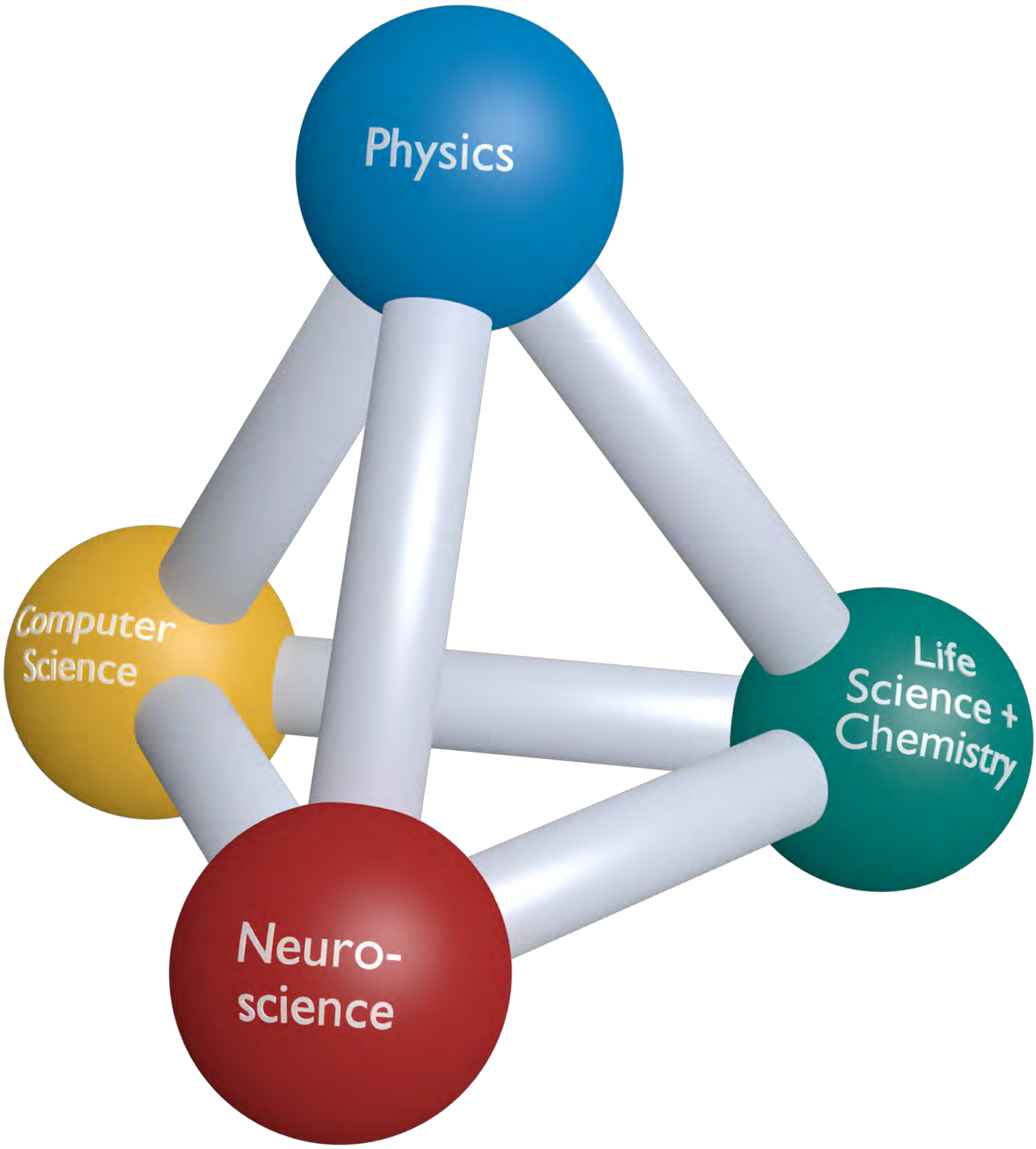
FIAS Frankfurt Institute for Advanced Studies



FIAS Scientific Report 2012

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FIAS Scientific Report 2012

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Preface

In the year 2012 FIAS has continued to carry out its mission as an independent research institute performing cutting-edge research in the natural and computer sciences. An account of recent scientific accomplishments can be found in the brief individual research reports collected in Section 4. In addition we document important developments at cooperating institutions, as well as colloquium schedules, conferences organized by FIAS, and the graduate teaching activities in the framework of the Frankfurt International Graduate School for Science (FIGSS).

