure (plus the educational component).

- The **JINR CMS Tier-1 site** is to obey to the performance and quantitative specifications foreseen in the agreement signed with CERN: **100% availability and reliability, capacities within agreed targets**.

Practical means to meet performance specifications:

- ***redundancy*** wherever possible (especially underlying engineering infrastructure)
- ***preventive*** and ***exhaustive monitoring***

- The **HybriLIT**: secures **hardware**, **software**, and **qualified expertise** for the development of efficient parallel codes.

Causes of decisions to build up the HybriLIT:

- **the wish to use efficiently the new hardware** (in connection with participation in modeling and computer simulation of the future CBM experiment, the new tasks related to the NICA-MPD experiment in the JINR itself).

Driving factors of the practical decisions:

- **scarcity of financial resources** (prevented buying from the very beginning a large cluster)
- **study of the TOP 500 list. Prevalent features:**
  = **modularity** of the large supercomputing structures;
  = **dominance of the Intel Xeon Phi and the NVIDIA CUDA GPU accelerators.**

- **Tailoring HybriLIT features to enhance performance:**

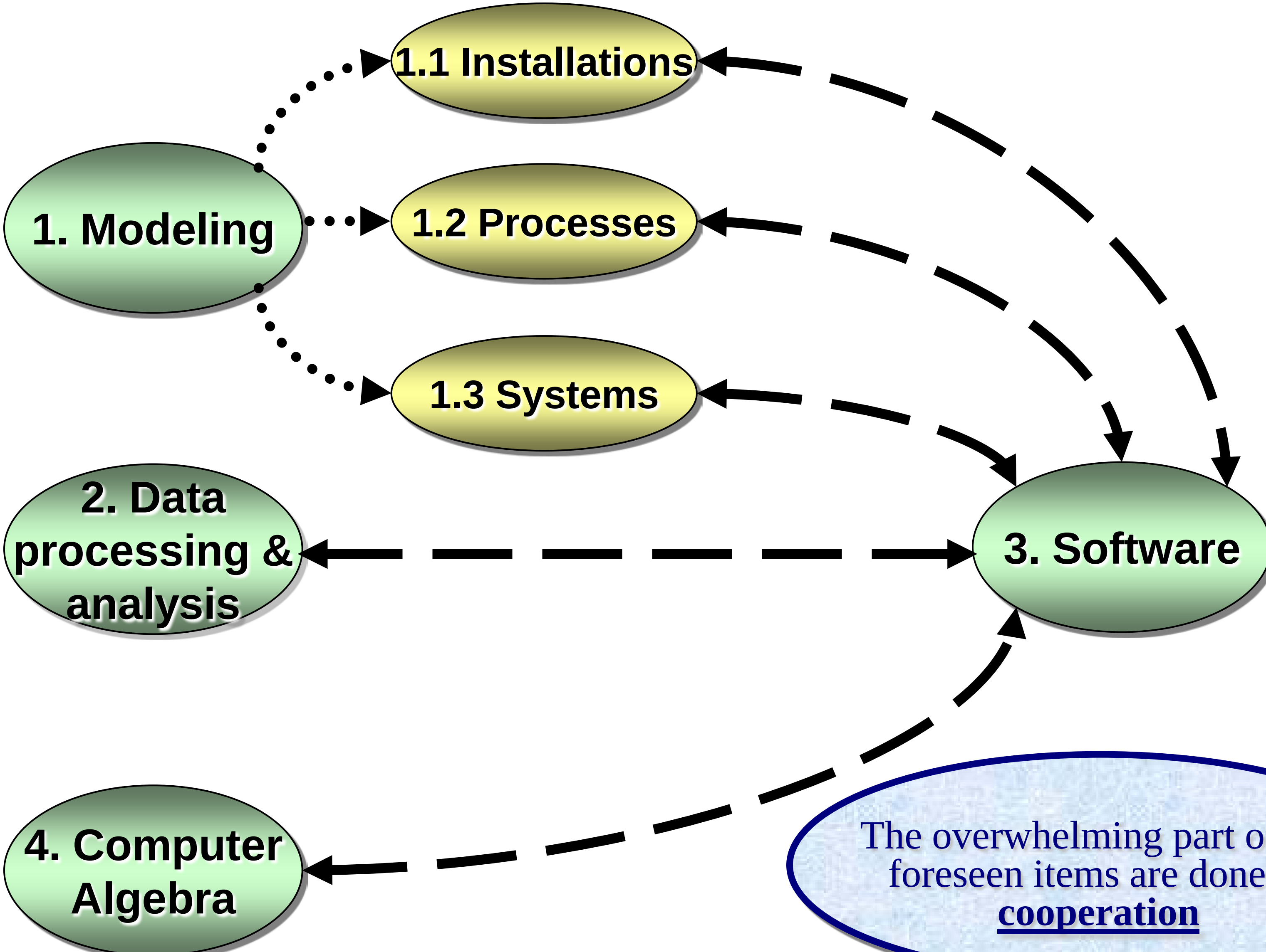
  - extensive testing of the Intel vs NVIDIA blades (has shown that, for the majority of the problems currently solved in JINR, the acceleration provided by the graphic units is faster than that provided by the many-core Intel Xeon Phi.)

  - standard hardware configuration offered by the vendors has insufficient RAM (this drawback was remedied at the acquisition of the last pair of NVIDIA K80 blades)

Outline

- Causes of changes in computer physics
- The Multifunctional Information and Computing Complex in LIT JINR
- **Instances of computer physics challenges**

Bird's-eye-view



The overwhelming part of the foreseen items are done **in cooperation**

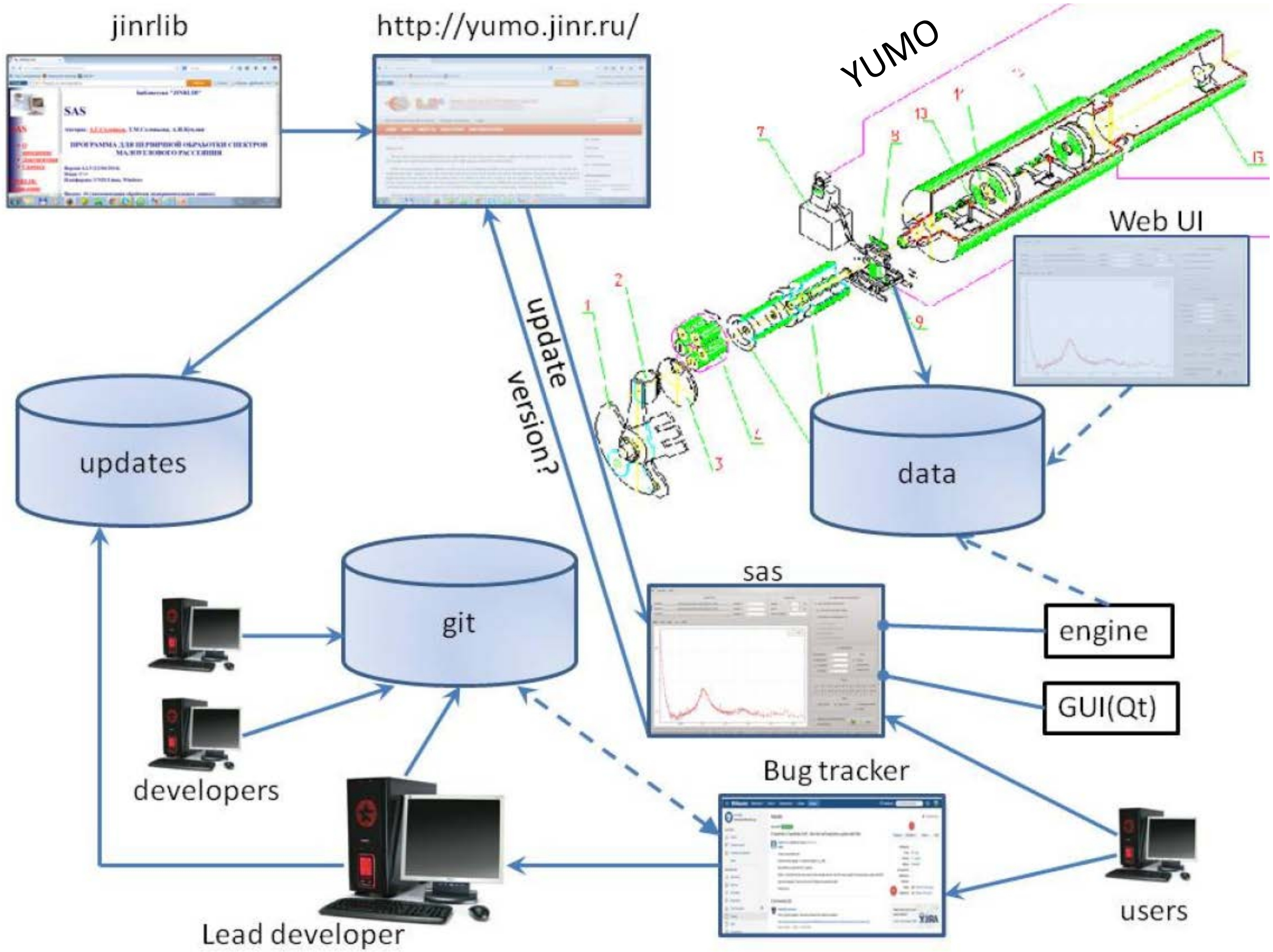
Software development in 2017-2023

- **Parallel software will be the mainstream [substantial reduction of CPU time & scale enhancement of the solved problems]**
  - Development and support of **program libraries** of general and special purpose
  - Creation and support of program libraries and software complexes implemented with **parallel programming techniques** CUDA, OpenCL, MPI+CUDA, OpenMP, etc.
  - Support and development of a **specialized service-oriented environment** for modeling experimental installations and processes and experimental data processing
  - **Tools and methods** for software development
    - flexible, platform-independent simulation tools
    - self-adaptive (data-driven) simulation development software

– **Automation upgrade of on-line data acquisition and processing**

[Instance: ●● For the future modernizations of

Automation of on-line data storage on modernized YUMO spectrometer



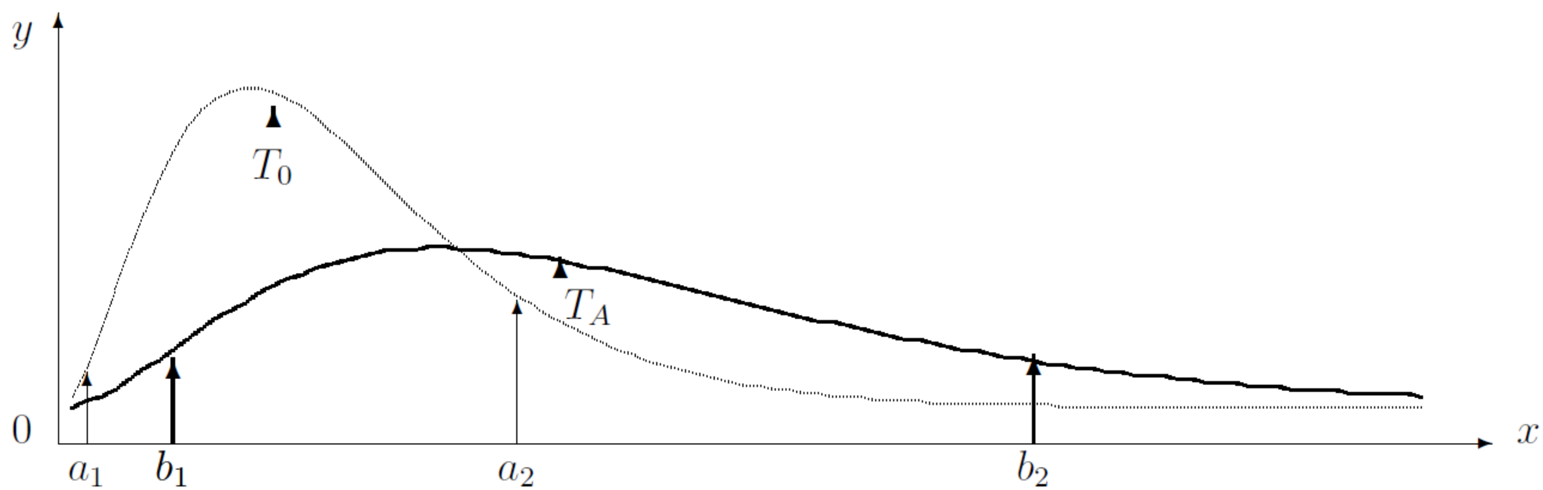
A.G. Soloviev, T.M. Solovieva (LIT), A.V. Rogachev, A.I. Kuklin (FLNP)

Confidence interval optimization for testing hypotheses under data with low statistics (Radioactivity: rare events)

New concept: **Optimal confidence interval** based on the order statistics, enables both the parameter (mean) estimation and the statistical tests. On the one hand, this provides clear and natural data interpretation, and, on the other hand, means a good compromise between the criteria: ”the shortest interval length” - ”the largest size of the covering probability”.

Application to the exponential distribution, which characterizes the radioactive decays and is very intolerant to the low statistics (m = 1-4 events): The gamma-distribution at m = 3.

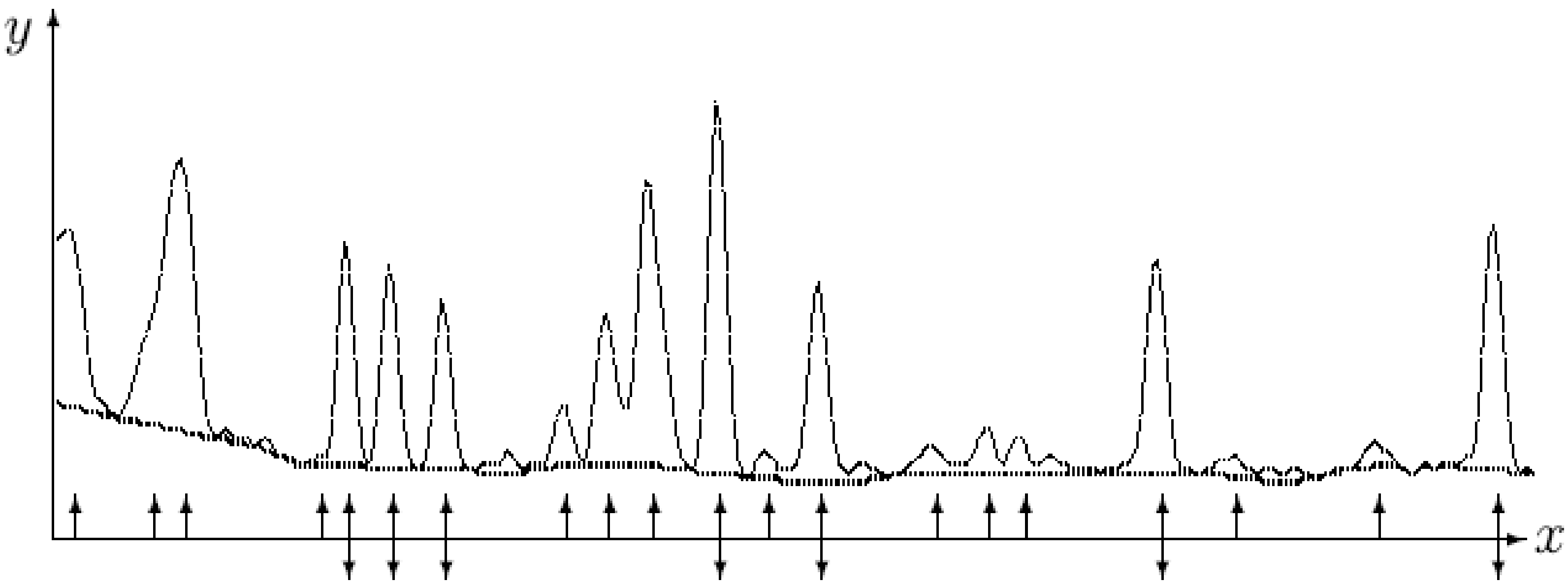
The confidence intervals [a_1, a_2] (thin line) and [b_1, b_2] (thick line) for the discrimination of the hypotheses T_0 = 20 and T_A = 40.



V.B. Zlokazov (LIT), CPC, 185 (2014) 933-938; PEPAN Letters., 12, No.2, 389-399 (2015)

VSHEC – A Program for the Automatic Spectrum Calibration

Nature of problem: Automatic conversion of detector channels into their energy equivalents.
Solution method: Automatic decomposition of a spectrum into geometric figures such as peaks and an envelope of peaks from below, estimation of peak centers and search for the maximum peak center subsequence which matches the reference energies in the statistically most plausible way.
An example of method usage to real data: A fragment of an alpha-spectrum of $^{nat}Yt + ^{48}Ca$. The thick curve is the non-linear background. The upward arrows indicate the found statistically significant peaks, the downward ones are those selected for calibration.



