Mathematical modeling of physical problems and high-performance computing on the heterogeneous cluster HybriLit

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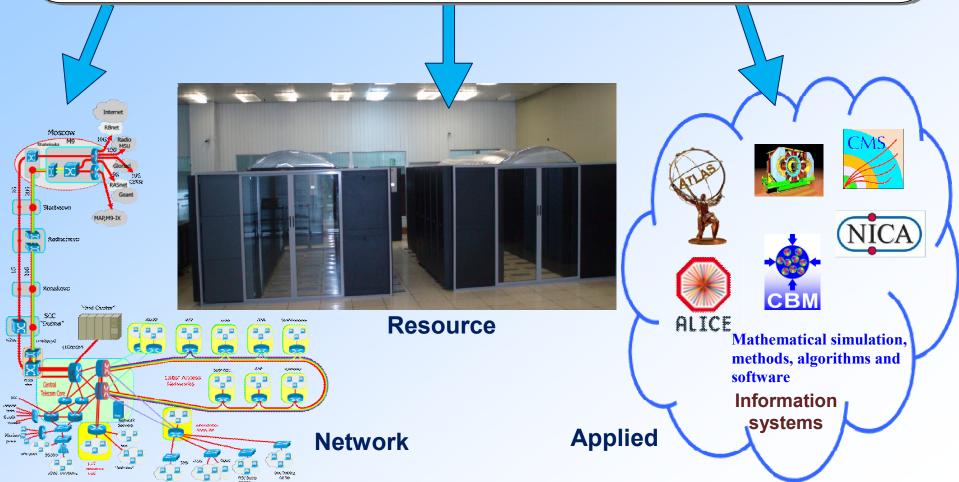
Invited Lecture at the RO-LCG 2014 conference, November 3-5, 2014

I. General

JINR Field of Research: Networking, Computing, Computational Physics LIT Topics in JINR Topical Plan:

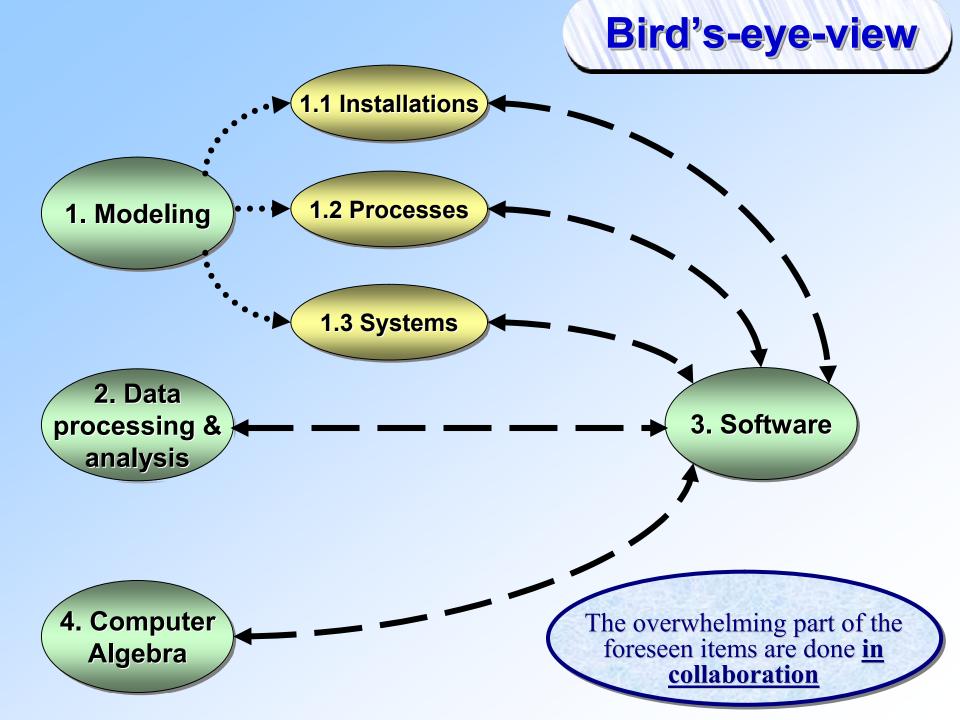
05-6-1118-2014/2016 Information and Computing Infrastructure of JINR

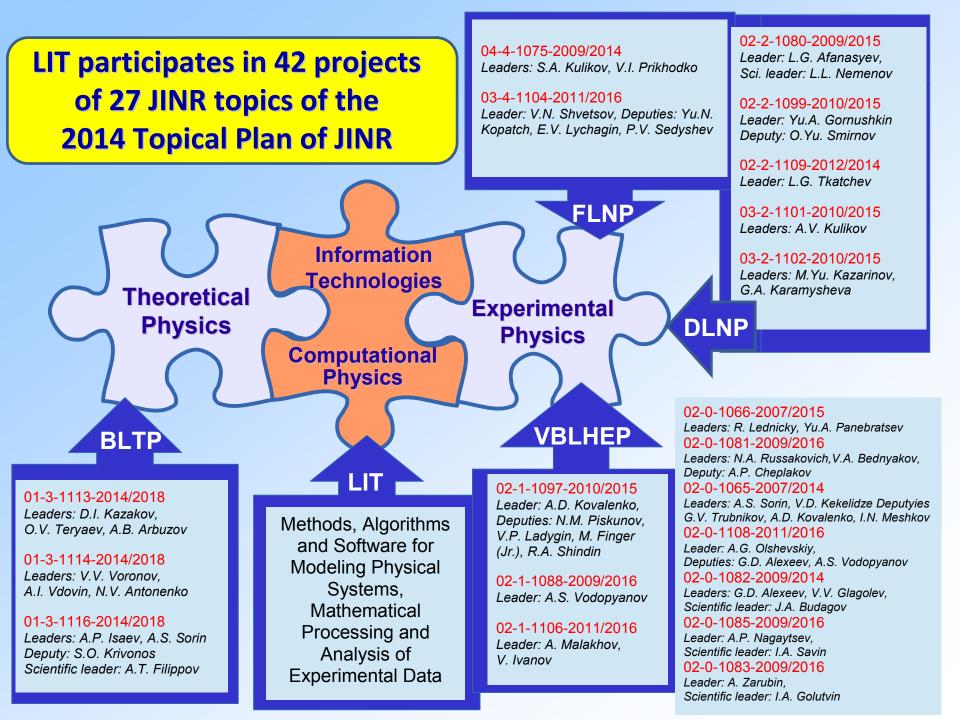
05-6-1119-2014/2016 <u>Methods, algorithms and software for modeling physical systems,</u> <u>mathematical processing and analysis of experimental data</u>



The four main tasks of the topic 1119

- 1. Development of mathematical and computational methods for modeling: new experimental facilities, accelerator complexes and their elements; nuclearphysical processes; complex physical systems.
- 2. Mathematical methods for data processing and analysis: development of new mathematical approaches for experimental data processing; algorithms and program complexes for solving topics in high energy physics, nuclear physics, condensed matter physics, including those at accelerator complexes LHC, NICA, FAIR, etc.
- 3. Development of numerical methods, algorithms, and software, computationally adapted to many-core and hybrid architectures, for solving physical models in high energy physics, nuclear physics, condensed matter physics, and nanotechnology.
- 4. Development of methods, algorithms, and software of computer algebra for modeling quantum systems and quantum informational processes, as well as for solving other applied mathematics topics.