In the year 2012 FIAS again has organized or co-organized a variety of scientific conferences and workshops on topics ranging from nuclear astrophysics or relativistic heavy ion physics to nanoscience and robotics. Many of these events were held at the premises in Frankfurt, e.g., three workshops of the ambitious Ernst Strüngmann Forum. Public outreach activities have concentrated on the lecture series "FIAS Forum" which presented a series of non-technical evening lectures on a variety of topics which were well received by the general public.

The year 2012 has brought a number of new faces and changes in the ranks of the senior scientific staff at FIAS. The computer scientist Ivan Kisel has joined FIAS as a new Fellow and at the same time was appointed to a professorship at Goethe University. Another newly appointed Fellow is Dr. Hannah Petersen who leads a Helmholtz Young Investigator Group and is designated for a professorship in the physics department. Three scientists were appointed to the title Research Fellow, the high-energy physicists Dr. Pasi Huovinen and Dr. Hendrik van Hees, and the neuroscientist Dr. Danko Nikolić. Dr. Nikolić is a veteran at FIAS, having served before as Junior Fellow for many years. A newly appointed Adjunct Fellows is Dr. Laura Tolos, Institute of Space Sciences, Barcelona, Spain, who had been Junior Fellow in the years 2006–2008.

Two former FIAS researchers have been appointed to professorships overseas: Rodrigo Picanço Negreiros at the Federal Fluminense University, Niteroi (Rio de Janeiro), and Manu Punnen John at the Union Christian College (part of Mahatma Gandhi University) in Aluva, Kerala province, India.

The computer science branch at FIAS could register a number of successes in the year 2012. Prof. Lindenstruth and his colleagues were commended by the initiative "Germany – Land of Ideas" for the LOEWE-CSC supercomputer and also received the German Computing Center Prize. Furthermore, the new supercomputer SANAM, built for KACST/Saudia Arabia, has qualified for place 2 on the list of the most energy-efficient high-performance computers worldwide and is ranked number 52 on the TOP500 list of the fastest computers.

After thorough discussions among the management and the scientists at FIAS, in 2012 an updated strategy plan "FIAS - Status and Perspectives" has been formulated. This will be regularly adjusted in order to account for future opportunities and challenges and to changes in the funding situation.

There are ongoing attempts to alleviate the structural imbalance of FIAS, which strongly tilts towards the branches of physics and neuroscience. Earlier efforts to fill the envisaged Helmut Maucher endowed professorship with a high-profile theoretical chemist or biologist had not been successful. As an alternative, presently the idea is pursued to apply the expertise of FIAS in complex systems and modeling to the area of economics and finance. In cooperation with the House of Finance at Goethe University, in September 2012 a pilot symposium "Systemic Risk: Economists Meet Neuroscientists" was organized. This may pave the way for FIAS to enter a promising new field of research.

Research highlights 2012

Physics

In the area of astrophysics the group of S. Schramm has made major progress in developing a two-dimensional code to describe the *cooling of neutron stars*. The two-dimensional modeling will, for the first time, allow the study of the stellar temperature evolution of fast spinning stars, including the spin-up from mass accretion in binary systems, with possible phase transitions in the interior of the stars that could lead to observable variations in the star's temperature evolution. This approach is an important tool to acquire more information on the equation of state of extremely dense matter as found in compact stars.

The Ultra-relativistic Quantum Molecular Dynamics (UrQMD) transport model for the description of *high-energy nuclear collisions* has been employed by M. Bleicher and collaborators in a number of studies. This includes: the transport properties of heavy quarks in the Quark-Gluon Plasma, the extraction of nuclear size information from two-pion HBT correlations at RHIC and LHC energies, and the production of dileptons in hot elementary matter.

Using experimental data on multihadron production at CERN LHC and SPS, R. Stock, M. Bleicher and colleagues were able to determine the position of the *parton-hadron phase boundary line* between deconfined partons and confined hadrons, in the plane of temperature and baryochemical potential (T, μ_B). The results of this analysis, which is based on the Statistical Hadronization Model (SHM) augmented with UrQMD simulations, agrees well with the predictions of lattice QCD.