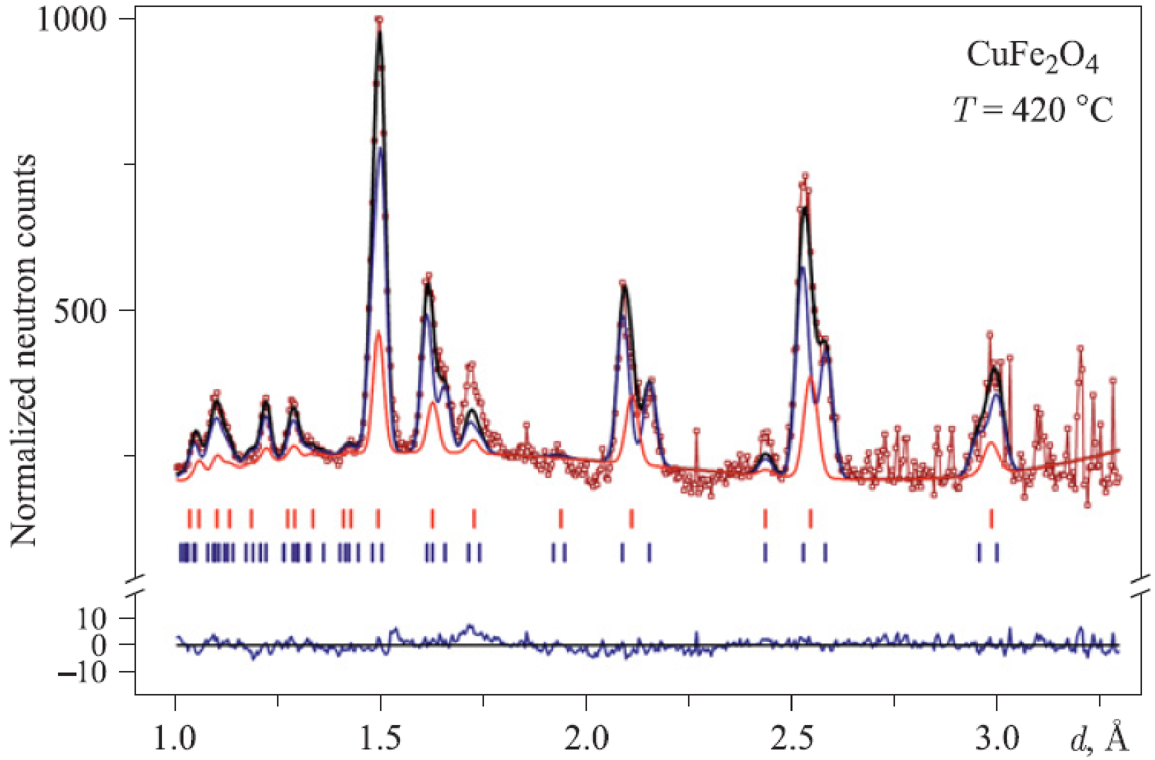
V.B. Zlokazov (LIT), V.K. Utyonkov, Yu.S. Tsyganov (FLNR), CPC 184 (2013) 428-431

Real-Time Visualization and Analysis of Neutron Diffraction Data

Packages MAPS and **SPEVA** were developed for preliminary analysis and final mathematical processing of large neutron diffraction data got in studies of transition processes in crystals. They secure automatic visualization of 2D data obtained at HRFD-diffractometer with time of flight scanning, respectively analysis of atomic structure changes during transition processes

An instance:

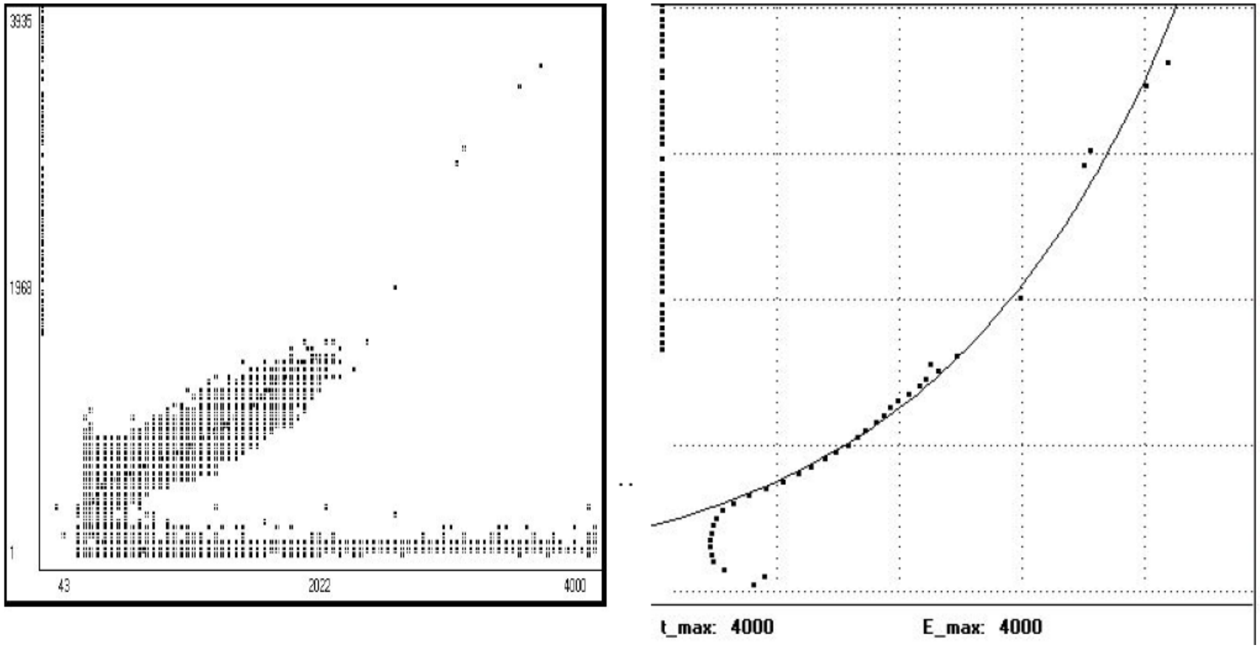
Structural phase transition between cubic (in red) and tetragonal (in blue) phases resolved in the diffraction spectrum of $CuFe_2O_4$ at the temperature T= 420 ^{0}C



V.B. Zlokazov, D.A. Balagurov, I.A. Bobrikov, N.Yu. Samoilova, A.M. Balagurov, JINR Preprint P3-2014-94

Robust Fitting for the Estimation of Hidden Parameters in Experimental Distributions on the Plane

The robust fitting is shown to be the only effective automatic approach to the derivation of the scintillator decay time τ from a measured energy dependence *E* = *g*(*t; τ*) with acceptable accuracy.



Left: A raw 2-dimensional record distribution *A*(*E; t*).
Right: The fitting function goes correctly through the points where it is adequate to the model, and ignores those where it is not (on the left side and at the bottom). The obtained result agrees with the known data (*τ*= 230*ns*)

V.B. Zlokazov (LIT), V.A. Morozov (FLNP), PEPAN Letters, 11, No.4, 748-752 (2014)

● Development of Modern Investigation Tools in Large Scale International Collaborations

– Contribution to the upgrade of Geant 4 package

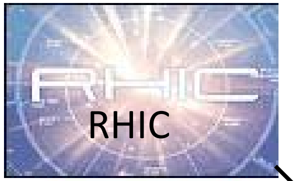
[Tasks: ●● Improvement of specific physics task modules of Geant 4;
●● Contribution to the code parallelization within Geant 4 modules;
●● **Grasp of Geant 4 and extension of its usage in addition to the high energy physics tasks]**

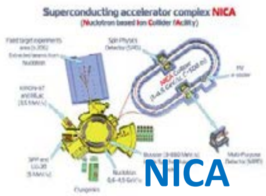
– CBM@GSI – Methods, Algorithms & Software for Fast Event Reconstruction

[Tasks: ●● Software parallelization for different detectors entering the CBM facility;
●● Development and implementation of the concept of CBM Databases;
●● Contribution to the development of the CBMROOT]

– CMS/LHC and BM@N/Nuclotron – New mathematical methods and emerging software for reliable data analysis

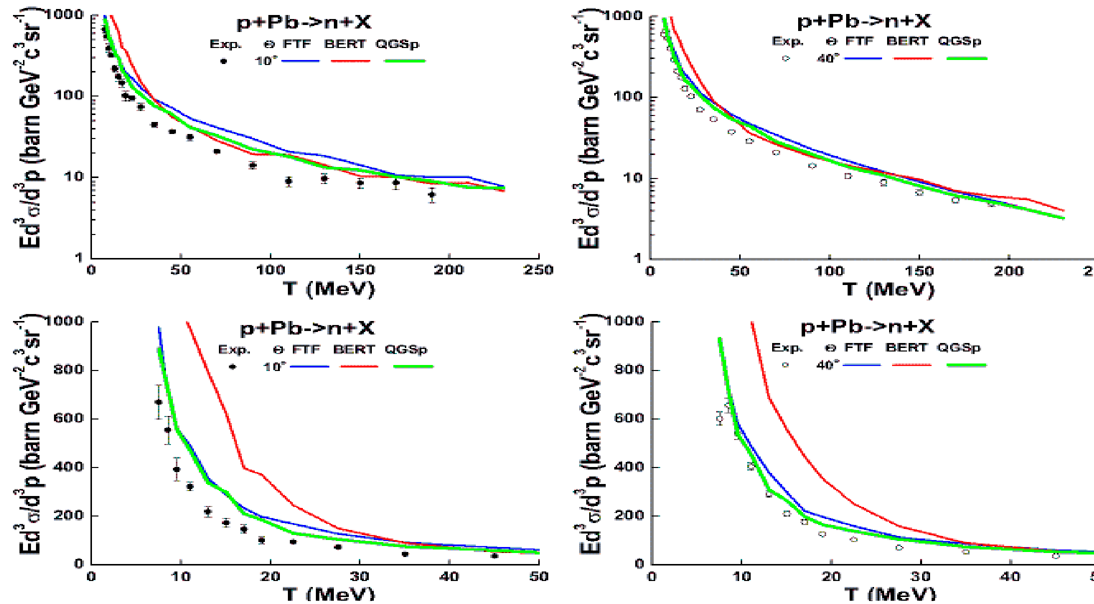
[Tasks: ●● CMS/LHC and BM@N/Nuclotron experimental data handling: development and improvement of pattern recognition algorithms]





Improvement of QGSp in Geant4

Physics List – QGSp_BERT used by ATLAS and CMS



Slow neutron production, ITEP experimental data (1983)

[Shower shape improvement]

Tasks solved (2015):

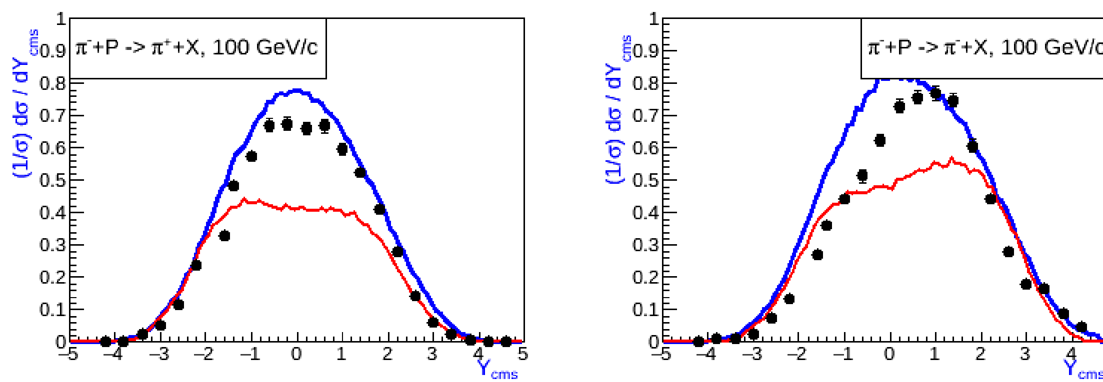
- Improvement of string fragmentation
- Improvements of processes cross sections
- Inclusion of the Reggeon cascading for correct description of nucleus breakups
- Improvement of parton momenta sampling

To do: fine tuning of model parameters

Improved QGSp will be available in G4.10.2.beta (end June 2015)
It is expected that new QGSp will improve calorimeter responses!

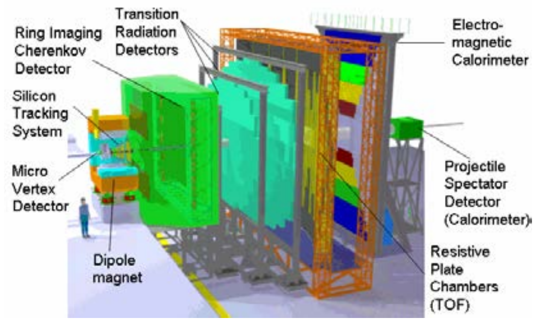
πP interactions at 100 GeV/c

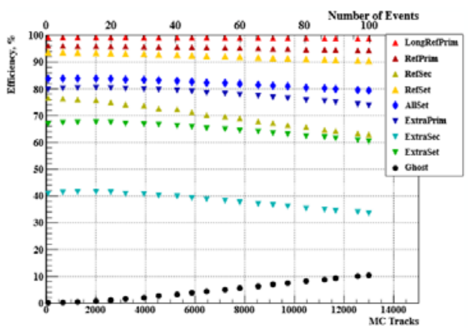
Red lines – old QGSp Blue lines – new QGSp

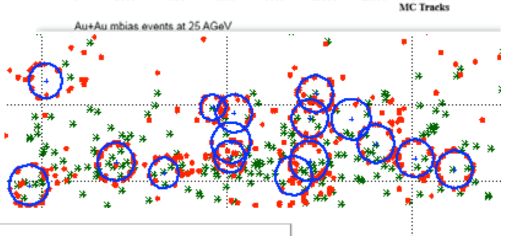


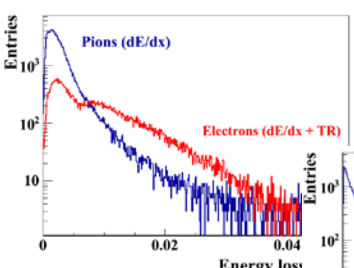
[Author of original code – N.S. Amelin (LIT, JINR)]
Developer – V.V. Uzhinsky (LIT, JINR)

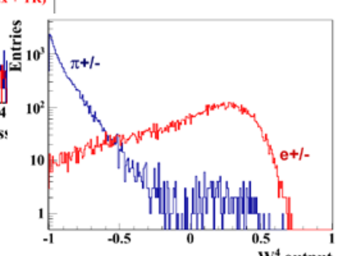
CBM@GSI – Methods, Algorithms & Software for Fast Event Reconstruction





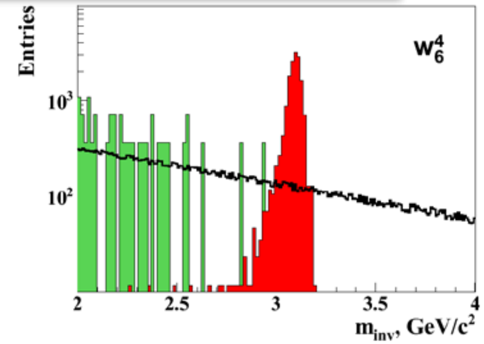






Tasks:

- 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, $J/\psi \to e^+e^-$ and $J/\psi \to \mu^+\mu^-$ reconstruction;

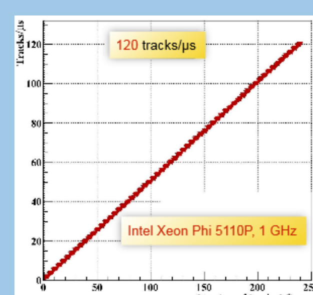


a: $S/Bg_{2\sigma}$, b: Efficiency (%), c: J/ψ per hour (10 Mhz)

	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:

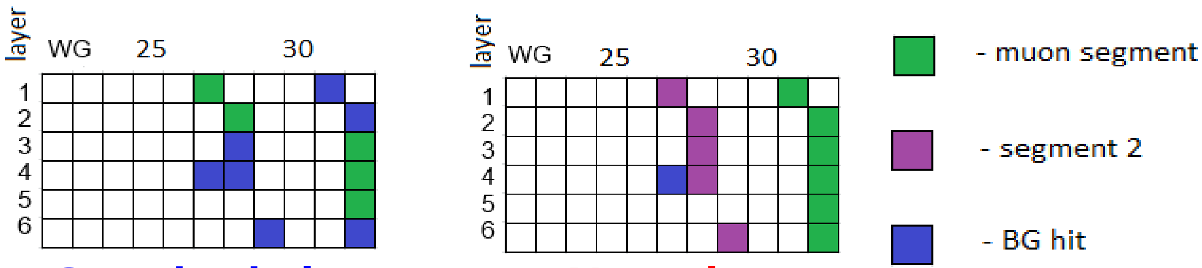
1) Vectorization (SIMD - Single Instruction Multiple Data) factor 2 to 4;
2) Multithreading – factor 4/3 ; 3) υ -Many core processor – factor υ. Total ≈ 4 υ



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.