II. Large scale international collaborations

Significant participation in large scale international collaborations

Sizeable specific contributions to:

Magnetic field calculations for new experimental

facilities and elements of accelerator complexes

- CBM dipole magnet;
- * SIS100 magnet elements at FAIR;
- * Profile optimization of the NICA collider dipole magnet;
- Booster quadrupole magnet at NICA;
- * 3D-dipole magnet for BM@N

Software upgrade for components of the improved ATLAS and CMS detectors, as part of JINR contribution
Modeling, algorithm and software for CBM@FAIR
Mathematical modeling of the hot and dense nuclear matter and spin physics phenomena within the flagman JINR NICA/MPD project

Contributions to the upgrade of the Geant4 package

JINR participates in 3 experiments at LHC : ATLAS, CMS, ALICE

Physics:



ALICE







> QCD @ Standard Model Physics

- Higgs Physics
- SUSY Physics > Exotics Physics













LIT JINR, in particular, takes part in muon reconstruction studies

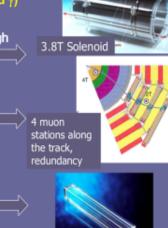
in the CMS experiment

🔀 The CMS Original Concept

Guiding channels: $H \rightarrow ZZ \rightarrow \ell^+ \ell^- \ell^+ \ell^-, H \rightarrow \gamma \gamma$ Optimized for high p_T leptons (and y)

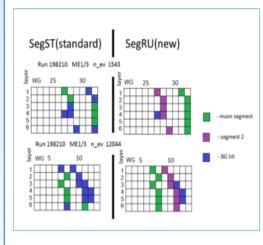
- Good momentum resolution with high B-field
- Excellent and redundant muon identification
- Very high energy resolution for electrons and photons

 ΔE



Current LIT activities: development of a new CMS muon segment builder

Fully active ECAL made of crystals



The new algorithm successfully decides the problems with background and multiplicity of hits, providing a correct muon segment building.

SegST – resulted from a current CMS code and SegRU – resulted from the new algorithm;

hitted Wire Groups are marked on the 6 Cathode Strip Chamber layers: blue - background, green - muon segment, violet - electromagnetic secondaries

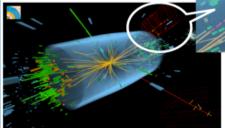
To be reported at CERN in November

By courtesy of V. Palichik and E. Tikhonenko (LIT)

A HIGGS CANDIDATE 4-JUL-2012

eeuu run 195099 evt 137440354

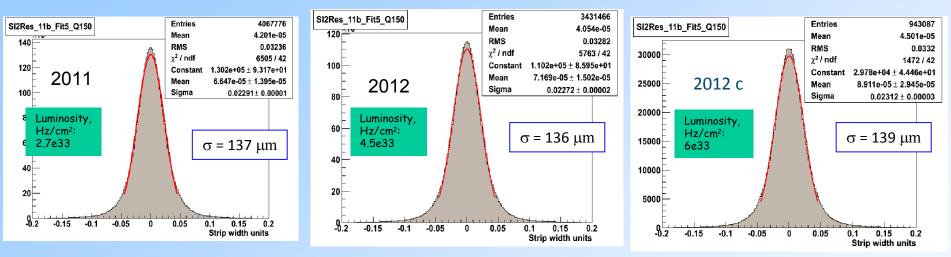
Higgs --> two Z-bosons, one of them decayed to 2 muons (red lines) and another - to 2 electrons (green lines)





One of the muons is reconstructed in the endcap muon system, part of which is of Dubna responsibility

CMS Cathode Strip Chambers Performance

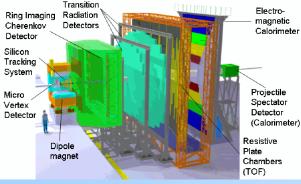


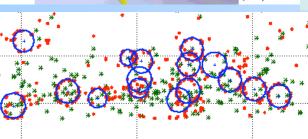
- Vladimir Palichik (LIT) is co-convenor of CMS CSC DPG (Detector Performance Group) since 2011.
- Outstanding contributions of LIT group to CMS during 2011-2013:
 - estimation of the cathode strip chambers spatial resolution and local reconstruction efficiency using 2012 collisions data;
 - ME1/1 chamber testing and troubleshooting;
 - offline validation of refurbished ME1/1 chambers with cosmic ray muons

Co-authorship to CMS Publications: 257 during 2011-2013 in refereed journals (Phys.Lett.B. Phys.Rev.D, Phys.Rev.Letters, The European Phys.Journal C, Journal of High Energy Physics and others); - 8 members of LIT staff are among the authors of the seminal CMS paper "Observation of a new boson at a mass of 125 GeV with the CMS experiment at the LHC", Physics Letters B 716 (2012) 30-61.

Left and Center: V.Palichik (LIT) report at CMS Run Coordination Workshop, Torino, Italy (Feb., 2013) Right: V.Palichik et al., Journal of Instrumentation, 8 (2013) P11002.