The group of E. Bratkovskaya has studied the parton-hadron matter in and out of equilibrium within the Parton-Hadron-String Dynamics (PHSD) transport approach for the *strongly interacting Quark-Gluon-Plasma (sQGP)*. In particular, the equilibration of observables and their fluctuations in the QGP as well as transport coefficients were studied in this way. The ratio of the shear viscosity to entropy density η/s was found to show a minimum close to the critical temperature T_c, while approaching the perturbative QCD limit at higher temperatures. The ratio of the bulk viscosity to entropy density ζ/s shows a maximum close to T_C.

The group of D.H. Rischke has investigated the derivation of the equations of motion of dissipative relativistic fluid dynamics from the underlying microscopic theory, the Boltzmann equation. A new method, based on moments of the single-particle distribution function and a systematic power-counting in Knudsen and inverse Reynolds number, was developed, allowing to systematically improve the calculation of transport coefficients. It was applied to situations where a naive power-counting fails.

In the area of nuclear structure physics, V.I. Zagrebaev and W. Greiner made new predictions for the synthesis of *superheavy nuclei*. They advocate the fusion of ^{48}Ca with transuranium nuclei to reach the "island of stability".

The topic of nuclear waste reduction has been addressed in a study modeling neutron production and transport in spallation targets made of Uranium and Americium (I. Mishustin, W. Greiner). This provides important input for the ongoing design of accelerator-driven systems (ADS) for *nuclear waste transmutation*.

Neuroscience

The activities of the group of J. Triesch mostly are concerned with the investigation of learning and self-organization processes in the brain using neural network models. In one study it was shown that the *distribution of synaptic strengths* and their pattern of fluctuations are explained by self-organization in a recurrent spiking network model combining spike-timing-dependent plasticity (STDP), synaptic scaling, structural plasticity, and intrinsic plasticity. The resulting dynamics produces lognormal-like weight distributions closely matching experimental data.

D. Nicolić, W. Singer, and colleagues have investigated the cortical *beta/gamma oscillations* (20-80 Hz) which are not yet fully understood. Exploration of networks containing either integrator or resonator inhibitory interneurons revealed that membrane resonance, as opposed to integration, promotes robust gamma oscillations having stable frequency via a mechanism called RING (Resonance INduced Gamma). The results compare favorably with measurements performed on the visual cortex of the cat.

In the framework of the Bernstein Focus Neurotechnology the group of J. Lücke studies novel approaches for *efficient and neurally plausible learning*. Basing their work on a probabilistic neuronal code they were able to train stimulus encoding models that are consistent with the stochastic activation of neurons and also match the observed neural response properties in primary visual cortex well. The model also was used to develop neural networks with optimal performance for the learning and classification of patterns.

Another line of research in the field of machine learning aims to exploit the principles of learning and development in biological organisms to build *autonomously learning robots*. This has led to the development of a curiosity-driven active vision system which autonomously explores its environment and learns object representations without any human assistance.

Life Science and Chemistry

Theoretical studies related to *heavy-ion tumor-therapy* are in the focus of several groups at FIAS. In 2012 the Monte Carlo Model for Heavy-Ion Therapy (MCHIT) developed by the nuclear physics branch (I. Mishustin, I. Pshenichnov, M. Bleicher) was used to simulate complex radiation fields generated by the impact of heavy ions. Microdosimetric characteristics were calculated for a broad selection of ions and beam energies, relevant for cancer therapy and also for predicting radiation exposure in space research. The MBN group has made predictions of possible direct thermomechanical biodamage, where The heat and pressure of the shock wave caused by passing ions is expected to directly produce DNA damage. Furthermore, the spatial dependence of the fluence of generated secondary electrons was calculated using a random walk model.

The Meso-Bio-Nano group at FIAS (A. Solov'yov) studies structure formation and dynamics of animate and inanimate matter, investigating a wide range of topics: atomic clusters, nanoparticles and biomolecules; collision, fusion, fission and fragmentation, self-organization and structure formation; assemblies of clusters/nanoparticles and bio-macromolecules, hybrid bio-nano systems, nanostructured materials; nanoscale phase transitions; thermal, optical and magnetic properties; collective phenomena; channeling effects, etc.