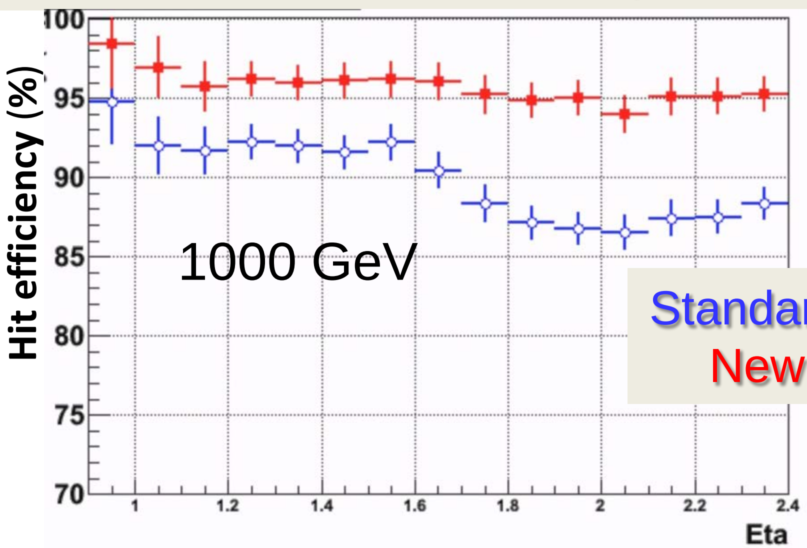
New findings for the Cathode Strip Chamber segment of CMS facility



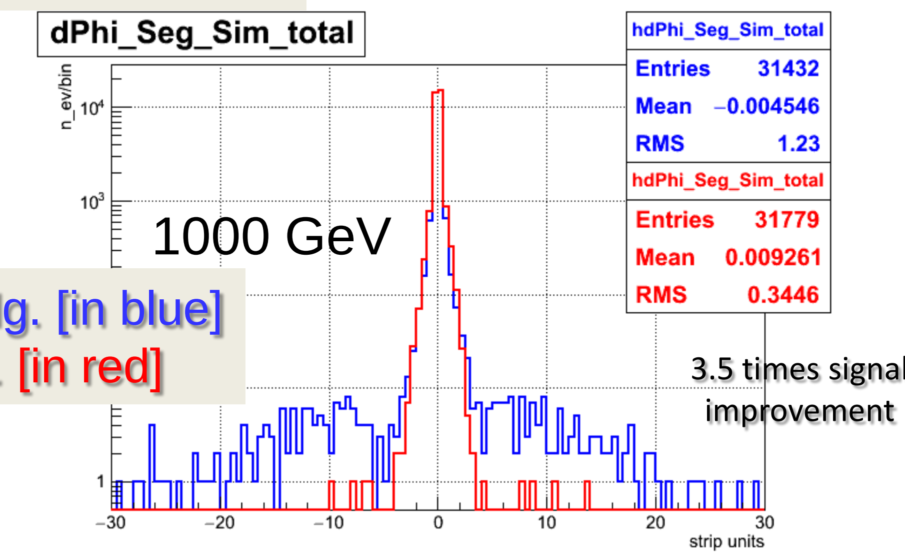
Standard alg. **New alg.**

- The IP is taken into account for non-bend plane view
- Base roads defined for bend-plane view using hits that are furthest apart in z
- Then add additional hits along road

Reported at CERN: 22.04.2015 and 11.05.2015;
the results were included into the CMS Spokesman's plenary talk at CMS week in May, 2015



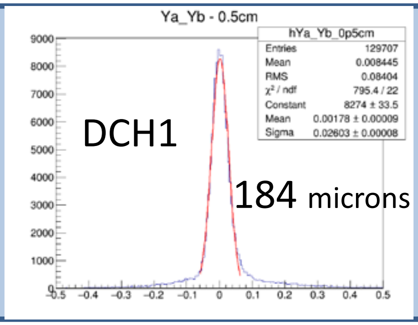
Standard alg. [in blue]
New alg. [in red]

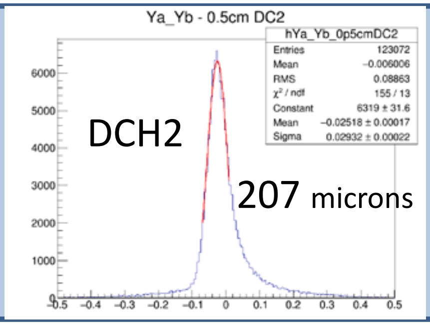


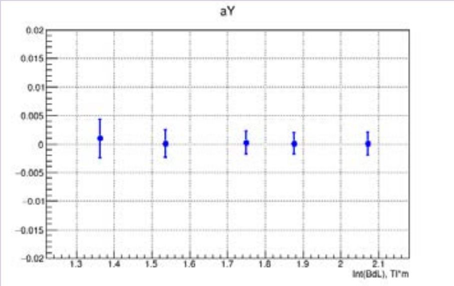
Vladimir Palichik and Nikolai Voytishin; LIT JINR

Track Reconstruction in Drift Chambers (DCH) and Momentum Estimation in BM@N experiment (excerpts)

***BM@N First Test Runs with Nuclotron beams** [February-March 2015]:*
Two DCHs have been used.
The best resolution was obtained for the Y-coordinate

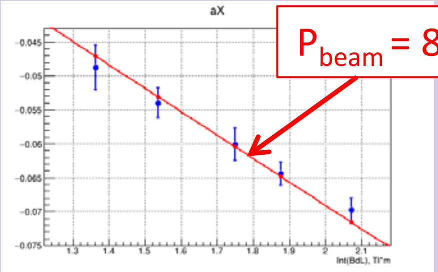






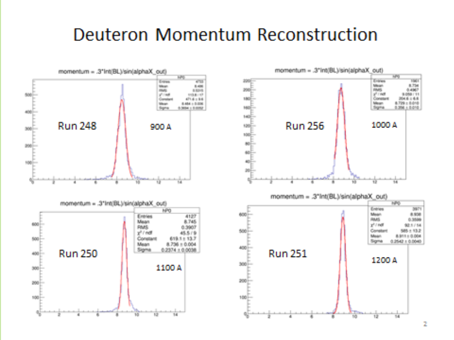
Y-slope is close to zero

***The DCHs have been aligned to the beam** (**track reconstruction with the both DCHs**):*

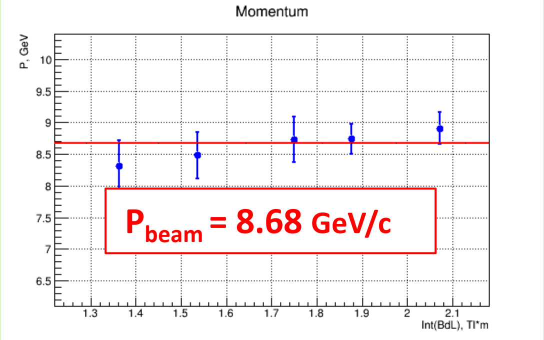


P_{beam} = 8.68 GeV/c

X-slope [extrapolated to magnetic field B=0] is close to zero



Estimation of deuteron beam momentum at different magnetic fields using X-slope



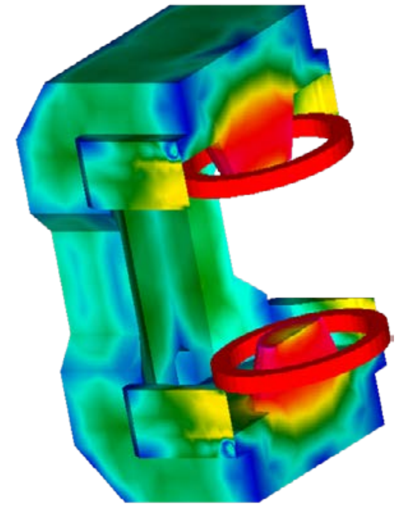
P_{beam} = 8.68 GeV/c

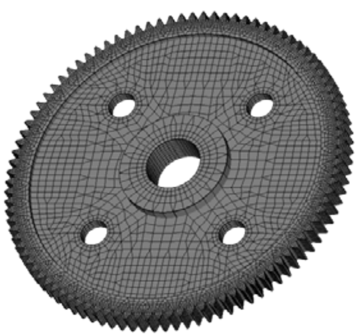
New Approach to Magnetic System Modeling

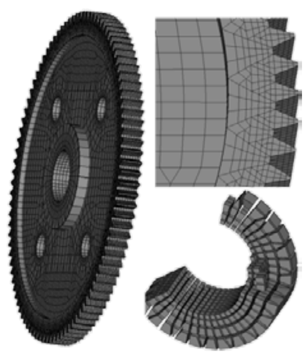
The **volume integral equations method** with integration over discretization elements (DE) was proposed for modeling magnetic systems.

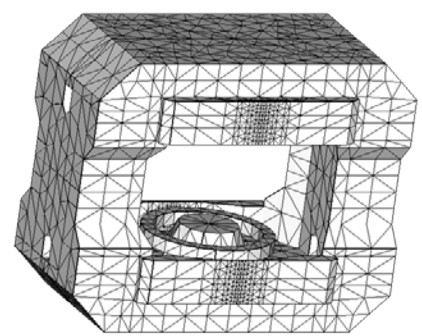
A generator of three-dimensional meshes, which implement the **finite element method**, has been created.

Instances of finite element decompositions are illustrated below.



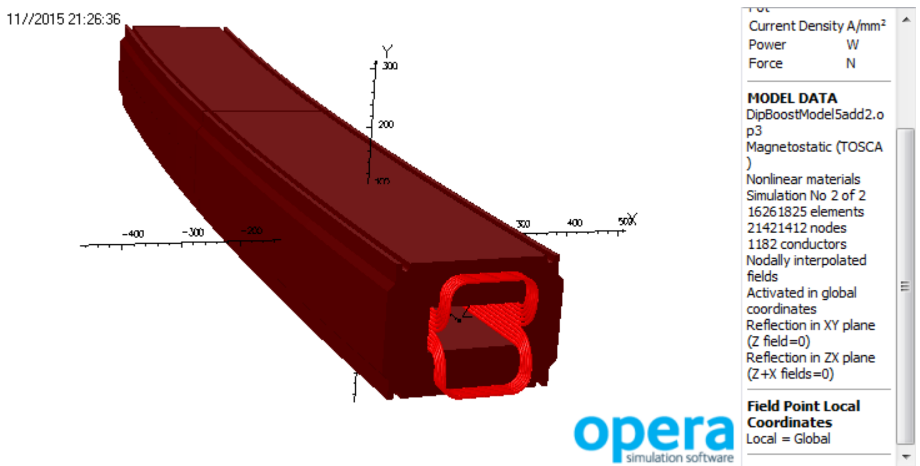




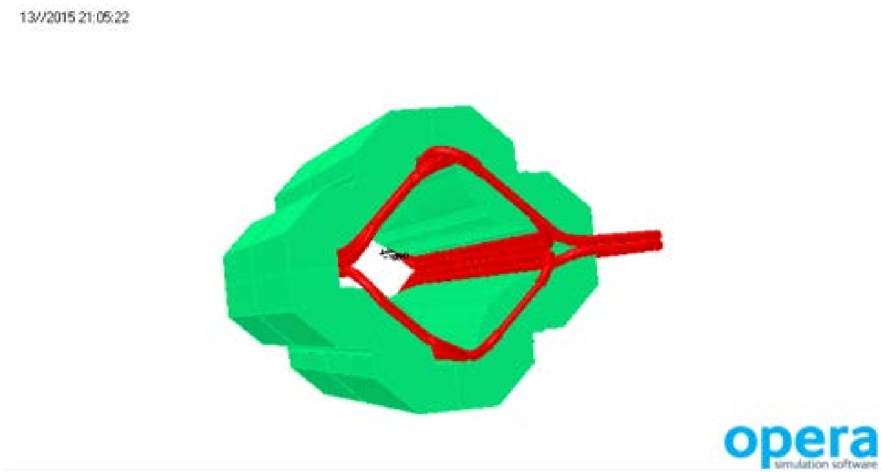


P.G. Akishin, A.A Sapozhnikov, Bull. PFUR, Ser. ®Mathematics.Information Sciences. Physics. 2014, No. 2.

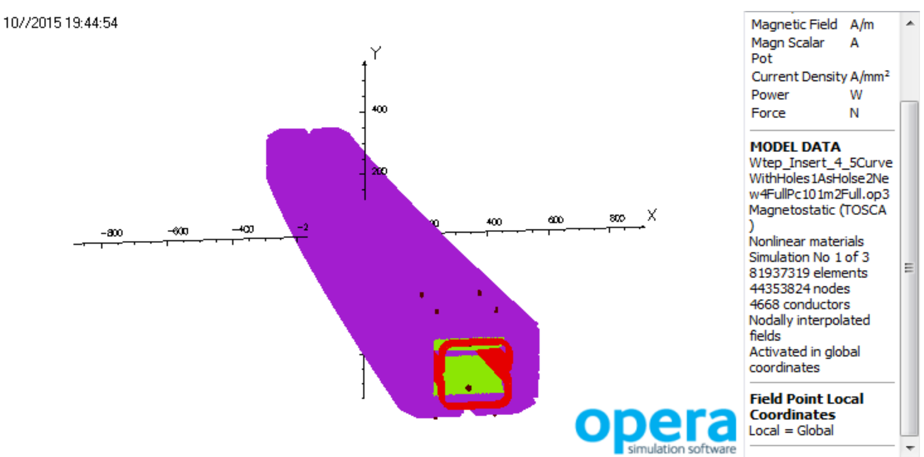
A Few Instances of 3D Magnetic System Modeling



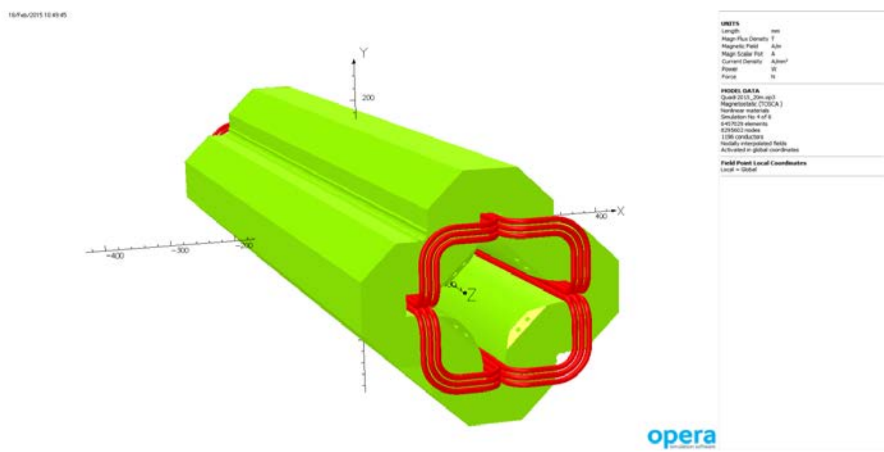
The booster dipole magnet (NICA)



The booster quadrupole magnet (NICA)



The booster dipole magnet of SIS100 (FAIR)



The booster quadrupole magnet of SIS100 (FAIR)

P.G. Akishin, 2015

• New Ways of Reducing Extreme Inner Problem Complexity

– **By developing problem adapted multiscaling algorithms**

[Examples: •• Matrix very ill-conditioning which cannot be tackled within the preconditioning approaches related to the Krylov subspace methods, such as GMRES;

•• Occurrence of unresolved inner isolated discontinuities (e.g., singularities, cusps, finite jumps, etc.) yielding more often than not unreliable numerical solution]

– **By dimensionality reduction**

[Examples: •• Dimension reduction in solving Feynman integrals uses the functional equation approach (developed in LIT) to replace an unsolvable problem by one of super-exponential (factorial) complexity by reducing the number of kinematical variables and masses

⇒ need of supercomputers with huge RAM and special OS]

– **By increasing the number of pivotal points for function expansions**

[Examples: •• In contradistinction to the existing floating point computing dogma, the **three-point basic element method** allows the ***reliable use*** of **high order polynomial expansions** :

= to reliably solve difficult data smoothing problems;

= to get efficient recognition and parametrization of high-dimensional patterns]

– **By embedding the original problem in different approximation space**

[Examples: •• Unified symbolic-numerical solution of boundary-value, resonance, and scattering problems by means of finite element method based on interpolation Hermite polynomials]

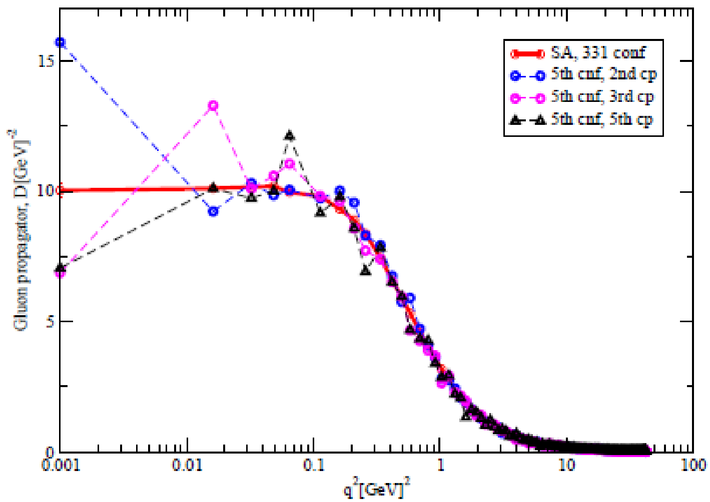
– **By combined use of analytical and numerical approximations**

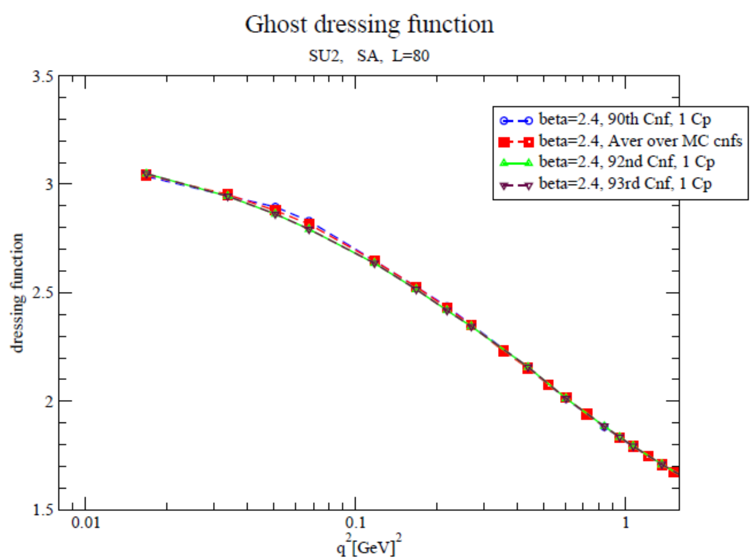
[Examples: •• Symbolic-numeric simulation of slender structures (rods, fibers, cilia, flagella, etc.)