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





Fast parallel algorithms developed for event reconstruction

- 1)Tracking: Kalman filter and track following;
- 2) Ring reconstruction: Hough Transform, COP, ellipse fitting;
- 3) Electron identification in RICH: ANN and cuts

Modern technologies for parallelization:

- 1) Vectorization (SIMD Single Instruction Multiple Data);
- 2) Multithreading (many cores CPU)

Results:

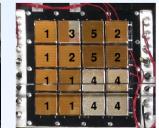
High efficiency of track and ring reconstruction (93-95%);
 Very fast algorithms (few ms per event)

Task	Initial Time [ms/event]	Parallel Time [ms/event]	Speedup
Tracking	730	1.5	487
Ring reconstruction	375	2.5	143

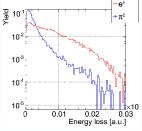


- 1) Development of methods, algorithms, and software for:
 - global track reconstruction;
 - event reconstruction in RICH;
 - electron identification in TRD;
 - momentum reconstruction;
- 2) Magnetic field calculations;
- 3) Beam time data analysis of the RICH and TRD prototypes;
- 4) Tools for quality assurance of the CBMROOT software;
- 5) Contribution to the CBMROOT development

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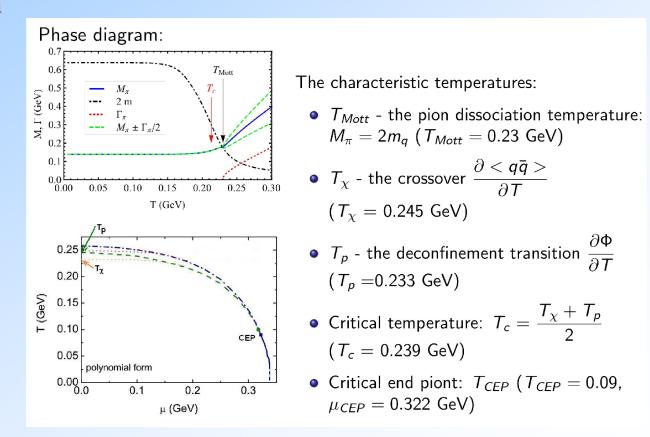






NICA/MPD: Development of a consistent QCD approach to the process modeling at finite temperature and density

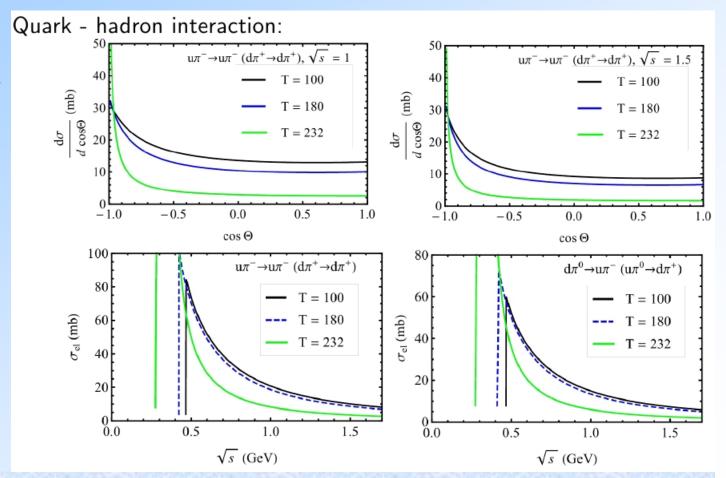
Consistent description of chiral symmetry breaking and its restoration at finite temperature Inclusion of the continuum state contribution to the scattering shift together with the Breit-Wigner ansatz for the resonance yields computed phase shifts obeying the Levinson theorem



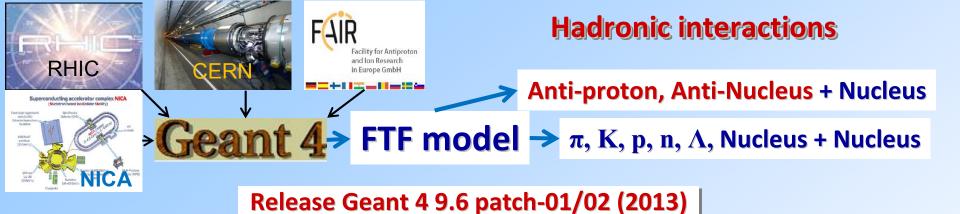
Yu.L. Kalinovsky (LIT), V.D. Toneev, A.V. Friesen (BLTP), D. Blaschke, A. Wergieluk (Univ. Wroclaw), P. Costa (Coimbra Univ.) PRD 85 (2012), PEPAN Lett. 9 (2012), Int.J.Mod.Phys A27 (2012), arXiv:1212.5245 (subm. PRD), arXiv:1304.7150 (subm. Nucl.Phys. A)

NICA/MPD: Development of a consistent QCD approach to the process modeling at finite temperature and density

Quark-meson interactions in a hot and dense medium can be confidently modeled to describe the kinetics of the processes



Yu.L. Kalinovsky (LIT), V.D. Toneev, A.V. Friesen (BLTP), D. Blaschke, A. Wergieluk (Univ. Wroclaw), P. Costa (Coimbra Univ.) PRD 85 (2012), PEPAN Lett. 9 (2012), Int.J.Mod.Phys A27 (2012), arXiv:1212.5245 (subm. PRD), arXiv:1304.7150 (subm. Nucl.Phys. A)



Hadron-nucleon process cross section

- Total, elastic and inelastic hadron-nucleon cross sections Cross sections of quark exchange processes Cross sections of anti-proton processes
- Cross sections of anti-proton processes
- Cross sections of diffractive and non-diffractive processes

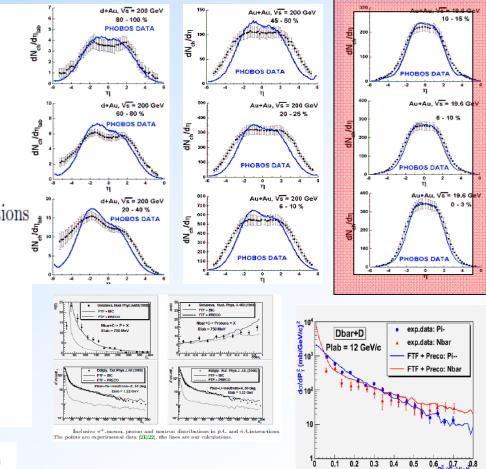
Simulation of hadron-nucleon interactions

Simulation of meson-nucleon and nucleon-nucleon interactions Simulation of anti-baryon-nucleon interactions

Simulation of nuclear interactions

- Sampling of intra-nuclear collisions
- Reggeon cascading
- "Fermi motion" of nuclear nucleons
- Excitation energy of nuclear residuals