Notable achievements of the MBN group in 2012 have been: development of a versatile semiempirical model to calculate the *ionization of biomolecules* after ion impact; self-consistent calculation of the electronic structure of noble-gas *endohedral fullerenes*; the study of collective electron oscillations (various types of *plasmons*) in nanostructures; micromechanical investigation of the unzipping of double-stranded DNA; molecular dynamics simulations of *nanoscale phase transitions* (folding, melting, solidification, sublimation, multifragmentation) for large atomic clusters;

Computer Science

The efforts of the team of V. Lindenstruth to develop novel fast and power-efficient computer architectures in 2012 culminated in the construction of the SANAM supercomputer, a joint project of FIAS, HIC for FAIR and KACST/Saudi Arabia. The SANAM system combines a large number of CPUs and GPUs and provides a peak computing performance of 540 TFlop/s. SANAM reaches an unprecedented power efficiency of more than 2.3 GFlop/Watt which secured it second rank on the list of the most power-efficient supercomputers worldwide (Green500).

Another major achievement has been the flawless operation of the High-Level Trigger HLT at the Large Hadron Collider/CERN. The HLT is part of the ALICE experiment and has been instrumental for its recent successful experimental run. The HLT is capable of full online event reconstruction. Running on GPUs and employing sophisticated parallel tracking routines, the HLT achieves speedup factors of more than two orders of magnitude.

The optimization of computer codes used for simulations in theoretical physics has been another focus of research of the computer science group at FIAS. E.g., a program for relativistic hydrodynamics has been ported to run on GPUs using the OpenCL language which resulted in speedup factors of up to 500. Similarly, codes for Lattice Quantum Chromodynamics (LQCD) have been adapted and optimized for GPU usage.

1. Partner Research Centers

HIC for FAIR
Helmholtz International Center

Development of HIC for FAIR in 2012

by Björn Bäuchle, Marcus Bleicher, Gabriela Meyer

HIC for FAIR in short

HIC for FAIR has been founded in 2008 in the first call of the Hessian LOEWE initiative (Landes-Offensive zur Entwicklung Wissenschaftlich-ökonomischer Exzellenz). The Universities of Frankfurt, Darmstadt and Gießen, the FIAS, GSI Helmholtz-Zentrum für Schwerionenforschung, and the Helmholtz Association have bundled their resources and research activities to foster FAIR-related research in Hesse. HIC for FAIR covers all four research pillars of FAIR including especially PANDA, CBM, nuclear astrophysics (NuSTAR), APPA and accelerator physics. Expertise and funding is provided for the development of the various experiments, theoretical investigations and large-scale computing via LOEWE-CSC (Center for Scientific Computing).

New LOEWE professorships, Helmholtz Young Investigators and young scientists

HIC for FAIR is actively promoting young scientists. Three Helmholtz Young Investigator (HYI) groups have succeeded in a competitive selection procedure of the Helmholtz Association and have joined HIC for FAIR in 2012. One of the groups, led by Hannah Petersen, started to work at FIAS in October. Also in 2012, HIC for FAIR scientists Pasi Huovinen and Hendrik van Hees started at FIAS as research fellows. The number of doctoral students affilitated to HIC for FAIR research in its graduate school HGS-HIRe has increased to 238 young scientists coming from 32 different nations in 2012, 22 % of these are female.

Conferences and physics days

To foster internal communications within the four expert groups, a new series of seminars – the "physics days" – have been started in the summer. The HIC for FAIR physics days bring together the scientists in each expert group from the HIC for FAIR partners to exchange ideas, present progress and discuss new projects. All research fields of HIC for FAIR have been covered, from elliptic flow in hydrodynamics via neutrinos from supernova explosions and experimental results about Lamb-shift in hydrogen-like gold ions to linear accelerator developments.

More than 30 international conferences and workshops have been organized by HIC for FAIR scientists, 10 of which have been supported by FIAS scientists. One of these is FAIRness, the first of a series of conferences dedicated to young scientists involved with FAIR. FIAS scientists Marcus Bleicher and Hannah Petersen were among the organizers of that conference. FIAS hosted 32 visiting scientists from all over the world who contributed to the scientific program at HIC for FAIR.

Fruitful discussion at Expert Group 2's first physics day in June 2012. FIAS scientist Prof. Dirk Rischke (standing) answers questions. Photo: © Bjørn Bäuchle, HIC for FAIR.