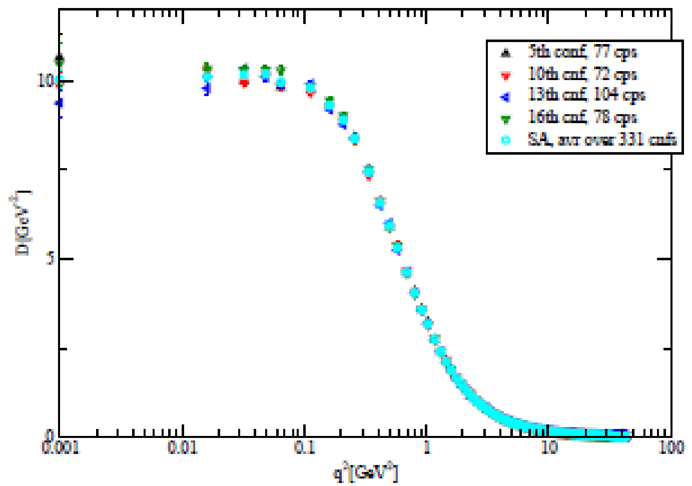
•• Phenomena in Josephson junction stacks]

Suppressing Gribov Noise in Gluon Propagators in Landau Gauge Gluodynamics

Left: Ghost dressing function $J(q^2)$ [at β=2.4, L=80] as compared to $J(q^2)$ averaged over 3 MC configurations
Right up: Gluon propagator $D(q^2)$ [at same β and L] and 3 Gribov copies at a single MC configuration as compared to standard $D(q^2)$ average over 331 MC configurations
Right bottom: Same as Right up, but average taken over many Gribov SA copies for a single MC config.







I.L. Bogolubsky, PoS(Baldin ISHEPP XXII)124, SISSA, ISSN 1824-8039 (2015) http://pos.sissa.it/

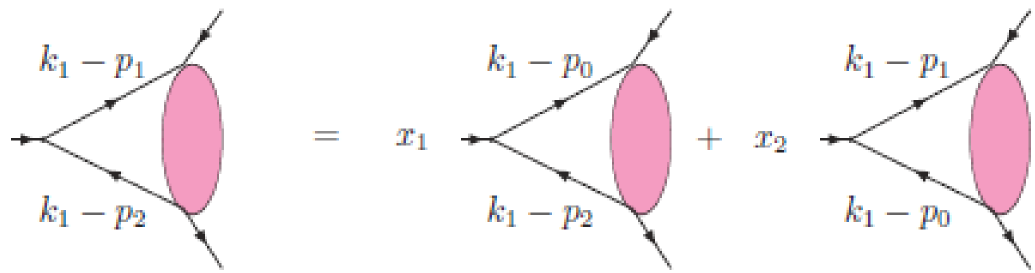
Dimension Reduction in Solving Feynman Integrals

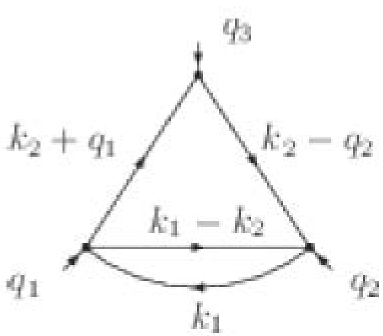
Problem: the analytic-numerical solution of high order **radiative corrections** described by multi-loop Feynman diagrams entering the ***theoretical description of the experimental data from the LHC***

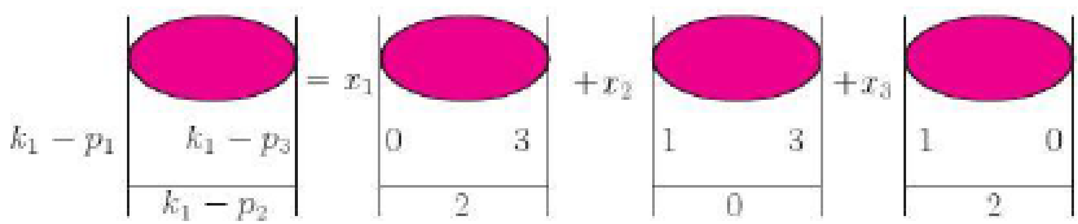
Method: the **functional equation (FE) approach (**developed in LIT) reduces the number of kinematical variables and masses

Computational challenge: FE replaces an ***unsolvable*** problem by one of ***super-exponential (factorial) complexity*** $\Rightarrow$ need of supercomputers with huge RAM and special OS

Instances of functional equations for one-loop (up) and two-loop (down) integrals

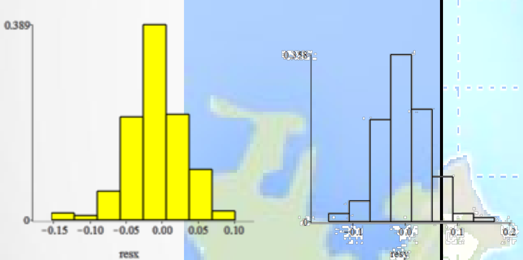


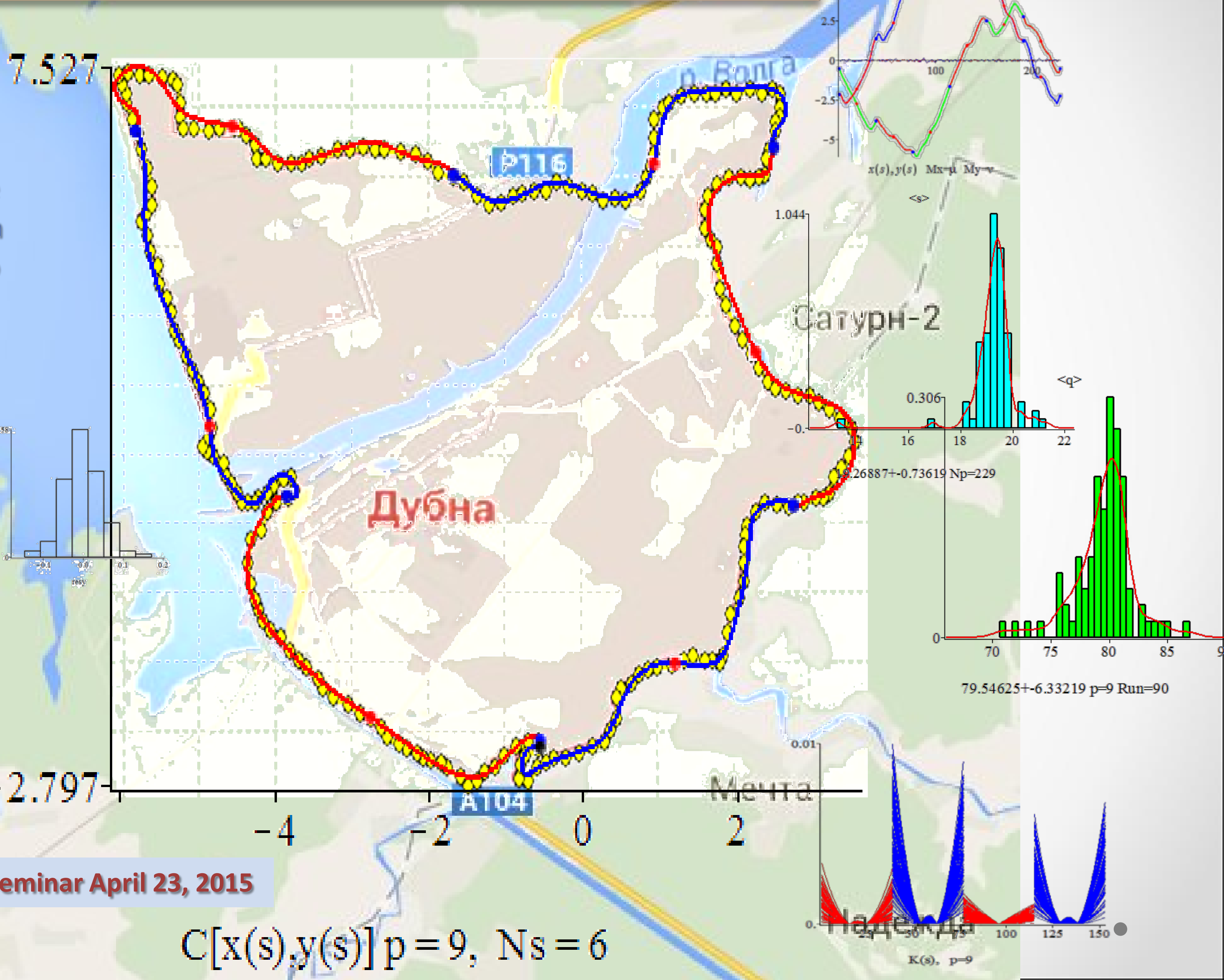




Efficient Recognition and Parametrization of a 2D Pattern

An instance of **parametric** piecewise 12-th order polynomial **smoothing** of the contour line of an object in order to get its **distinctive features**





Resonance tunneling of clusters through repulsive barriers

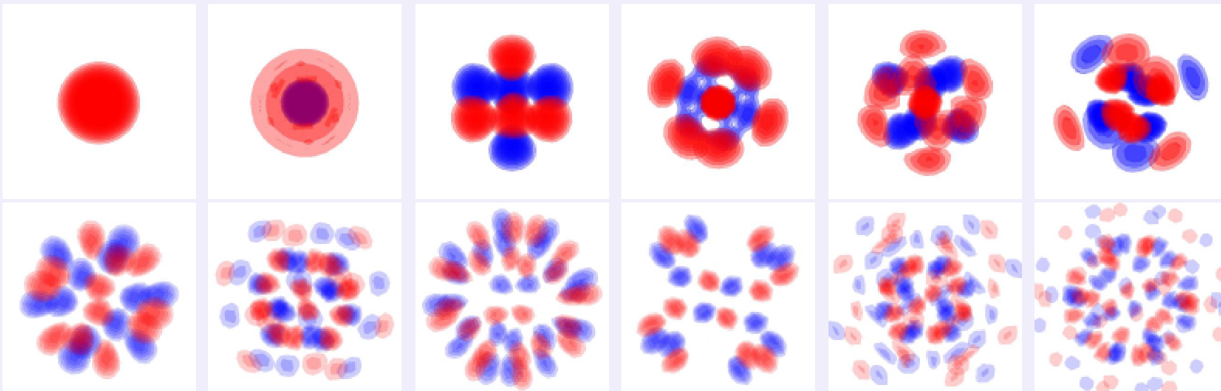


Fig. 1. Profiles of the first six oscillator symmetric (upper) and antisymmetric (lower) eigenfunctions for 4 particles in coordinate frame (ξ_1, ξ_2, ξ_3).

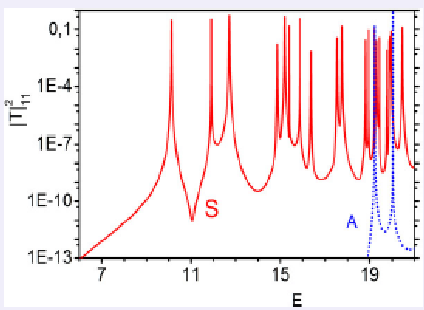
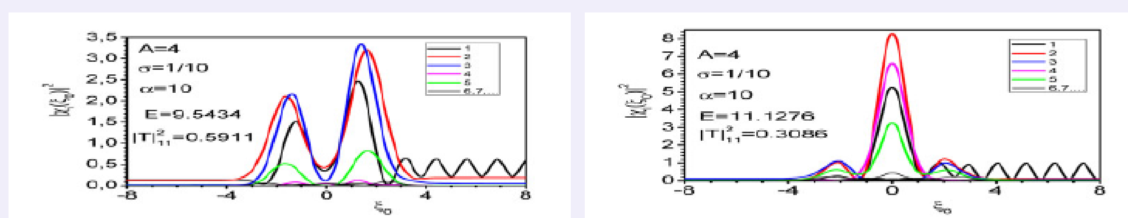


Fig. 2. The transmission coefficient $|T|^2_{11}$ vs collision energy E (osc. u.) of symmetric (S) and antisymmetric (A) states for tunneling of composite system of four identical particles (A=4) on a line with the pair oscillator interactions through narrow repulsive Gaussian barrier $V(x_i) = \alpha/(2\pi\sigma^2)^{1/2} \exp(-x_i^2/\sigma^2)$, $\alpha = 20$, $\sigma = 0.1$.

Fig. 3. The probability densities $|\chi_i(\xi_0)|^2$ of the coefficient functions of symmetric states for transmission of four particles $(\alpha = 10)$.



A.A. Gusev, O. Chuluunbaatar, S.I. Vinitsky, V.A. Rostovtsev (JINR), V.L. Derbov (SSU, Saratov), Int'l Workshop on Computer Algebra, 26-27 May 2015

Solution of boundary-value problems using finite element method with interpolation Hermite polynomials

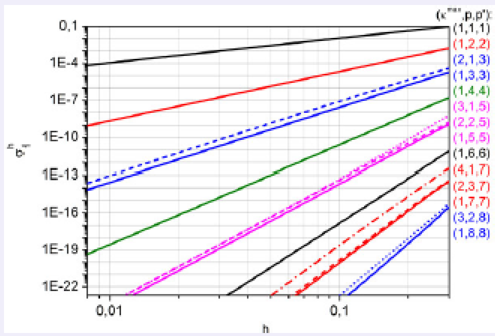


Fig. 1 Absolute error $\sigma_1^h = |\varepsilon_1^{exact} - \varepsilon_1^h|$ for the ground state of Pöschl-Teller potential vs the grid step h calculated using approximation by Interpolation Hermite Polynomials of order p' with different multiplicity of nodes $\kappa^{\max}$ and number of subdomains on a finite element p.

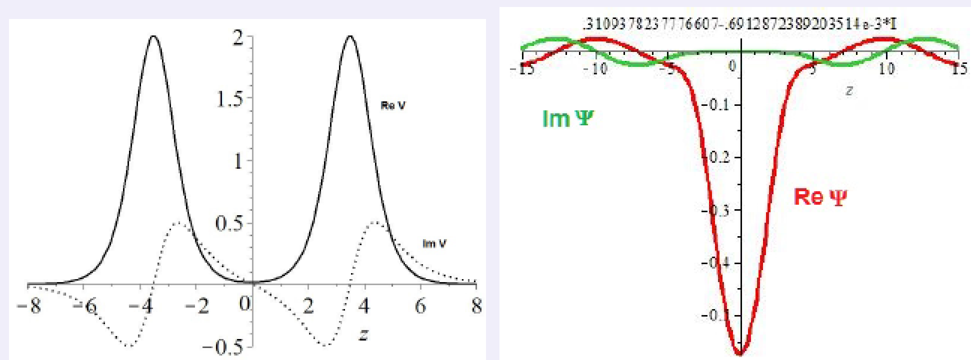


Fig. 2. The system of two complex Scarf potentials (left panel) and the function of resonance metastable state with the energies $2E_1^r = 0.31094 - 0.00069\imath$ (right panel).

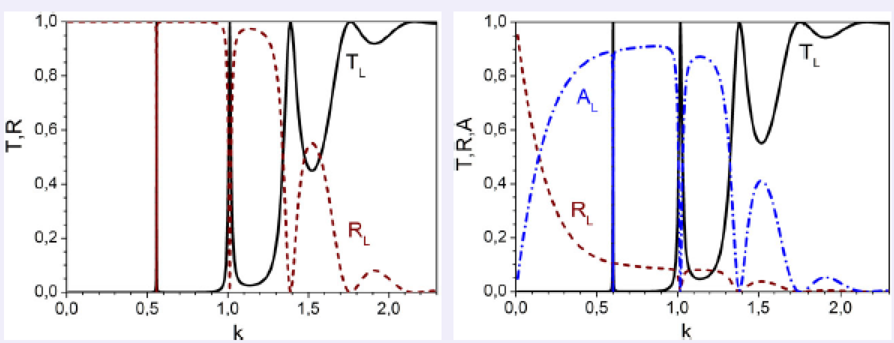


Fig. 3. The coefficients of transmission T_L, reflection R_L, and absorption A_L versus the wave number $k = \sqrt{2E}$ for the systems of two purely real (Pöschl-Teller) potentials (left panel) and complex (Scarf) potentials (right panel).

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

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

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

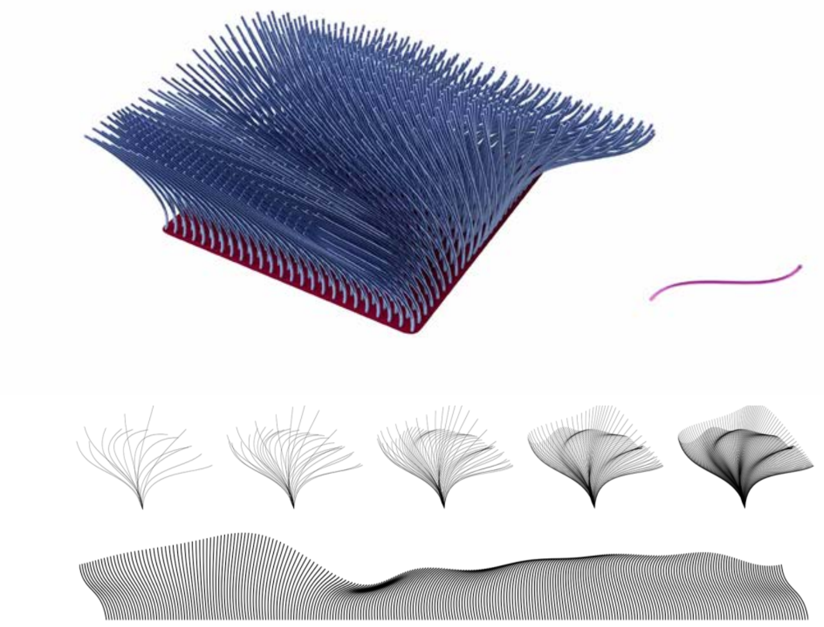
To obviate stiffness, the solution derived by the authors from LIT JINR and HMTI-BAS (Minsk) combined computer algebra and numerical methods: analytical solution of the parameter-free part of the system and numerical for the remaining part.

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.

Animation (video):

http://www.dmichels.de/casc2015/CiliaCarpet.mp4



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

V.Gerdt (LIT JINR), D.Lyakhov (HMTI, Minsk), D.Michels (Compt. Sci. Dept., Stanford Univ. , CA), G.Sobottka and A.Weber (Multimedia, Simulation and Virtual Reality Group, Univ. Bonn). To be publ. in Lecture Notes in Computer Sci. (2015)

• Tackling Complexity Coming from Nonlinearities by Parallel Programming

– Addition of new features (**essentially non-linear**) **to make the models more realistic resulted in outcomes characterized by two essential features:**

●● **Increased computational complexity** asking for **substantially large** CPU time.