A. Galoyan (VBLHEP), V. Uzhinsky (LIT)



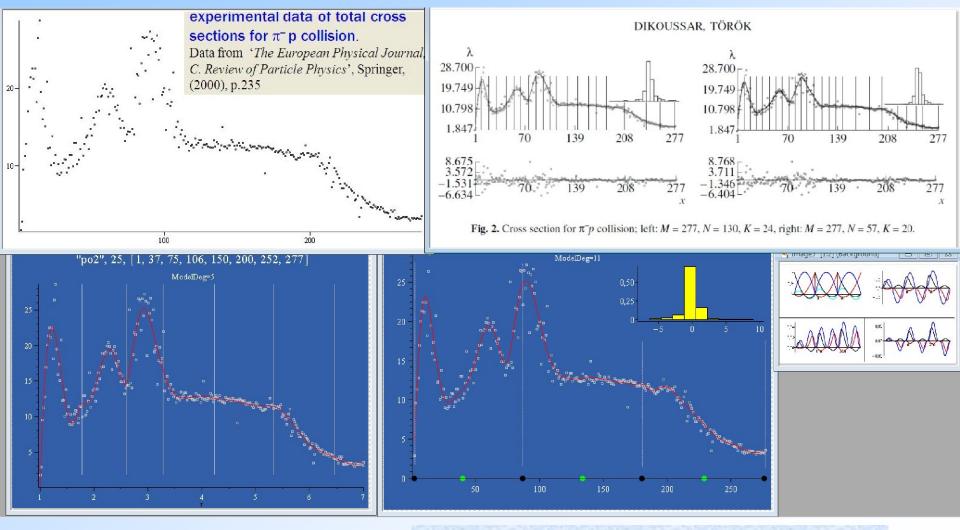
III. Mathematical methods

New mathematical method for experimental data processing and analysis

Polynomial approximation and robust data smoothing within the basic element method: Previous research directed to the development of approximation methods, resulting in smoothing algorithms able to encompass features of the apparently irreconcilable point-wise Taylor and interval-wise Chebyshev series expansions, has resulted in a fundamentally new approach, called the basic element method (BEM) to the numerical solutions of the data smoothing problem.

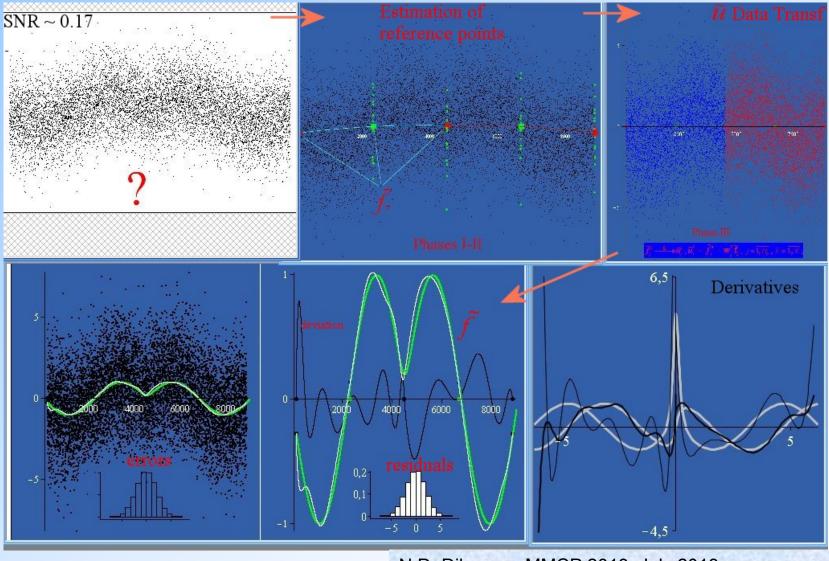
The BEM is characterized by exceptional flexibility and robustness, as well as by a remarkably low computational complexity (orders of magnitude lower than that of the well-known spline function method). The time is ripe for building proper interfaces of the BEM to actual data smoothing problems asked by various experiments.

BEM vs. Splines for solving a typical smoothing problem



N.D. Dikousar, Matematicheskoe Modelirovanie (2014)

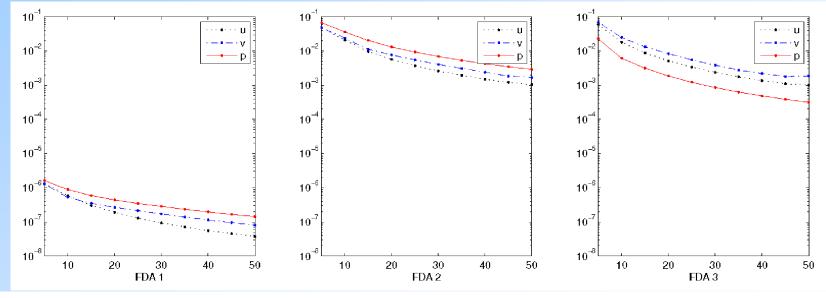
BEM solution of "Mexican Hat" smoothing problem for a low signal to noise ratio



N.D. Dikousar, MMCP 2013, July 2013

Consistent discretization of non-linear PDE by finite-difference approximations

We prove that the *inheritance of the algebraic properties* of differential equations by the finite-difference approximation (FDA) discretization *is of fundamental importance for consistent numerical solution*.

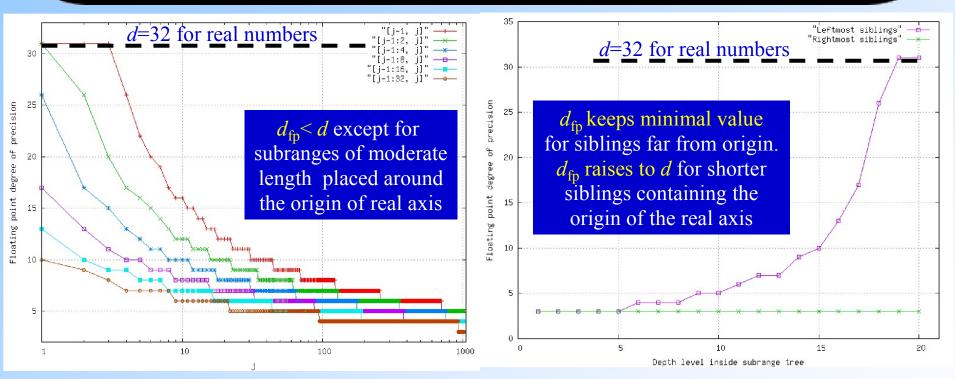


Computer experiment demonstration is provided for the two-dimensional Navier-Stokes equations (NSE) describing an incompressible viscous fluid.

Relative errors for the velocity components (u,v) and pressure (p) are plotted vs. the number of discretization knots. FDA1 preserves NSE algebraic properties, whereas FDA2 and FDA3 do not.