ExtreMe Matter Institute EMMI

by Carlo Ewerz

The Extreme Matter Institute EMMI was founded in 2008 in the framework of the Helmholtz Alliance 'Cosmic Matter in the Laboratory' and is funded by the Helmholtz Association. The institute, which is managed by the GSI Helmholtz Center for Heavy Ion Research in Darmstadt, is dedicated to research in the area of matter at the extremes of density and temperature, ranging from the coldest to the hottest and densest forms of matter in the Universe. This comprises in particular the four key areas a) quark-gluon plasma and the phase structure of strongly interacting matter, b) neutron matter, c) electromagnetic plasmas of high energy density, d) cold quantum gases and extreme states in atomic physics. This research is carried out with a special emphasis on interdisciplinary aspects and common underlying concepts connecting the different research areas.

EMMI research is carried out in close collaboration with its 13 national and international partner institutions; the German partners are the universities of Darmstadt, Frankfurt, Heidelberg and Münster, the Forschungszentrum Jülich, the Max-Planck-Institut for Nuclear Physics in Heidelberg, and FIAS. To the latter EMMI has particularly close ties. The Scientific Director of EMMI, Prof. Peter Braun-Munzinger, is also a Senior Fellow of FIAS. The four EMMI Fellows (leaders of EMMI Fellow Groups) are also Fellows at FIAS.

In 2012, more than 400 scientisty contributed to the activities in EMMI, among them more than 150 doctoral students and more than 100 postdocs. The structured graduate education of doctoral students within EMMI is organized in close collaboration with the surrounding graduate schools, for example with the Helmholtz Graduate School for Hadron and Ion Research (HGS-HIRe), the Heidelberg Graduate School of Fundamental Physics (HGSFP), and the Helmholtz Research School Quark Matter Studies (H-QM).

In 2012, EMMI members have published more than 300 papers in refereed journals, and more than 100 contributions to conference proceedings. EMMI runs an active workshop program. 7 EMMI workshops and one four-week EMMI program with strong international participation were organized in 2012. In addition, 29 'EMMI Seminars' were organized in 2012 in which external experts and guest scientists present their work on subjects related to EMMI. These seminars, mostly taking place in Darmstadt, form a nucleus for frequently attracting EMMI members from the nearby partner institutions. 12 renowned experts have visited EMMI partner institutions for extended periods in 2012 as EMMI Visiting Professors, and have made progress in their collaborations with EMMI members. These and further EMMI activities are listed at www.gsi.de/emmi.

Since 2012, EMMI provides the possibility to have talks at EMMI workshops recorded on video. The recorded talks are made available to all EMMI members and other interested scientists.

EMMI organized two masterclass events for high school students in 2012. In these masterclasses the students analyzed actual data from the ALICE experiment at the Large Hadron Collider at CERN. The total number of participants was about 50.

Bernstein Focus Neurotechnology Frankfurt

by Visvanathan Ramesh and the BFNT PI team

The Bernstein Focus Neurotechnology: Frankfurt is aimed at bringing together an interdisciplinary team to design and implement a cognitive vision framework that demonstrates autonomous learning and multiple cue fusion in the context of specific applications such as security, surveillance and robotics. Since the project start, a number of scientific results have been produced in areas such as: developmen-tal psychology, unsupervised machine learning, architectural models for vision, and high-performance computing. A key challenge of this interdisciplinary project was in the setup the organization, processes, and in the establishment of common mindset and goals that balance scientific and engineering goals. In the year 2012, a key achievement has been the setup of a distributed, modular organization with efficient interfaces for integration that allows balance between components and systems research. Coordination between science and engineering threads are achieved through established management and software engineering processes.

Execution is now in two threads as envisioned in our revised plan – a scientific research thread, and a systems science and engineering thread focused on development of advanced models, architectures, and implementation of visual cognition systems. In the systems science and engineering thread, we have developed a rapid application engineering platform for computer vision and have verified the utility of the platform and processes by developing a video surveillance system. We have also made key progress in fusion of architectural views from systems engineering with neuroscience. The architectural model involves massively parallel modules performing feed-forward decomposition of input visual signal into constituent modalities (e.g. color, motion, texture, shadow, reflection, contours, etc.) that allow for indexing into a rich memory structure. Generated hypotheses are then refined via a dynamic, recurrent process to converge to an interpretation. While both engineering and neuroscience views of the architecture are in agreement at this higher level, practical considerations present a multitude of options on module selection, learning and inference approaches, and memory representation schemes. Our systems engineering methodology allows for parallel execution and exploration of the tradeoffs and systematic comparison of alternative models and approaches necessary. Progress has been made this year in alternative methods for hypotheses generators motivated from physics based modeling and machine learning. These methods have been incorporated into prototype demonstrators for video surveillance.