●● Occurrence of "natural parallelism" enables easy implementation of parallelization by means of modern programming techniques

[Instances: ●● Modeling **and prediction of hadron properties at finite temperature and density**

●● Modeling **nuclear processes** within **free-parameter-less models**

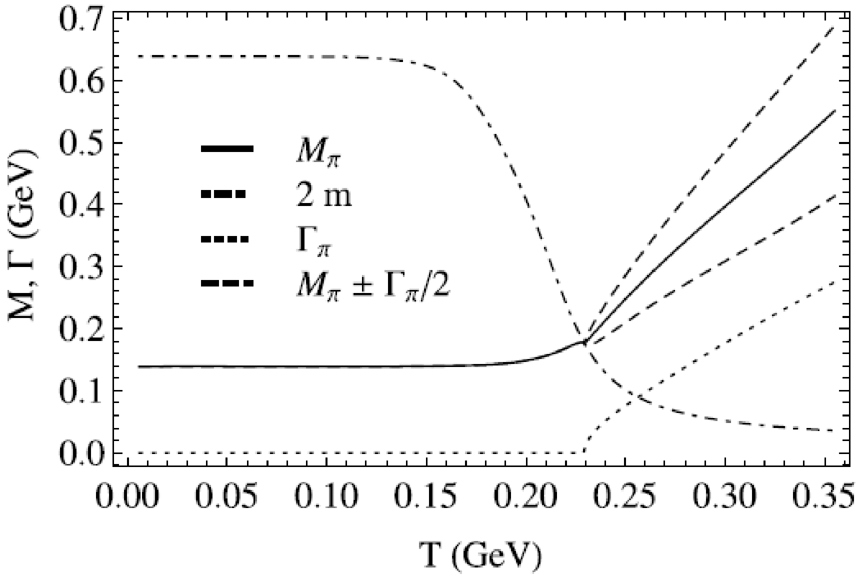
= optical nucleus-nucleus potential computations of elastic scattering and fragmentation processes

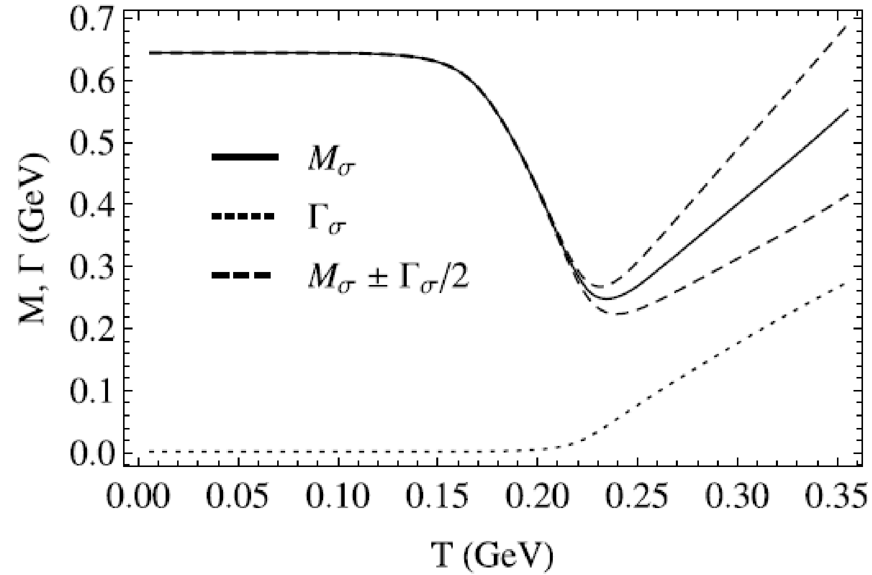
●● Structural analysis of **vesicular systems** from small-angle synchrotron scattering

●● Dynamical model of the hydrated electron (**polaron**)]

●● Accurate numerical solution of the heat propagation processes arising in the interaction of energetic charged particles with materials]

Modeling and prediction of hadron properties at finite temperature and density





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 the meson width $\Gamma_{\pi/\sigma}$

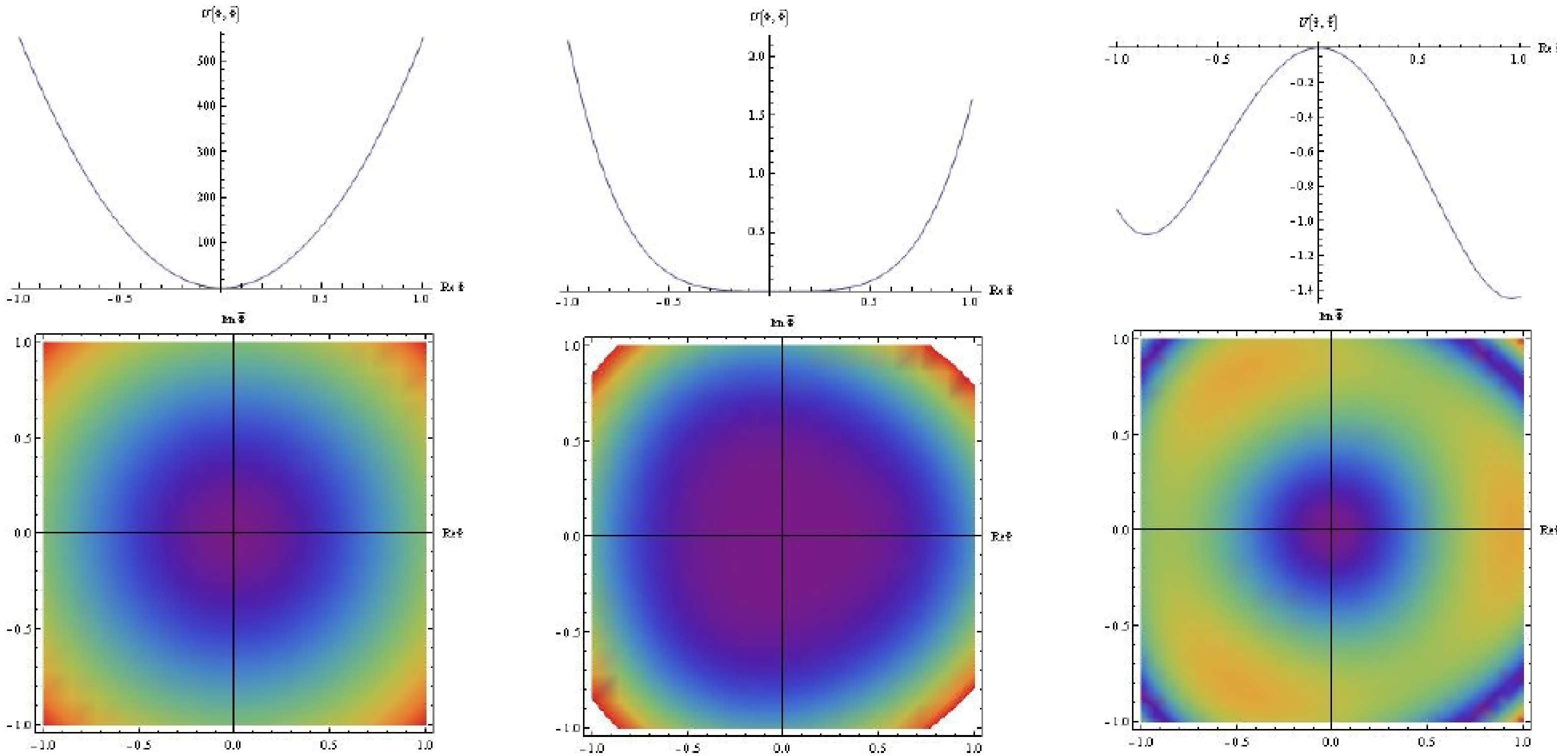
A.V. Friesen, Yu.L. Kalinovsky, V.D. Toneev, Nuclear Physics A 923 (2014) 1–18

Plans: – ***Study of the hadron properties*** in the framework of effective QCD motivated models at finite temperature and density ***in the vicinity of the Mott transition***: wave functions, quadratic radius, hadron dissociations, chemical freeze out.
– Comparison of the results obtained for the chiral fluctuations with those from Lattice Gauge Theory (LGT) modeling and the RHIC and NICA data.

Deconfinement transition description using the Polyakov loop

Hadron – hadron cross sections in the medium taking into account the quark exchange diagrams and box diagrams: damping rates, relaxation time.

[The effect of the medium was implemented through a temperature dependent π-π cross-section in the collision integral which is obtained by including one-loop self-energies in the propagators of the exchanged ρ and σ mesons]



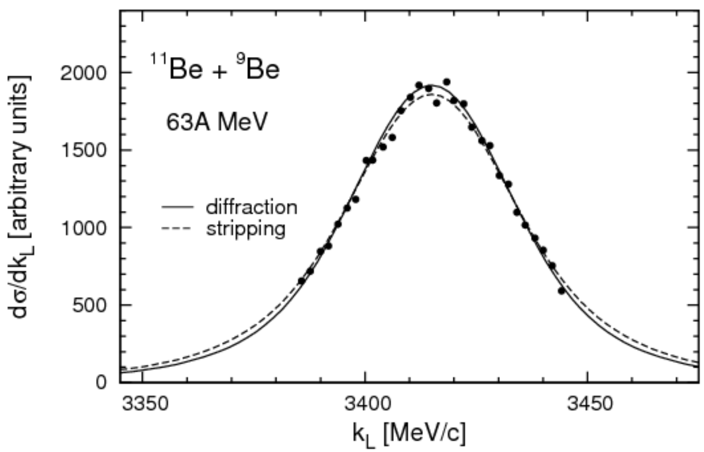
Y. Kalinovsky, (2015)

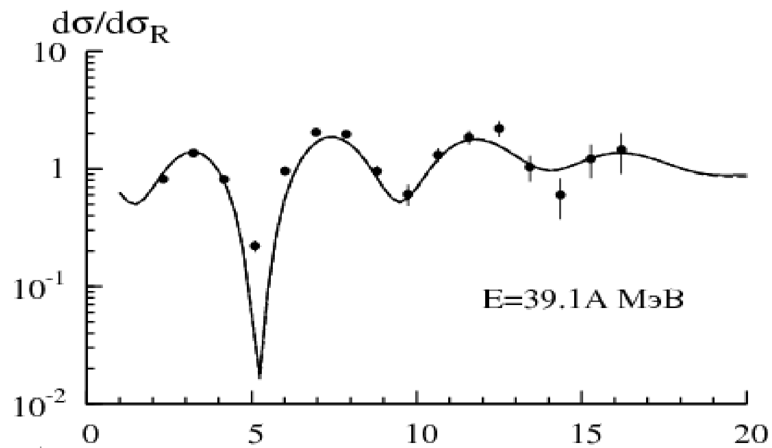
Hybrid Optical Potential Description of Elastic Scattering and Fragmentation Processes

Computer time vs number of processes and discretization N. Calculations on the HybriLIT cluster of the microscopic OP for $^{6}He+^{28}Si$ at 50 Mev/Nucleon.

Number of processes	1	2	4	8	16	32
N=201	1156	399	153	75	66	76
N=401	15697	8106	4098	1745	834	968

Most recent results of analysis of elastic scattering and fragmentation processes of $^{10}Be+^{12}C$ from [Phys. Rev. **C 91** (2015) 034606]

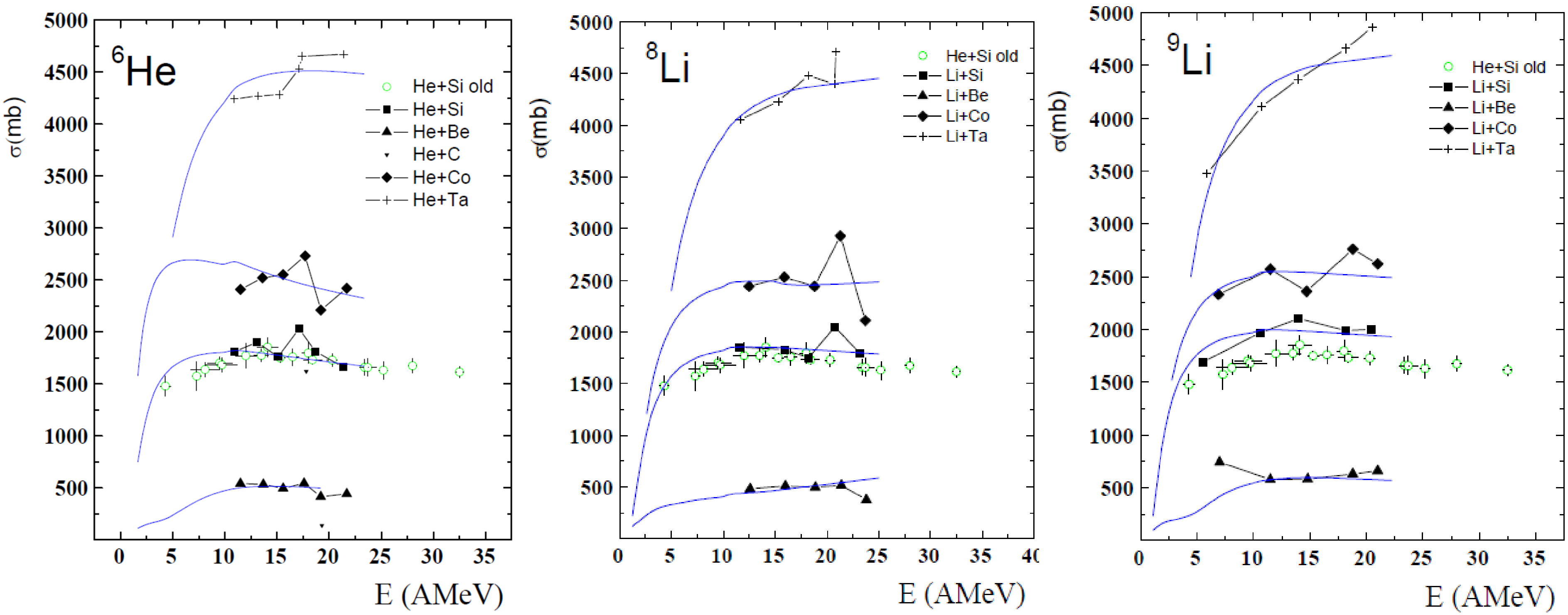




V.K. Lukyanov, D.N. Kadrev, E.V. Zemlyanaya, K. Spasova, K.V. Lukyanov, A.N. Antonov, M.K. Gaidarov, PRC 91, 034606 (2015)

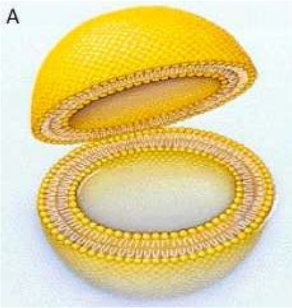
Hybrid Optical Potential Computation of Total Interaction Cross-Sections of Exotic Nuclei

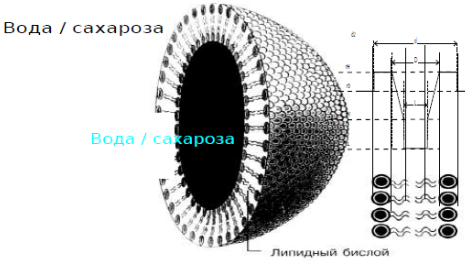
Optical potential computations and comparison with experimental data of total interaction cross-sections of the exotic nuclei ^{6}He and ^{8,9}Li with different nuclei over a large range of energies and masses

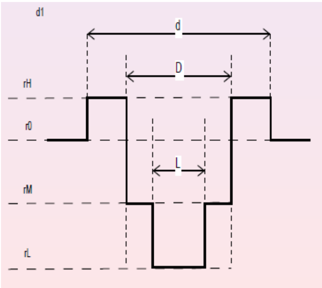


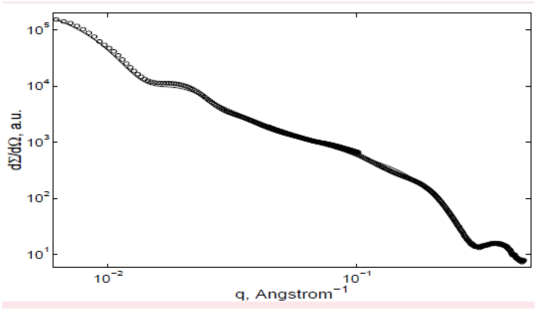
K.V. Lukyanov et al., EXON-2014, to be publ. in the Conference Proceedings (2015)

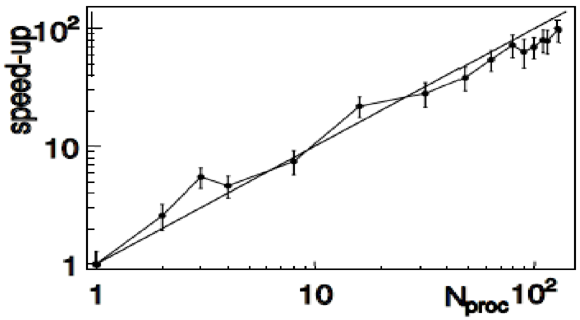
ADE-SFF Structural Analysis of Vesicular Systems

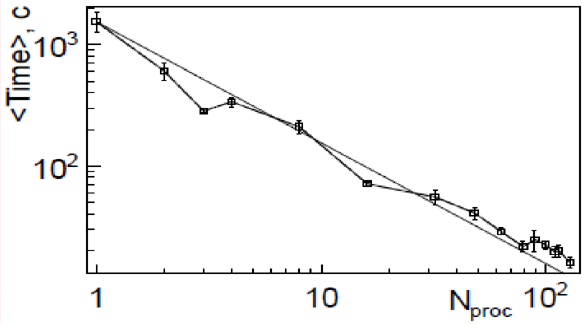












The structure of the ***poly-dispersed lipid DMPC*** (1,2-dimyristoyl-sn-glycero-3-phosphocholine) ***vesicles*** solvated in 40% sucrose solution was investigated.