V.Gerdt et al., On Consistency of Finite Difference Approximations to the Navier-Stokes Equations, Lecture Notes in Computer Science 8136, 2013, pp. 46—60.

Floating point degree of precision of a quadrature sum



Computations done over the *machine floating point number set* need a fundamentally different characterization of the integrand properties.

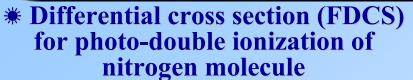
The plots point to the property of the *floating point degree of precision* of a *quadrature sum* $(d_{\rm fp})$ of showing significant deviation from the *algebraic degree of precision* (d) which holds over the field of the real numbers.

This entails substantial modifications of the implementation of *Bayesian automatic adaptive quadrature*.

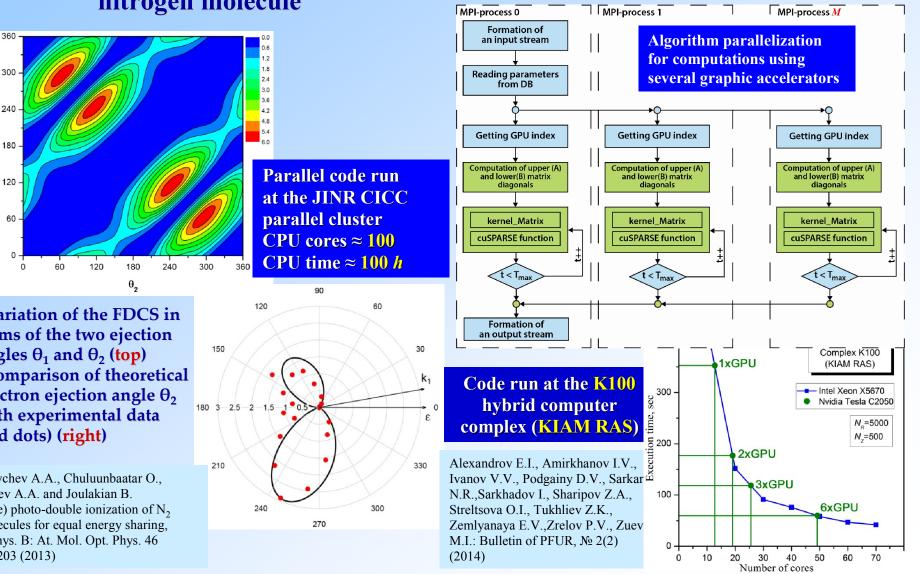
S. Adam, Gh. Adam, LNCS 7125, Springer (2012)

IV. Early parallel computations

Early codes adapted to multi-core and hybrid architectures



***** Modeling thermal processes in materials irradiated by ion beams



 Variation of the FDCS in terms of the two ejection angles θ_1 and θ_2 (top) Comparison of theoretical electron ejection angle θ_2 with experimental data (red dots) (right)

300

240

180 θ

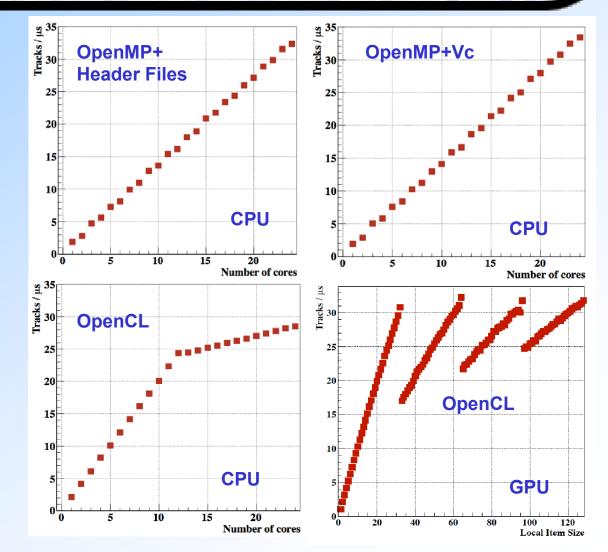
120

60

Bulychev A.A., Chuluunbaatar O., Gusev A.A. and Joulakian B. $(\gamma, 2e)$ photo-double ionization of N₂ molecules for equal energy sharing, J. Phys. B: At. Mol. Opt. Phys. 46 185203 (2013)

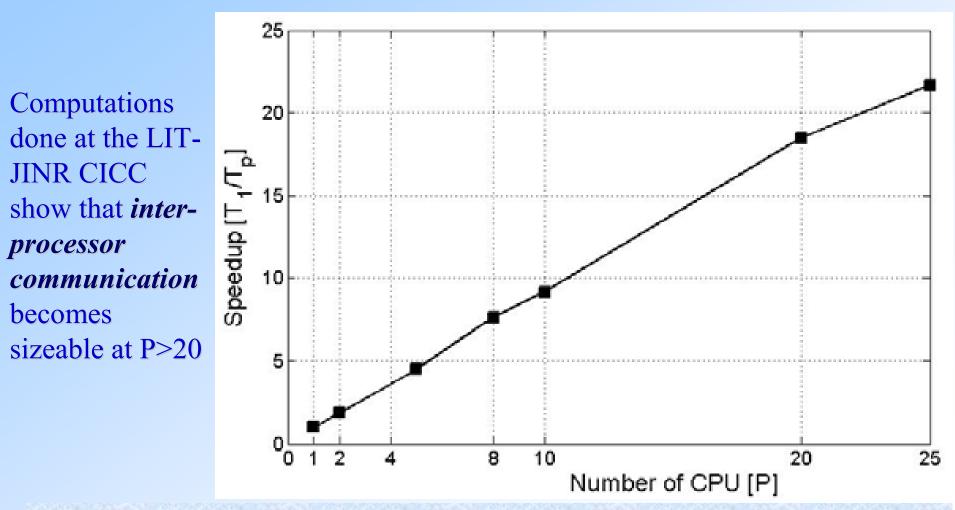
Many-core computer experiments on Kalman filter based track reconstruction algorithm

LIT implementations have reached *strong scalability* of four Kalman filter based *track reconstruction algorithms for* CBM *experiment*, under different computing paradigms.