Our research in scientific components involves autonomous learning, self-organization, cue-integration and fusion. We have continued to investigate autonomous learning of visual representations with the iCub robot and have developed a self-calibrating system that learns representations of binocular images and so-called vergence motor commands to direct both cameras to the same point on an object. On the other hand we are continuing to develop our system for curiosity-driven learning of object representations. Recent efforts in parallelizing various aspects of the software have led to significant speed-ups in the corresponding modules, paving the way for large-scale experiments in the coming year. In the area of self-organization, we have studied random recurrent networks of firing rate neurons as a model of cortical circuits involved in object recognition and have demonstrated spontaneous formation of feature selectivities in a random recurrent neural network model of V1. Specifically, we examined selectivity for stimulus motion, probed by driving the network with a moving grating stimulus and illustrate that, for increasingly heterogeneous connections, increasingly strong levels of selectivity arise spontaneously in the network. In the area of machine learning, we have explored connections between Bayesian learning and bio-inspired learning architectures. One research highlight is our investigation of biologically relevant implementations for learning between hierarchical stages (single-cause hierarchical model) and the demonstration of equivalence of neutrally plausible learning to specific generative model based learning. Specifically, studies of single-cause Poisson mixture models were conducted, and it was shown that neurally plausible learning can be optimal, neurally plausible and corresponding optimal learning was implemented. Another key progress in machine learning from this year, involves the autonomous learning of mappings between frames in videos and the application of deep learning architectures to activity classification from video. We have published several peer-reviewed papers at international conferences and journals.

In summary, the BFNT team has made considerable progress in executing towards the goals of the project. In parallel, we have made significant strides in the last year to link to key academic and industrial partners in Europe, US and Asia and are establishing the foundations towards our longer-term goal of establishment of a strong systems science and engineering research network that will advance theory and practical construction of intelligent systems.

2. Graduate Schools

Helmholtz Graduate School for Hadron and Ion Research

and

Helmholtz Research School for Quark Matter Studies

by Henner Büsching and Gerhard Burau

In the past three years education of doctoral students associated with the GSI Helmholtzzentrum für Schwerionenforschung has seen a paradigm shift. The concept of structured doctoral education has been established and novel systematic education approaches in the training of doctoral students have been sucessfully introduced.

The Helmholtz Graduate School for Hadron and Ion Research (HGS-HIRe for FAIR) was established in October 2008 as a joint endeavor of GSI and the universities at Darmstadt, Frankfurt, Giessen, Heidelberg and Mainz together with FIAS to promote and support structured doctoral education for research associated with GSI and FAIR. It is supported by the Initiative and Networking Fund of the Helmholtz Association. In 2012 the Helmholtz Research School for Quark Matter Studies (H-QM) [originally a joint project of the GSI Helmholtzzentrum, Goethe-Universität Frankfurt and FIAS to specially support a selected group of highly talented students performing research in the field of heavy-ion physics] has been fully integrated in the structure of HGS-HIRe. Moreover, HGS-HIRe provides and centrally organizes, strongly supported by FIAS, the successful doctoral scholarship programs of GSI, HIC for FAIR and EMMI.

From the very beginning, we esteemed the possibilities of the Helmholtz Graduate School initiative very high as a tool to initiate novel structures and to assess nonstandard instruments and innovative measures in the fields of structured doctoral education. With more than 300 doctoral students and 90 alumni at the end of 2012 - nearly 30% of them with an international background - HGS-HIRe has succeeded in implementing many new structures for the benefit of the scientific community at GSI, FIAS and the partner universities. Even more important, we believe, in the past three years HGS-HIRe has strongly enhanced, improved and facilitated the educational, scientific and social life of many young researchers.