The method of **Separate Form Factors** (SFF) was modified in order to include the fluctuations of the lipid bilayers and was adapted to the analysis of low-angle scattering of synchrotron radiation data.

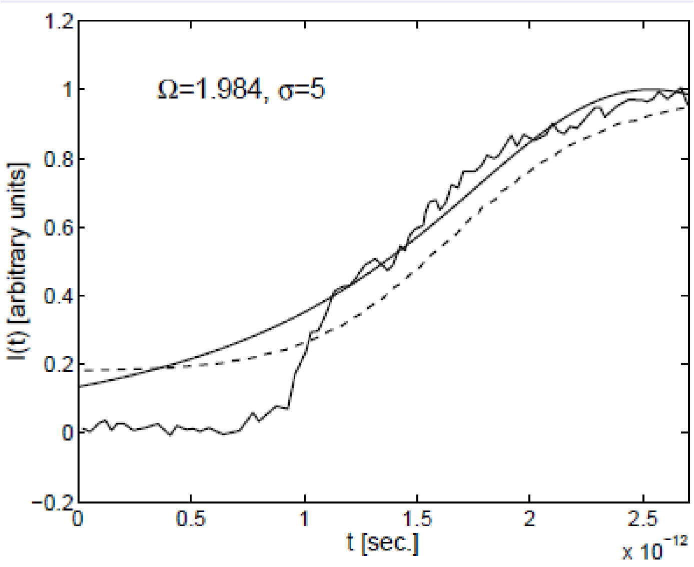
The fitting of the parameters responsible of the vesicular structures was based on the ADE (Asynchronous Differential Equation) algorithm.

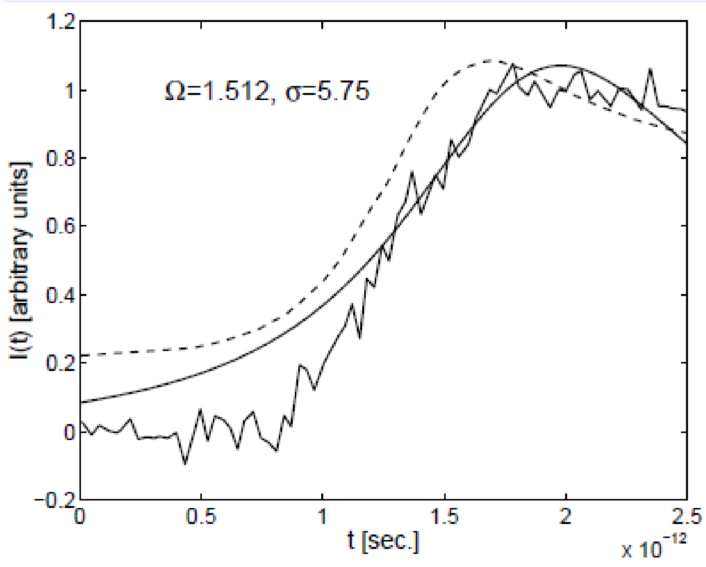
Performance enhancement by the developed MPI/C++ code is shown in the figures.

Plan: Computer ***investigation of vesicular systems*** using the ADE-SFF approach with the aim at ***creating new nano-medical remedies*** (collaboration with FLNP)

М.А.Киселев, Е.В.Земляная, Е.И.Жабицкая, В.Л.Аксенов. Кристаллография, Т.60, вып.1, сс.140-145, 2015

Dynamical model of the hydrated electron (polaron)



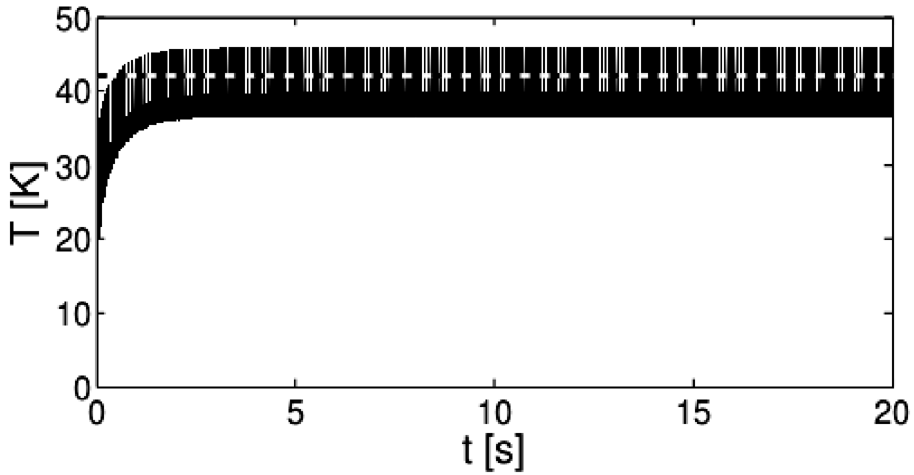


The boundary value problem of the polaron model was formulated and solved using our MPI/C++ code. The comparison of numerical outputs with experimental data (see figures) has shown that the developed model consistently describes the dynamics of the electron photoemission in water under the laser radiation in the ultra-violet range.

Plans: - Numerical investigation of the polaron dynamics in other condensed matter.
- Optimization of the computational scheme, including parallel implementations.
- Improvement of the polaron model by taking into account the time dependence of the width of the absorption band.

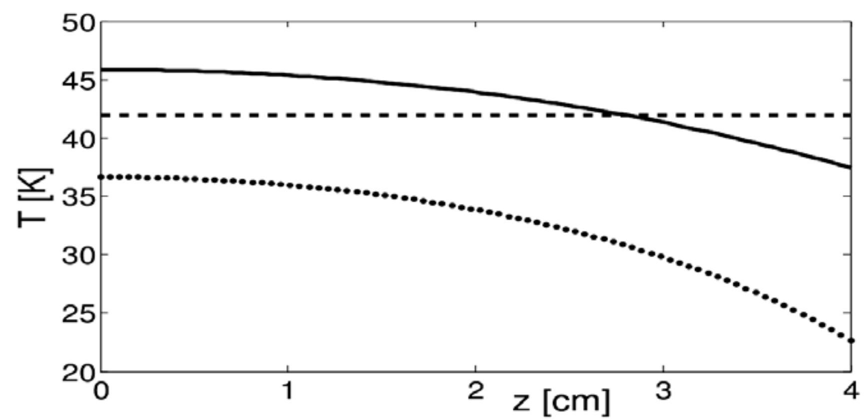
В.Д.Лахно, А.В.Волохова, Е.В.Земляная, И.В.Амирханов, И.В.Пузынин, Т.П.Пузынина. Поверхность, 1, 82-87, 2015

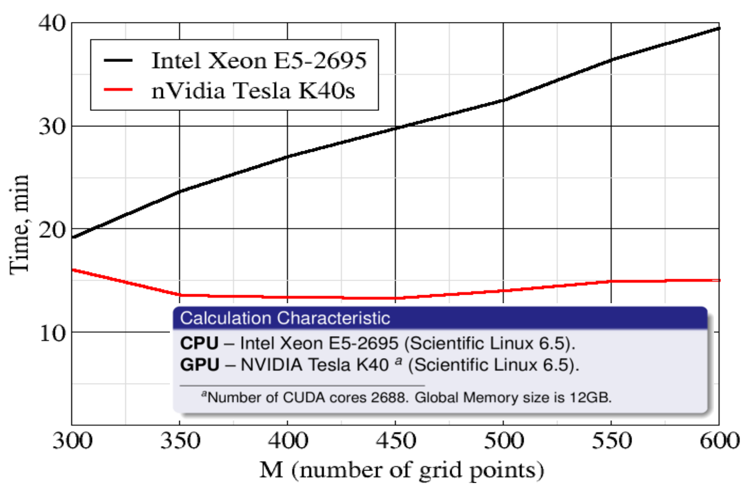
Optimization and Design of an Ion Source Cryogenic Cell



Left: Surface temperature evolution at z = 0 (solid line), critical temperature of the working gas evaporation and condensation (dashed line). The result shows that the initialization time of the cryogenic cell is about 5-10 seconds.

Right: Temperature profile of the stable regimes at moments just before source switching on (dotted line) and source switching off (solid line). The dashed line points to the critical temperature

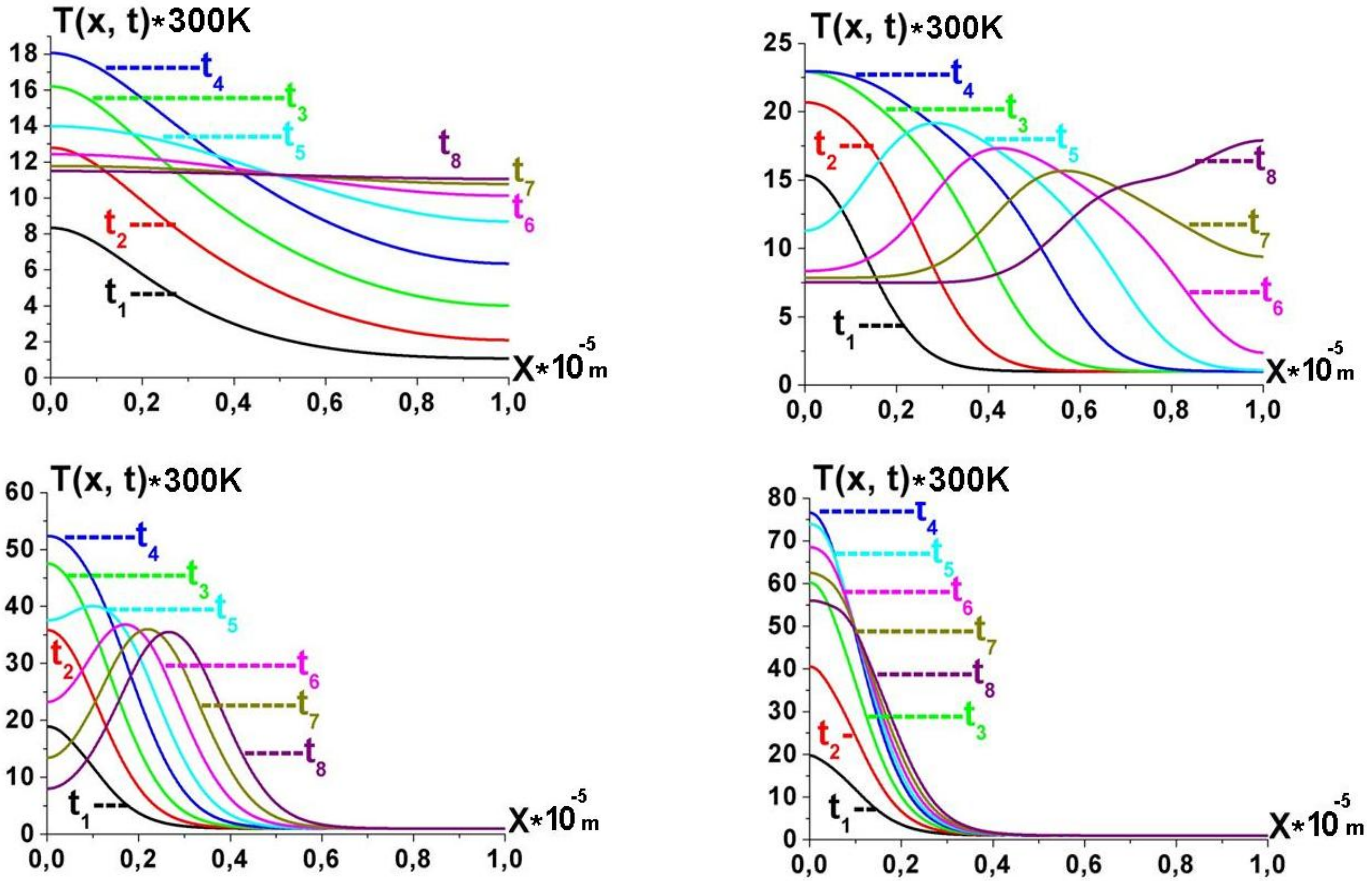




Left: OpenCL GPU implementation of the developed algorithms shows three-times acceleration as compared to the sequential code implementation

A. Ayriyan et al. PFUR Bull. Ser.: Math. Inf. Phys. (2015) 1, 54-60
A. Ayriyan et al. ArXiv:1408.5853

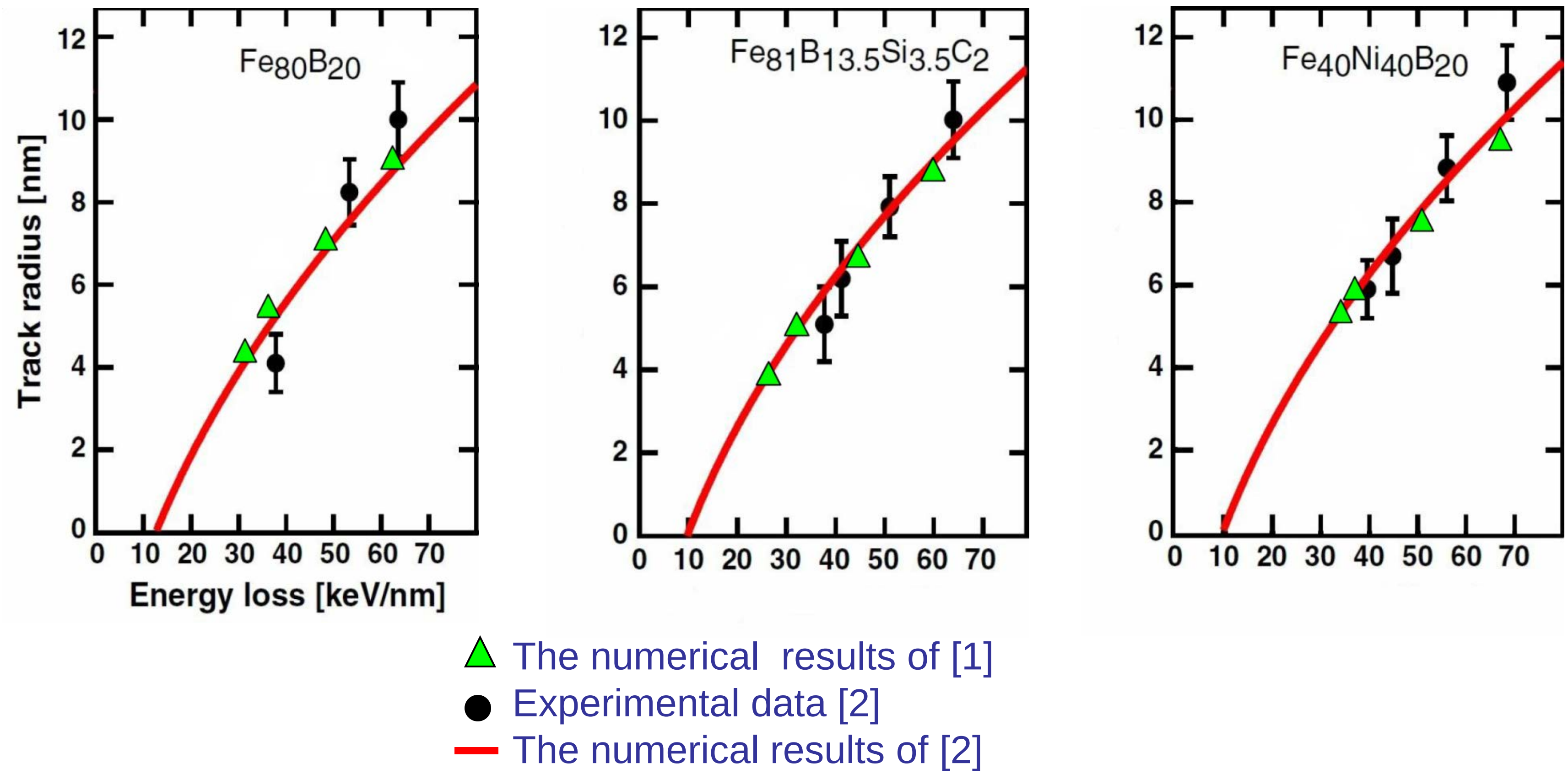
Numerical simulation of thermal processes in materials, with heat equation obeying initial-boundary conditions



Dynamics of temperature profiles for hyperbolic heat conduction equations (τ = 0, 1, 10, 100) at times $t_i = 0.25 \cdot i$ (i=1,2,…,8), where τ stays for the time of relaxation of the heat flux

I.V. Amirkhanov, N.R. Sarker, I. Sarkhadov, Z.A. Sharipov, Z.K. Tukhliev, 2015

Modeling the track formation in amorphous iron alloys exposed to high-energy heavy ion bombardment



[1] I.V. Amirkhanov, A.Yu. Didyk, I.V. Puzynin, T.P. Puzynina, N.R. Sarker, I. Sarkhadov, Z.A. Sharipov, Z.K. Tukhliev, to be publ.
[2] M.D. Rodriguez, B. Afra, C. Trautmann, et. al., Journal of Non-Crystalline Solids 358 (2012) 571-576.