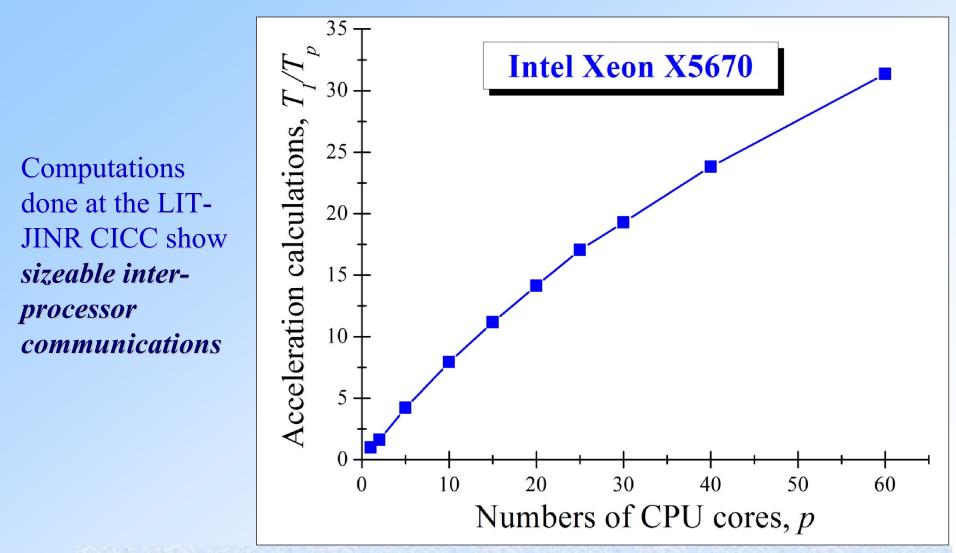


V.V. Ivanov et al., (2013)

Parallel solution of the heat flow simulation inside a cylindrical cryogenic cell subject to millisecond electric discharges: algorithm scalability



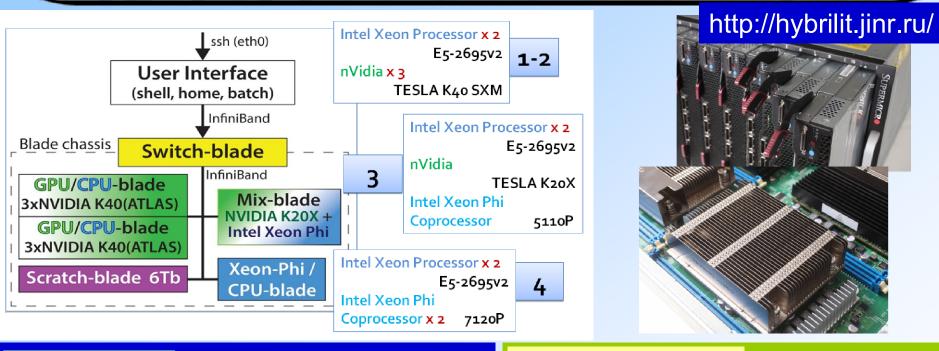
A. Ayriyan, E. Ayryan, E. Donets, J. Pribis, in Math. Modeling and Comp. Sci., Springer, LNCS 7125 (2012); A. Ayriyan, E. Donets, J. Pribis, poster to the 39-th Session of PP-PAC, June 2013. **Parallel solution of the simulation of thermal processes in materials irradiated by heavy ion beams : algorithm scalability**



E.I. Alexandrov, I.V. Amirkhanov, V.V. Ivanov, D.V. Podgainy, N.R. Sarkar, I. Sarkhadov, Z.A. Sharipov, O.I. Streltsova, Z.K. Tukhliev, E.V. Zemlyanaya, P.V. Zrelov, M.I. Zuev, poster to the 39-th Session of PP-PAC, June 2013.

V. Parallel computing on HybriLIT

The heterogeneous computing cluster HybriLIT



Resources

CPU 96 cores GPU 19968 cuda cores PHI 182 cores

Performance

RAM 512 Gb EOS storage 14 Tb **Ethernet** InfiniBand 40 Gb/s

Max. single-precision Max. double-precision

46,914 Tflops 17,979 Tflops

Power consumption: 10 KW

Software installed:

Scientific Linux 6.5. CUDA Toolkit 5.5, CUDA Toolkit 6.0 **OpenMPI 1.6.5, 1.8.1 OpenMP GCC, ICC** Intel Cluster Studio 2013 JDK-1.7.0, JDK-1.8.0

Compilers used:

nvcc

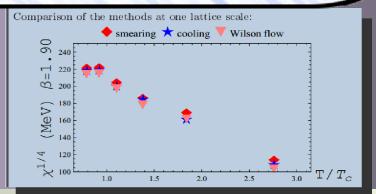
mpic++, mpicc, mpicxx, mpif77, mpif90, mpifort, icc, ifrort mpiicc, mpiifort

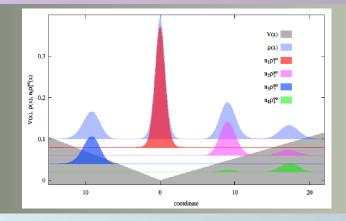
First parallel runs on HybriLIT

Smearing techniques in lattice QCD:

F. Burger (IP HU, Berlin, Germany),M. Müller-Preussker (IP HU, Berlin, Germany),E.-M. Ilgenfritz (BLTP&VBLHEP JINR),A. M. Trunin (BLTP JINR)

http://theor.jinr.ru/~diastp/summer14/program.html#posters





Investigation of Bose-systems:

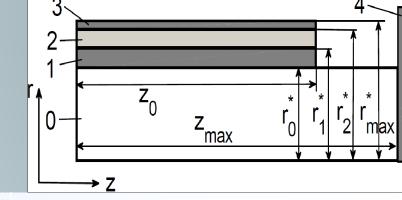
Alexej I. Streltsov ("Many-Body Theory of Bosons" group at CQD, Heidelberg University, Germany), Oksana I. Streltsova (LIT JINR)



Optimized temperature work cycle of a multilayer cylindrical object (source of multiply charged ions)

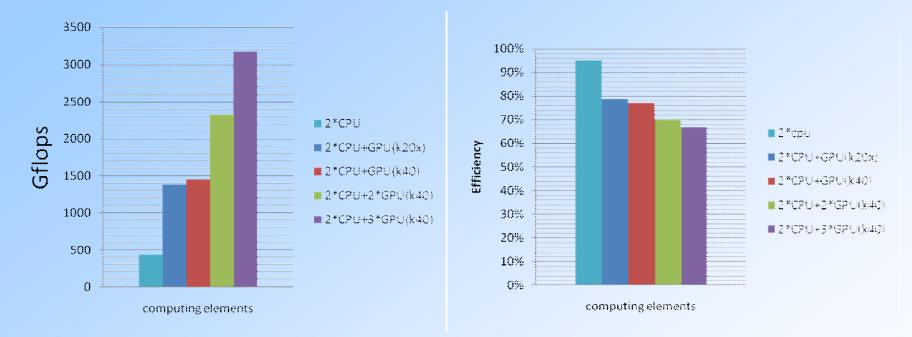
A. Ayriyan (LIT JINR), J. Busa Jr. (TÚ of Kŏsice, Slovakia),
E.E. Donets (VBLHEP, JINR),
H. Grigorian (LIT JINR,;Yerevan State University, Armenia),