The strategic goals of HGS-HIRe for the first three years have been reached and have even been excelled in many aspects:

- Structured doctoral education has been commonly established at GSI and FAIR as well as at FIAS and the partner universities in the research fields of GSI and FAIR.
- New innovative concepts such as interdisciplinary Lecture Weeks, specialized Power Weeks and transferable skills training have been developed and are implemented.
- An active social and academic network within the local community of doctoral students has been established and has brought together students from the different participating institutions, different fields or theoretical and experimental groups, emphasizing the strong interdisciplinarity of the research at GSI and FAIR.
- Participating students are trained on a broader scientific basis and gain a comprehensive overview of their own and neighboring research fields.

- Organizational structures have been established to conduct and sustain a structured, high quality doctoral training.
- HGS-HIRe has gained international visibility and has started to build up a reputation for excellent doctoral education on a very high level.

In the year 2012 ten lecture weeks on various theoretical and experimental topics, three specialized power weeks, a total of thirteen seminars on transferable skills, and several HGS-HIRe Perspectives events have been organized by HGS-HIRe and H-QM. Last but not least three special events have been continued within the HGS-HIRe programm of 2012: The second joint Helmholtz-Rosatom School for Young Scientists at FAIR (held in Bekasova/Russia), a new issue of the international HGS-HIRe Summer Student Program at GSI, and finally the 4th HGS-HIRe Graduate Days held in the Alte Lokhalle in Mainz with more than 200 participants! Altogether these activities demonstrate impressively the manifold program of HGS-HIRe and H-QM.

The participants of HGS-HIRe contribute significantly to the scientific progress of their research fields. In the next years the Helmholtz Association together with its national and international partners is constructing the FAIR accelerator complex at GSI, one of the largest investments in fundamental research in Europe at this time. Participants of HGS-HIRe are trained and educated to lead and take responsibilities in this great scientific endeavor.

The success of the new measures has significantly raised acceptance of structured doctoral education among cooperating researchers, universities and doctoral students.

In our perception structured doctoral education shall give guidance, provide rich opportunities and support. It shall motivate and challenge and enable the students to excel to the best of their personal ability. Furthermore it shall set strategic goals and develop measures for structural, sustainable developments and improvements for the academic partners. The art and challenge of structured doctoral education on large scales as Helmholtz Graduate Schools is therefore to establish functional structures to address the individual needs of an increasing, large number of participants with a dedicated personalized approach. It needs to be structured education for every single, individual participant who hopes to profit strongly for his personal education and career. And it needs to be structured education with constant improvements, adaptations, modifications and a strong innovative spin for the scientific and academic community. We believe HGS-HIRe is on the right way in its first years of operation to excel on both sides of this delicate balance.

Special encouragement and motivation was a special recognition in early 2012: HGS-HIRe was selected as the only graduate program to be featured in the BMBF-documentation on examples of the Joint Initiative for Research and Innovation “Neue Dynamik in der Forschung - Beispiele aus dem Pakt für Forschung und Innovation”.

The best source to get an impression of the manifold, colorful, rich life in HGS-HIRe is our webpage `www.hgs-hire.de`.

FIGSS

The Frankfurt International Graduate School for Science

by Jochen Triesch

The Frankfurt International Graduate School for Science (FIGSS) is the graduate school of FIAS. It provides a framework for doctoral education at FIAS, while PhD degrees are officially granted by Goethe University. The students are encouraged to obtain their PhD within three years, but often take longer. They are typically funded by research grants to their advisors, since FIGSS does not have its own funding. Conventional funding mechanisms for graduate schools such as training grants of the DFG („Graduiertenkollegs“) or other agencies typically require a strong thematic focus, which is at odds with the breadth of research topics pursued at FIAS.

The number of FIGSS students has stabilized over the last years. Enrollment in December 2012 was 61 compared to 56 in 2010 and 66 in 2011. Six PhDs were awarded in 2012. This number is comparatively low, but only reflects a „natural“ fluctuation. We expect a substantially higher number for 2013. The fraction of female students has stayed at 15%, and the student population remains very international with 54% of our students being foreign nationals. The composition of FIGSS with respect to the different research disciplines was as follows (December 2012): Physics (39%), Neuroscience (25%), Computer Science (21%), Chemistry and Biology (15%).