• Numerical Studies of Physical Processes in Exotic Materials

[Instances: •• **Studies of Bose-Einstein condensates**

= Self-consistent theory of Bose-Einstein condensate of **cold atoms in traps and optical lattices**

= Analysis of critical properties of Bose-condensed systems close to the point of phase transitions

= Numerical investigation of strongly nonequilibrium condensates in traps with modulated potentials

= Self-similar approximation theory and scale separation approach for an accurate description of properties of cold bosons in traps

•• **Coherent radiation and fast magnetization reversal in magnets with exchange interactions**

= Applications to **graphene**, **graphite**, **carbon nanotubes**, and related materials

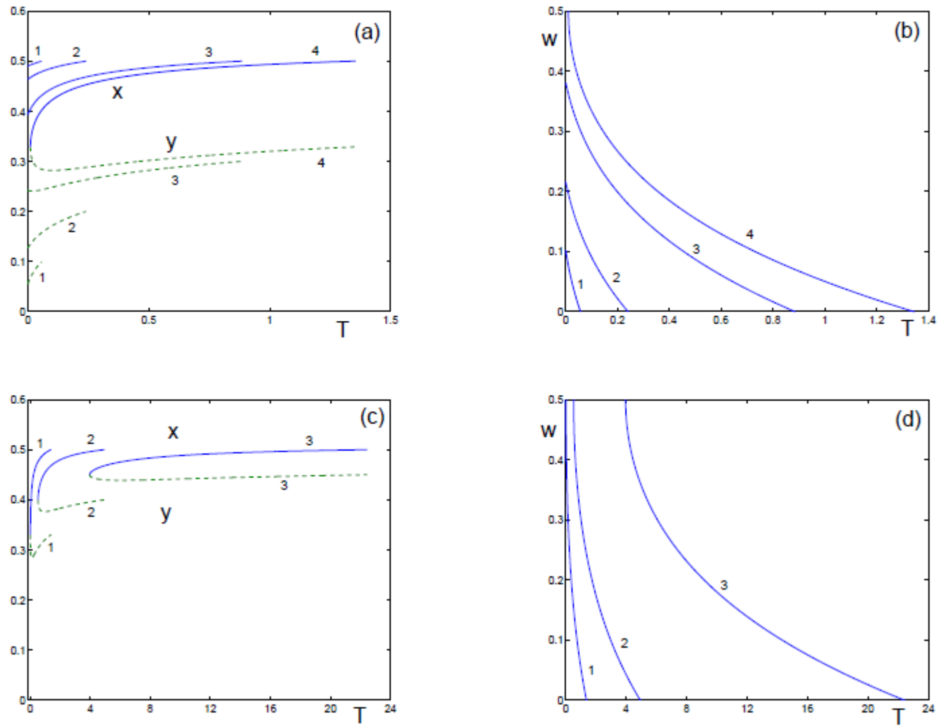
•• **Modeling electromagnetic and thermal processes in superconductors**

= Study of the quench behavior of **MgB_2 conductors** optimized for use in high current transfer lines: work is requested within the **planning upgrade of the LHC machine** at CERN.]

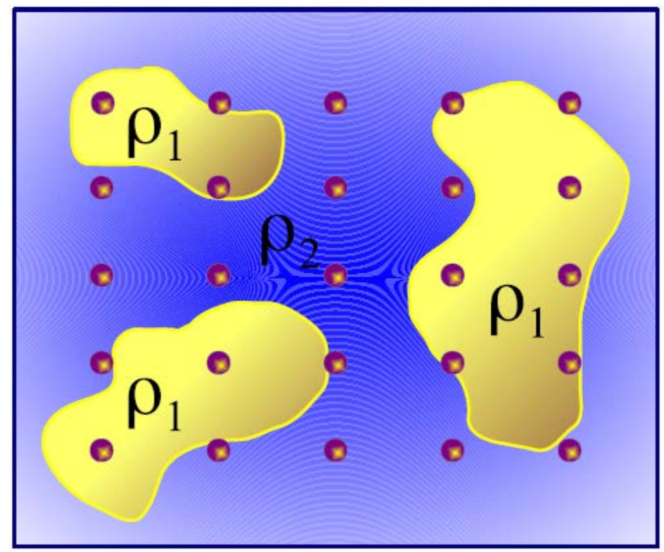
Optical lattice with heterogeneous atomic density

Problem: The formation of heterogeneous states in optical lattices characterized by a spontaneous mesoscopic separation into spatial regions with different atomic densities.

Numerical result: Such states can arise if there are repulsive interactions between atoms in different lattice sites and the filling factor ν is less than one-half.



Snapshot of a heterophase two-density lattice system. Regions of higher density ρ_1 are randomly immersed into the matrix of lower density ρ_2, with $\rho_1 > \rho_2$.



Solutions as functions of the dimensionless temperature T for different filling factors:

(a) order parameters x (solid line) and y (dashed line) for $\nu=0.1$ (line 1), $\nu=0.2$ (line 2), $\nu=0.3$ (line 3), and $\nu=0.328$ (line 4);

(b) dense-phase probability w for the same filling factors and enumeration as above;

(c) order parameters x (solid line) and y (dashed line) for $\nu=0.33$ (line 1), $\nu=0.4$ (line 2), and $\nu=0.45$ (line 3);

(d) dense-phase probability w for the same filling factors and enumeration as in (c).

V.I. Yukalov and E.P. Yukalova, Laser Phys. 25 (2015) 035501

Investigation of the Quench Behavior of MgB_2 Conductors Optimized for Use in High Current Transfer Lines

S. Giannelli‡, G. Montenero‡, A. Ballarino‡, B. Bordini‡, A. Chervyakov+

‡CERN - European Center for Nuclear Research, Geneva, Switzerland, +JINR - Joint Institute for Nuclear Research, Dubna, Russia

The context: MgB_2 trasfer lines and superconducting links

MgB_2 conductors have been proposed in recent years for the development of high-current electric transfer lines. **Helium gas-cooled MgB_2 cables** are being developed and tested at CERN in the framework of the Superconductig Link project as part of the High-Luminosity upgrade of the LHC[1].

A **20m-long, 20kA MgB_2 cable** has been **successfully tested** in the Superconducting Link Test Station at CERN[2]. The performance of the cable in the temperature range 20-35 K is in accordance with the expected critical current values as calculated from the short-sample properties, indicating a fair homogeneity of the conductor properties over long lengths as well as no major degradation induced by the cabling process. The cable was also a demonstator for a power transmission line studied in the framework of a collaboration agreement between CERN and IASS[3].

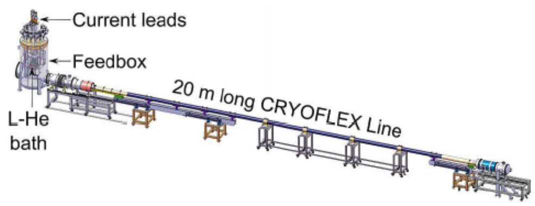
In parallel to the ongoing R&D activities concerning conductor development, cabling processes and installation issues, attention is being paid to the problem of the quench protection of these lines. The design of a reliable and yet practicable **quench protection** system requires a deep understanding of the thermo-electrical stability properties of the conductor, at the wire as well as at the cable level. Both experimental and modelling activities are being performed in order to assess the quench behaviour of MgB_2 wires and cables.

References

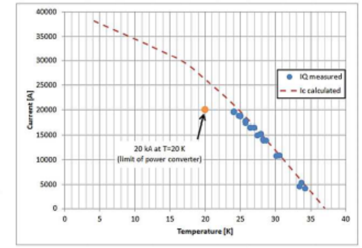
[1] Ballarino A, Development of Superconducting Links for the LHC Machine, Supercond. Sci. Technol. 27 044024, 2014

[2] Giannelli S, Ballarino A, Bordini B, Hurte J, Jacquemod A, First Measurement of MgB2 Cables Operated in Helium Gas Up to 35K, *Cern Internal Note*

[3] www.iass-potsdam.de/research-clusters/earth-energy-and-environment-e3/scientific-program/long-distance-energy-transport

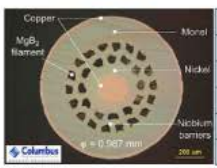


20kA MgB_2 cable successfully tested in February 2014 in the Superconducting Link Test Station at CERN



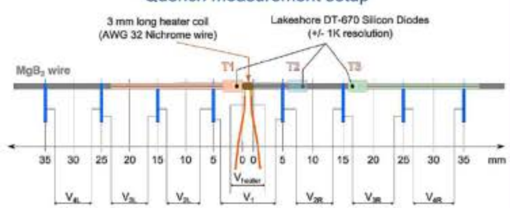
Quench propagation tests on MgB_2 wires

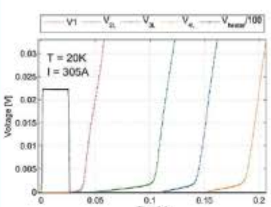
MgB_2 wire

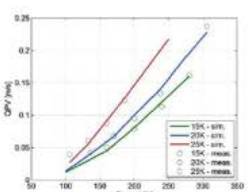


Material	%
MgB_2	9.6
Copper	12.4
Nickel	24.8
Monel	41.2
Niobium	12

Quench measurement setup

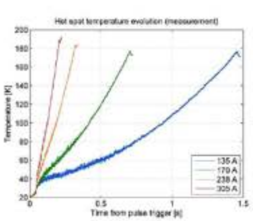


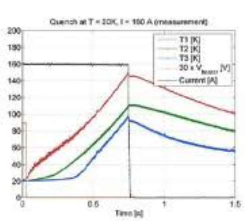


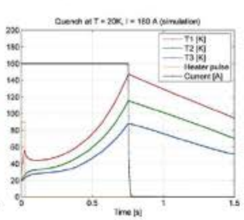


Quench propagation velocities

Quench propagation velocities have been measured by the time-of-flight method based on the voltage traces. The measured values have been compared with the results of a 1D, fully nonlinear electro-thermal model of a single wire.



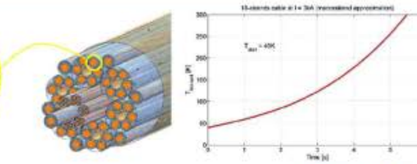




Contact resistances in MgB_2 cables with copper core stabilization

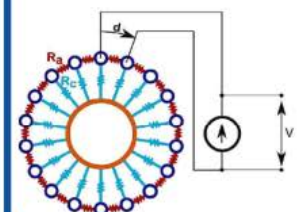
The problem

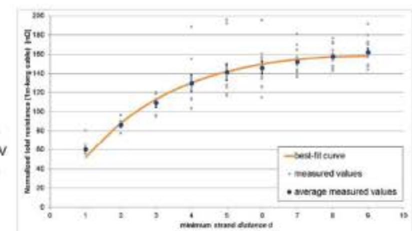
- In LHC the time constant for current decay is fixed by the magnet string: 1-3 s → need for external stabilization
- The quench load of a cable with 12 mm^2 Cu core is sufficient to limit the hot-spot temperature to acceptable values in the *macrostrand* approximation **but** good current sharing is required → depends on contact resistances



Methodology

- The total resistance R_{tot} between strands used for current injection is measured
- Varying the minimum strand *distance* **d** between the chosen strands, a curve $\mathbf{R_{tot}(d)}$ is obtained which implicitely depends on $\mathbf{R_a}$ and $\mathbf{R_c}$
- An electrical model (Simulink) of the cable has been built and R_a, R_c have been calculated by a least-square fit of the measured $\mathbf{R_{tot}(d)}$ curve via a nonlinear optimization routine (Matlab)





Best-fit values (1m-long cable)	
R_a	63.5 nΩ
R_c	472.6 nΩ
Normalized conductance	
G_a	$1.57 \cdot 10^7\ (\Omega m)^{-1}$
G_c	$2.12 \cdot 10^6\ (\Omega m)^{-1}$

Multi-strand model of quench in cables (...work in progress)

- The 1D model of a strand is used as the building block for a multi-strand quench model of cables
- Full thermal, electric and magnetic coupling between the different electrical/thermal elements (strands, cores) is considered
- Investigations will be performed of the effectiveness of current sharing with the Copper core (using measured G_a, G_c) and of the electromagnetic/thermal coupling of different electrical lines sharing the same cryostat

• Developments in Computer Algebra and Quantum Computing

– **New approaches to the derivation of involutive Groebner bases**

[Tasks: •• Down-up approach to the derivation of compact bases;

•• Parallel algorithms for the construction of compact involutive bases;

•• Generation of finite difference schemes inheriting the algebraic properties of the ancestor partial differential equations;

•• Numerical algorithm applications to the analysis of low dimensional nanostructures and other composite quantum systems in molecular, atomic and nuclear physics]

– **Modeling and control of quantum information processes**

[Tasks: •• Entanglement description in systems of qubits as the main resource in quantum information and communication;

•• Study of systems of charged particles under strong laser radiation;

•• Modelling quantum dynamics of elementary particles and nuclei interacting with strong laser radiation. Proposals for the European project “Extreme Light Infrastructure (ELI)”, Prague (Chezh Republic) and Măgurele (Romania)]

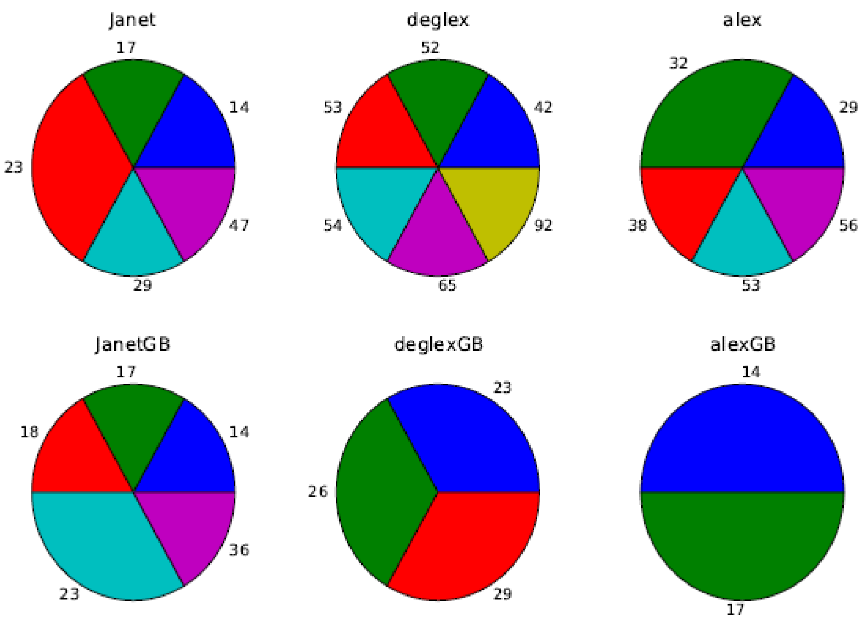
– **Design of algorithmic methods of discrete quantum mechanics**

[Tasks: •• Description of quantum gates;

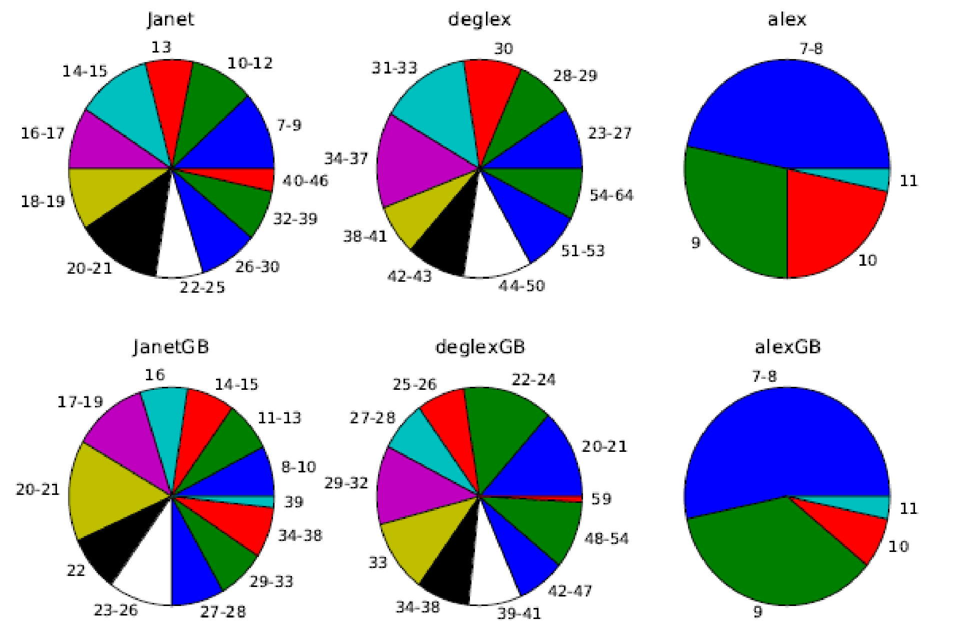
•• Applications to quantum information processes]

$\succ_{alex}$ – a compact involutive basis

Completion of $\{\, x_1^{10}, x_1^7 x_2, x_1^4 x_2^2, x_1 x_2 x_3^3, x_2^4 \,\}$



Completion of $\{\, x_1^2 x_2^2 x_5, x_2^2 x_3 x_5, x_2 x_4, x_3^2, x_3 x_4 x_5^2 \,\}$



Computational superiority of $\succ_{alex}$ -division over Janet division follows from:

= a smaller number of nonmultiplicative prolongations

= a higher stability under permutation of the variables

Description of entanglement space of 2-qubit states

Nonlocal quantum correlations (***entanglement***) ***of quantum states*** is the main resource of quantum computation, information and communication. Its understanding ***is an open problem***.