J. Pribis (LIT JINR; TU of Kŏsice, Slovakia)



arXiv:1408.5853v2 [physics.comp-ph] 7 Sep 2014

Linpack benchmark of HybriLIT (preliminary)



Linpack testing parameters corresponding to the data reported in figures:

- For CPU, the default version defined on the intel studio (composer_xe_2013_sp1.2.144), with the CPU frequency = 2.4 GHz of the E5-2695 v2 Intel processor

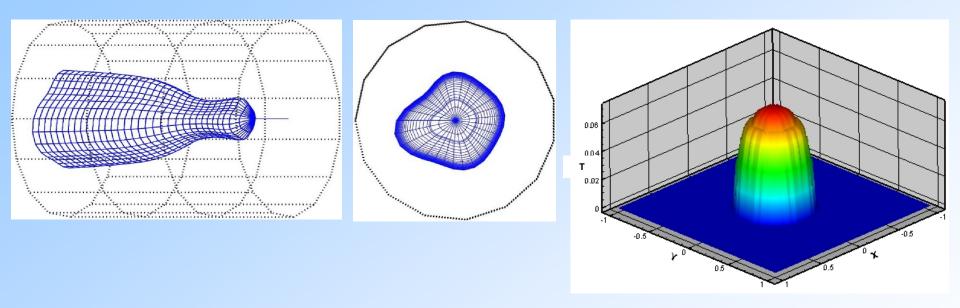
- For GPU, the version hpl-2.0_FERMI_v15, downloaded from the official NVIDIA site

- The data correspond to:

the order of the coefficient matrix A, N = 120 000, the block partitioning factor NB = 1 024, 24 CPU per 1 GPU for a single K20x or K40, 6 CPU per 1 GPU for 2*K40, and 4 CPU per 1 GPU for 3*K40

VI. Testing HybriLIT vs. K100 hybrid cluster at **KIAM RAS**

GIMM FPEIP : package for simulation of thermal processes in materials irradiated by heavy ion beams



Alexandrov E.I., Amirkhanov I.V., Zemlyanaya E.V., Zrelov P.V., Zuev M.I., Ivanov V.V., Podgainy D.V.,
 Sarker N.R., Sarkhadov I.S., Streltsova O.I., Tukhliev Z. K., Sharipov Z.A. (LIT)
 Principles of Software Construction for Simulation of Physical Processes on Hybrid Computing Systems
 (on the Example of GIMM_FPEIP Complex) // Bulletin of Peoples' Friendship University of Russia. Series
 "Mathematics. Information Sciences. Physics". — 2014. — No 2. — Pp. 197-205.

Computational Task

Solve a system of coupled PDE describing heat conduction within the thermal spike model in cylindrical coordinates (z axis is perpendicular to the ion momentum hitting the surface)

$$C_e(T_e)\frac{\partial T_e}{\partial t} = \nabla(\lambda_e(T_e)\nabla(T_e)) - g(T_e - T_i) + A_e(\mathbf{r}, t)$$
$$C_i(T_i)\frac{\partial T_i}{\partial t} = \nabla(\lambda_i(T_i)\nabla(T_i)) - g(T_e - T_i) + A_i(\mathbf{r}, t)$$

Here *e* and *i* label the electron gas and ion lattice subsystems, characterized by the unknown temperature fields $T_e(\mathbf{r}, t)$ and $T_i(\mathbf{r}, t)$, respectively.

 $C_e(T_e)$, $C_i(T_i) \& \lambda_e(T_e)$, $\lambda_i(T_i)$ denote the specific heat capacity and thermal conductivity coefficients of the electron gas and respectively the lattice;

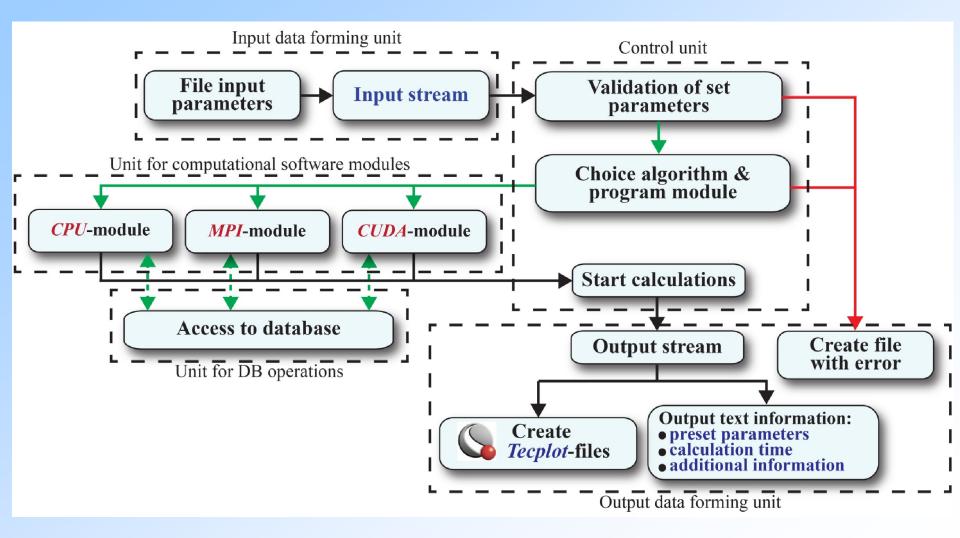
g denotes the electron-phonon interaction;

 $A_e(\mathbf{r}, t)$ and $A_i(\mathbf{r}, t)$ denote the volumetric energy densities induced by the incident ion flux into the electron gas and ion lattice subsystems.

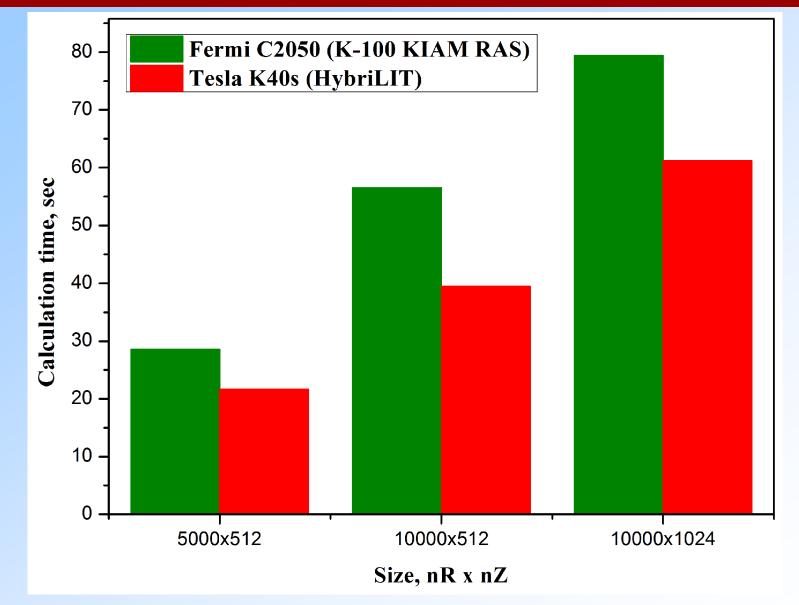
$$T_{e,i}(r,\varphi,z,t) = T_{0,e,i}(r,z,t) + \sum_{m=1}^{M} T_{m,e,i}(r,z,t) \left(c_{1m} \cos m\varphi + c_{2m} \sin m\varphi\right)$$

Size of problem: $N_R \times N_Z \times M$ Multi-GPU

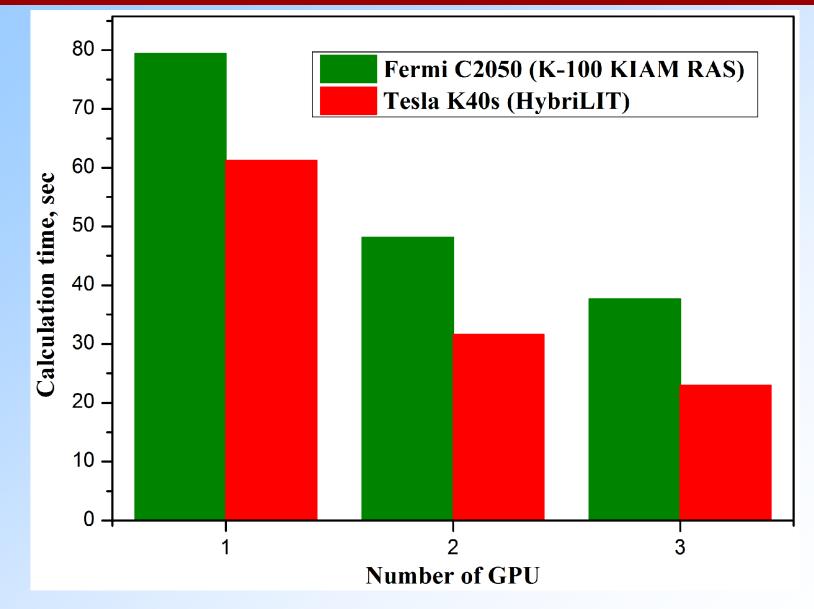
GIMM FPEIP: Logical scheme of the algorithm



GPU calculations



Multi-GPU calculations



VII. Invitation to MMCP 2015 (High Tatras, Slovakia)

Mathematical Modeling and Computational Physics (MMCP'2011) July 4 - July 8, 2011 Stará Lesná, Slovakia

Organizers:

- Laboratory of Information Technologies,
- Inst. Exp. Physics, SAS, Košice,
- Technical University, Košice,
- Pavol Jozef Šafárik University, Košice,
- Union of Slovak Mathematicians and Physicists, Košice, Slovakia

Topics:

-mathematical methods and tools for modeling complex physical and technical systems;

- methods, software and computer complexes for experimental data processing;
- methods, algorithms and software of computer algebra;
- computational chemistry, biology, and biophysics;
- distributed scientific computing;
- computing tools of a new generation.



MATHEMATICAL MODELING AND **COMPUTATIONAL PHYSICS 2011**

Stará Lesná, High Tatra Mountains, Slovakia

July 4 — 8, 2011

Joint Institute for Nuclear Research, Laboratory of Information Technologies (Dubna)

Organizers





Conference chairmen: V.V. Ivanov (JINR) P. Sovák (UPJŠ)

Program Committee

I. Antoniou (Greece) S. Adam (JINR) O. Iliev (Germany) S. Dimova (Bulgaria) K. Flachbart (IEP, Slovakia) V. Friese(Germany) V.P. Gerdt (JINR) U.H.E. Hansmann (USA) Sh. Hayryan (Taiwan) J. Honkonen (Finland) D. Horváth (Slovakia) Ch.-K. Hu (Taiwan)

I. Kisel (Germany) N. Kolkovska (Bulgaria) P. Kopčanský (IEP. Slovakia) V.D. Lakhno (Russia) V.S. Melezhik (JINR) S. Scott (North Ireland) M. Pavluš (Slovakia) R.V. Polozov (Russia) I.V. Puzynin (JINR) L.A. Sevastianov (Russia) P.N. Vabishchevich (Russia) P. Zinterhof (Austria) P.V. Zrelov(JINR)

Topics

Institute of Experimental Physics (Košice, Slovakia)

Technical University (Košice, Slovakia) Pavol Jozef Šafárik University (Košice, Slovakia)

- mathematical methods and tools for modeling complex physical and technical systems
- software and computer complexes for experimental data processing
- methods, algorithms, and software of computer algebra
- computational chemistry, biology, and biophysics
- new generation computing tools, distributed scientific computing





E-mail: mmcp2011@saske.sk http://www.tuke.sk/busa/mmcp2011.htm

Organizing committee

Chairmen: Gh. Adam (JINR) and M. Hnatič (UPJŠ&IEP) Scientific Secretaries: J. Buša (TU) and T.A. Strizh (JINR)

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D.V. Podgainy (JINR)	P. Murin (UPJŠ, Slovakia)
O.I. Streltsova (JINR)	J. Pribiš (FEI TU)
P.V. Zrelov(JINR)	Š. Schrötter (FEI TU)
J. Buša, jr. (FEI TU)	

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Gheorghe Adam Ján Buša Michal Hnatič (Eds.)

Mathematical Modeling and Computational Science

-NCS 7125

International Conference, MMCP 2011 Stará Lesná, Slovakia, July 2011 Revised Selected Papers



Book Performance Report 2013 June 2014

Dear Gheorghe Adam,

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- -4. distributed scientific computing and big data;
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