Example : 3-paramer family of 2-qubit density matrices

$$\rho = \frac{1}{4}\begin{pmatrix} 1+\alpha & 0 & 0 & 0 \\ 0 & 1-\beta & i\gamma & 0 \\ 0 & -i\gamma & 1+\beta & 0 \\ 0 & 0 & 0 & 1-\alpha \end{pmatrix}$$

PG-criterion of separability →

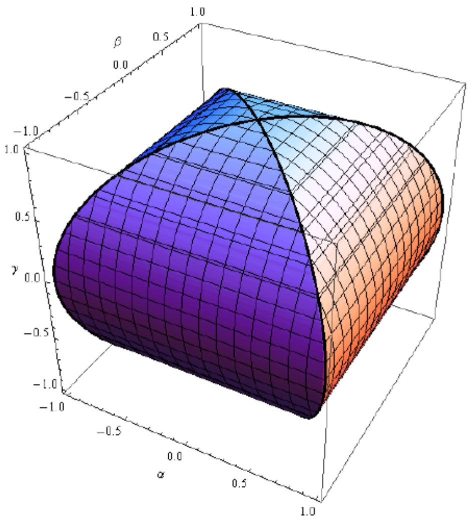
Separable states

$$\alpha^2 \le 1, \quad \beta^2 + \gamma^2 \le 1$$

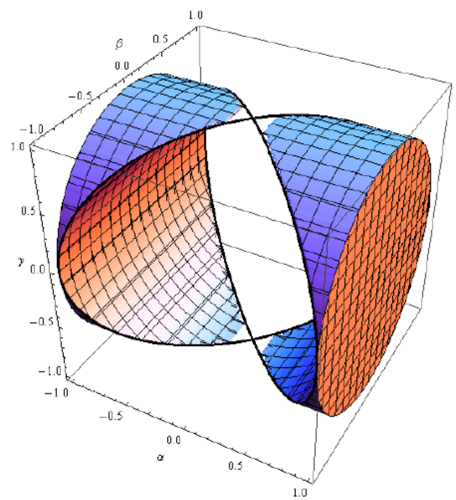
and

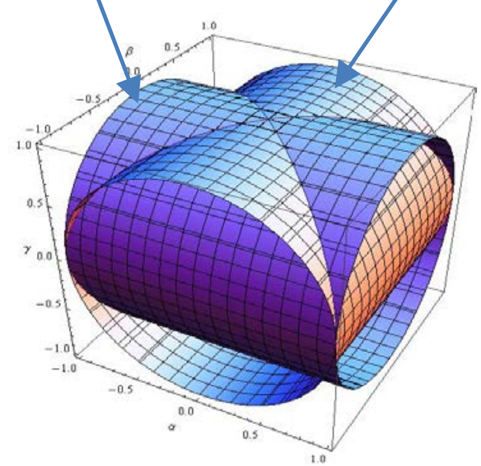
$$\beta^2 \le 1, \quad \alpha^2 + \gamma^2 \le 1$$

Separable states



Entangled states

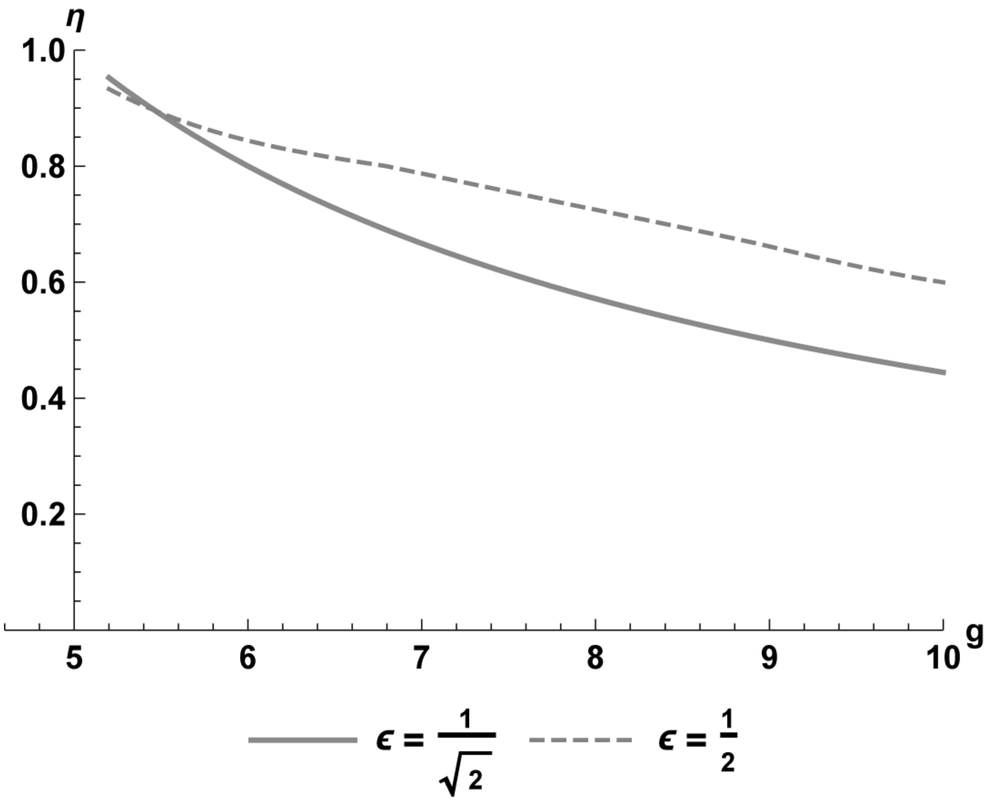




V.P. Gerdt, A. Khvedelidze, Yu. Palii, Phys. Atom. Nucl. 74, 6 (2011), 893--900 ; Zapiski POMI RAN 432, (2015), 111--126

Systems of charged particles under strong laser radiation

The modelled locus of points of (dimensionless) intensity (η) in terms of polarization (ε) and gyromagnetic ratio (g) for which the spin-flip resonance occurs



Perspective Developments: are of interest for the European project *"Extreme Light Infrastructure* (ELI)", Prague (Czech Republic) and Măgurele (Romania)

A. Khvedelidze, I.A. Rogojin, Mathematical Modelling 27, 7 (2015) , 118-125

● HybriLIT Based Future Software Developments

– **Efficient parallel computing** on the heterogeneous hybrid cluster **HybriLIT**

[Tasks: ●● Development of a user friendly information-computing environment enabling efficient exploitation of the HybriLIT Intel parallelism and NVIDIA-CUDA parallelism, respectively;

●● Deriving new HybriLIT-adapted methods and algorithms able to effectively solve topics of the highest interest for the JINR research projects;

●● Development of a HybriLIT-based parallel computing library of wide interest to the JINR users;

●● Infrastructure development for tutorials on parallel programming techniques]

– **Hybrid Programming Based Cross-Platform Software Implementing the MultiConfigurational Time Dependent Hartree (for) Bosons** (**MCTDHB**) **Method**

[●● Method founders: **Lorenz S. Cederbaum, Ofir E. Alon, Alexej I. Streltsov**

●● Main Implementation: **Many-body theory of bosons group in Heidelberg, Germany** http://MCTDHB.org

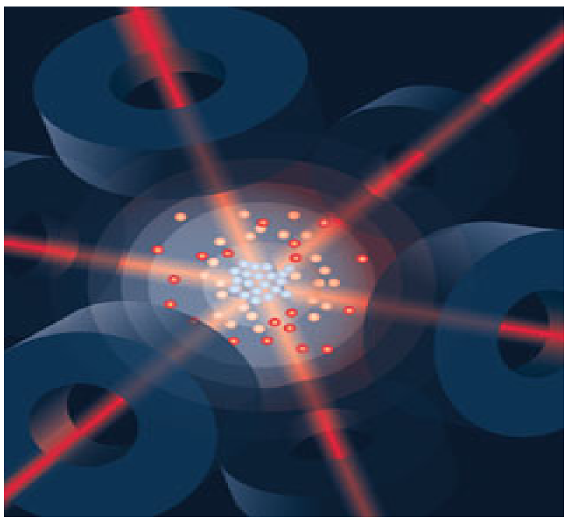
●● **Hybrid Programming**: MPI+OpenMP, MPI+OpenMP+CUDA **done at LIT-JINR since 2013**

●● User Friendly GUI **MCTDHB-Lab** is **under development** (**Univ. Heidelberg + LIT JINR**).
This is a free-for-download cross-platform software working on Mac, Windows and Linux]

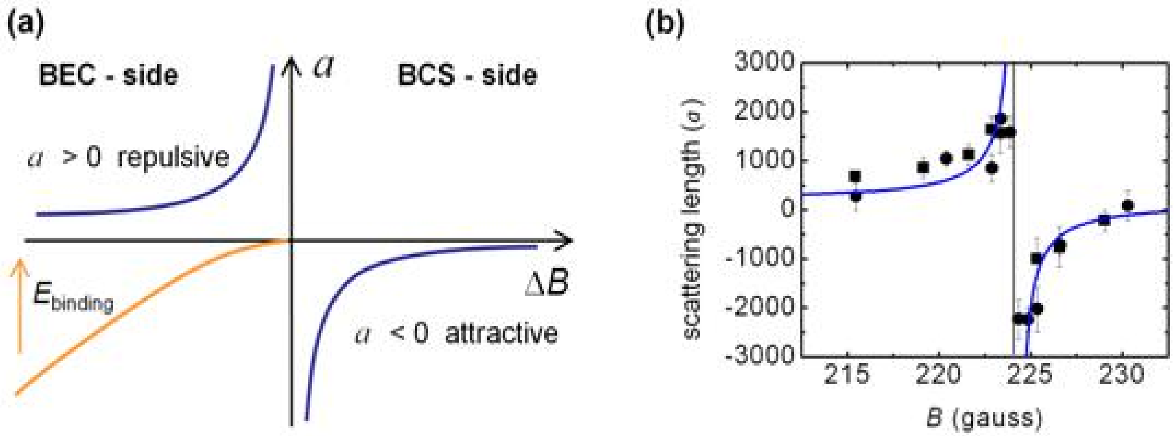
MultiConfigurational Time Dependent Hartree (for) Bosons

$$\hat{\mathbf{H}} = \sum_{i=1}^{N}\left(-\frac{1}{2m}\nabla_{\vec{r}_i}^2 + V(\vec{r}_i;t)\right) + \sum_{i<j}^{N}\lambda_0 W(\vec{r}_i,\vec{r}_j;t)$$

BECs of alkaline, alkaline earth, and lanthanoid atoms
(^{7}Li, ^{23}Na, ^{39}K, ^{41}K, ^{85}Rb, ^{87}Rb, ^{133}Cs, ^{52}Cr, ^{40}Ca, ^{84}Sr, ^{86}Sr, ^{88}Sr, ^{174}Yb, ^{164}Dy, and ^{168}Er)



Magneto-optical trap $\longrightarrow \mathbf{V}(r,t)$



The interatomic interaction can be widely varied with a magnetic Feshbach resonance… (*Greiner Lab* at Harvard)

1D-2D-3D: Control on dimensionality by changing the aspect ratio of the trap

$$\mathbf{V}(x,y,z) = \tfrac{1}{2}m\omega_x^2x^2 + \tfrac{1}{2}m\omega_y^2y^2 + \tfrac{1}{2}m\omega_z^2z^2$$

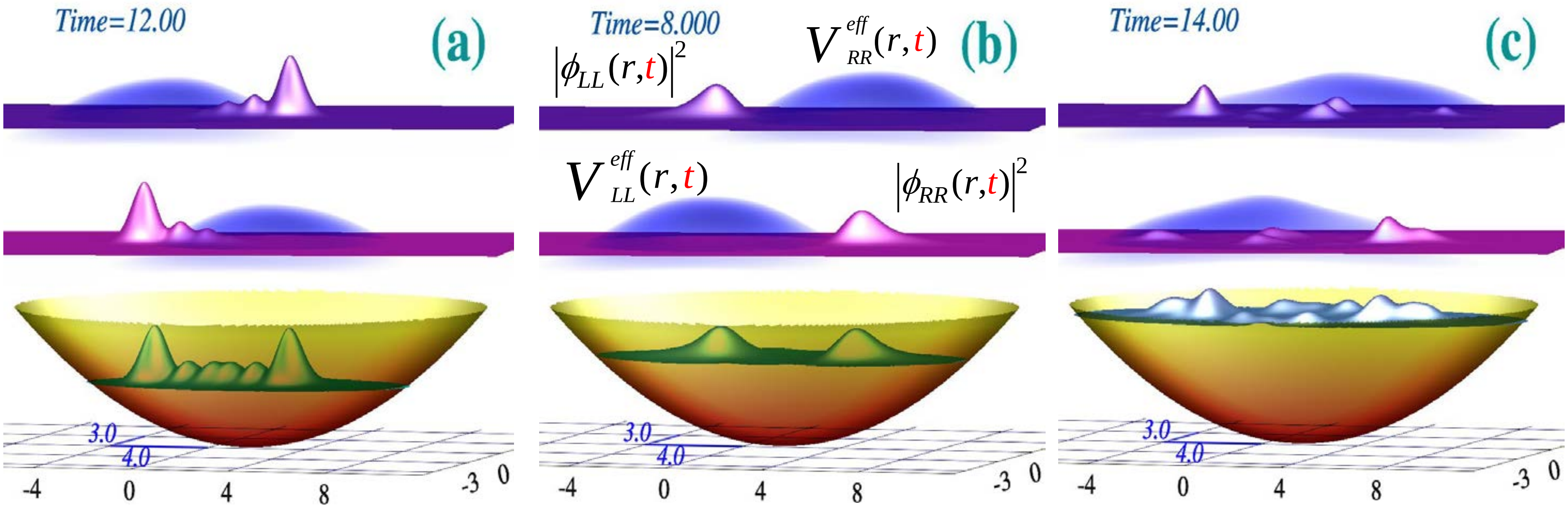
Highly-non-equilibrium quantum dynamics in trapped systems of ultra-cold atoms and molecules

(N=100: sudden displacement of trap and sudden quenches of the repulsion in 2D)

Trap displacement: $\mathbf{V}(x,y) = \frac{1}{2}x^2 + \frac{3}{2}y^2 \rightarrow \mathbf{V}(x-1.5, y-0.5)$

Inter-particle repulsion quench is described by the variation of the parameter λ_0

$\lambda_0 = 0.5 \rightarrow 0.1$ $\lambda_0 = 0.5 \rightarrow 0.7$ $\lambda_0 = 0.5 \rightarrow 0.8$



Two generic regimes: (i) Non-violent (under-the-barrier) and (ii) Explosive (over-the-barrier)

O.Streltsova (LIT), O.Alon, L.Cederbaum, A.Streltsov, Phys. Rev. **A89**, 061602(R) (2014)

Center for Quantum Dynamics

Many-body theory
of bosons group
Heidelberg, Germany

PD Dr. Alexej I. Streltsov
UNIVERSITÄT HEIDELBERG

Dr. Oksana I. Streltsova
LIT JINR, DUBNA

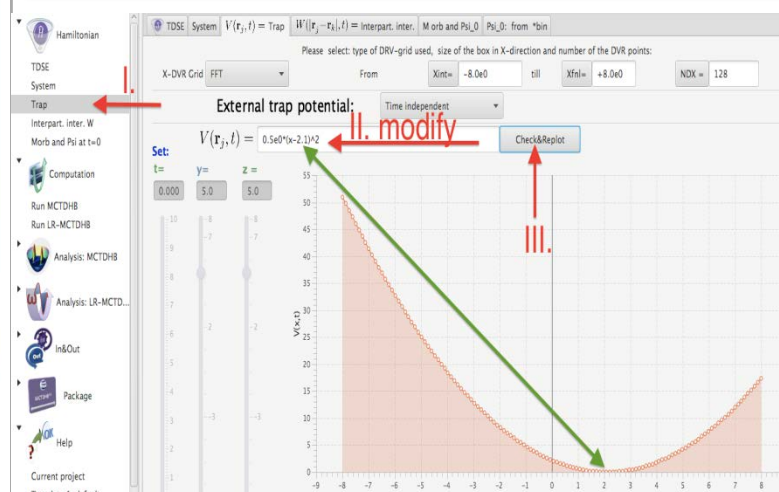
hYBRI

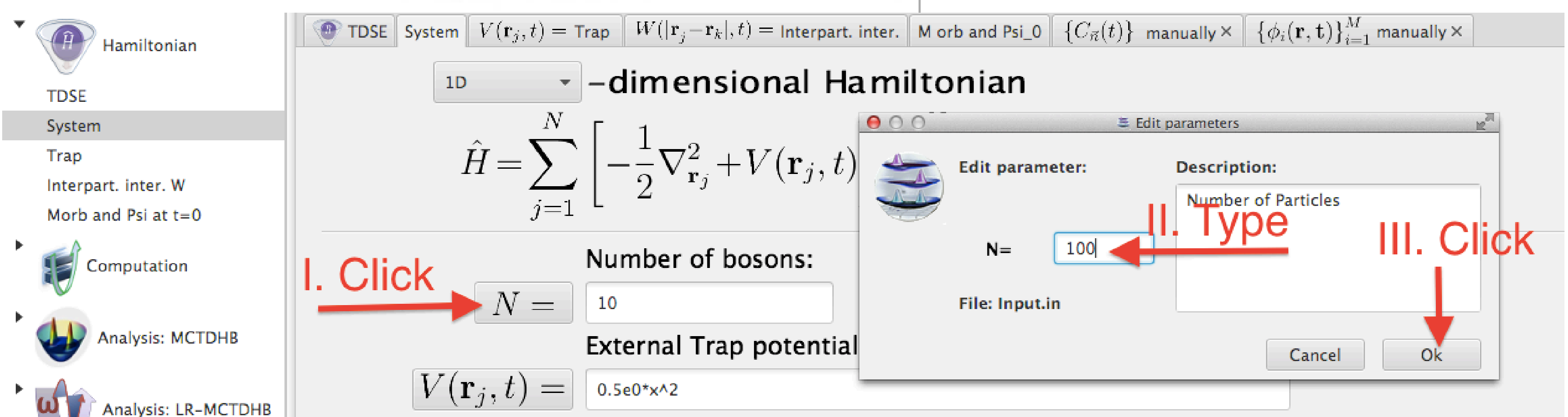
Heterogeneous Computations
HybriLIT - team

http://QDlab.org

MCTDHB-Lab is a free-for-download cross-platform software working on Mac, Windows and Linux

http://QDlab.org





Conclusions

- *Following the worldwide trend, the computing and software will become overwhelming*
- *In addition to the high energy physics, other investigations are also seeking novel computing models*
- *Computing is essential to R&D, science and technology, operations and management*
- *The development of numerical methods and algorithms for parallel and hybrid calculations in scientific research will become pervasive*
- *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*

Thank you for your attention !