A core activity of FIGSS continues to be its weekly seminar, held in the form of a lunch seminar with free pizza, where FIGSS students and post-docs report on the status of their PhD work. Care is taken that the talks are of high quality and understandable to an interdisciplinary audience. To this end, we use feedback forms that attendees fill in after every presentation and presentations are videotaped to give speakers feedback about their presentation style. The best presentation of each semester is awarded a bottle of Champagne.

Courses offered at FIGSS

Summer Semester 2012

J. Triesch	Methods for the study of complex systems, 2+1h
W. Greiner	Gauge Theory of Weak Interactions 2, 2h
I. Mishustin	Dynamical models for relativistic heavy-ion collisions, 2h
A. Solov'yov	Theoretical and computational methods in Meso-Bio-Nano Science, 2h
T. Burwick	Visual System - Neural Structure, Dynamics, and Function, 2h
S. Schramm	Quantum theory on the lattice, 2+1h
E. Engel	Quantum molecular dynamics, 2+1h
H.-J. Lüdde	Nonlinear dynamics and complex systems, 2+2h
D. Schuch	Nonlinearities and Dissipation in Classical and Quantum Physics, 2h
J. Triesch	Systems Neuroscience, Seminar, 2h

Winter Semester 2012/13

J. Triesch M. Kaschube	Theoretical Neuroscience, 2+1h
T. Burwick	Brain Dynamics: From Neuron to Cortex, 2h
I. Mishustin	Physics of Strongly Interacting Matter, 2h
A. Solov'yov	Theoretical and computational methods in Meso-Bio-Nano Science, 2h
C. Sasaki	Chiral thermodynamics of hot and dense QCD matter, 2h
P. Nicolini	Classical and quantum physics of black holes, 2+1h
S. Schramm	Nuclear and Neutrino Astrophysics, 2h
D. Schuch	Riccati and Ermakov Equations and the Quantum-Classical Connection, 2h

Regularly held seminars

FIGSS Seminar	– FIAS Fellows
Interdisciplinary FIAS Colloquium	– FIAS Fellows
Seminar on Meso-Bio-Nano-Science	– Solov'yov, Greiner
Current topics in theoretical neuroscience	– Triesch
NeuroBio Theory seminar series	– Kaschube, Triesch
Nuclear/Heavy ion group meeting	– Mishustin
Machine learning lunch seminar	– Lücke
Astro meeting	– Mishustin, Schramm
Journal club in high-energy physics	– Nicolini

Ph.D. degrees received by FIAS/FIGSS students in the year 2012

1	Tim Schuster	16.03.2012	Hadron ratio fluctuations in heavy-ion collisions
2	Thomas Weisswange	04.06.2012	Development of cue integration with reward-mediated learning
3	Mykhaylo Zynovyev	29.06.2012	Conceptual design of an ALICE Tier-2 centre integrated into a multi-purpose computing facility
4	Sohrab Saeb	05.09.2012	Learning active vision: from kinematics to decision making
5	Jaber Dehghany	10.10.2012	Mathematical modeling of insulin-secretory granules' dynamics in pancreatic beta-cells
6	Jochen Thäder	31.10.2012	Commissioning and Jet Physics with the ALICE High-Level Trigger

3. FIAS Scientific Life

Seminars and Colloquia at FIAS in the year 2012

The organization of common colloquia and seminars has played an inportant role for fostering an interdisciplinary spirit at FIAS. From the beginning, in the weekly “Interdisciplinary FIAS Colloquium” distinguished speakers were invited to give overview talks covering all scientific areas represented at FIAS. Since 2006 the “FIGSS Student Seminar” has been held, mainly as a platform for Ph.D. students to present their work. These events are addressing the ‘general public’ at FIAS and bring together the researchers and students from all scientific branches. In addition, various group seminars are held with a more focussed specialization. Their schedules are not listed in the following.

19.01.2012 **Prof. Dr. Matthias Kaschube,** Frankfurt Institute for Advanced Studies
Collective behavior in living systems

26.01.2012 **Prof. Dr. Visvanathan Ramesh,** Goethe University Frankfurt and FIAS
Systems science & engineering for computer vision

09.02.2012 **Prof. Dr. Laszlo Csernai,** Department of Physics and Technology, University of Bergen, Norway
Can we see consequences of low viscosity of Quark-Gluon Plasma?

16.02.2012 **PD Dr. Katia Parodi,** Heidelberg Ion Beam Therapy Center at the Heidelberg University Hospital, Heidelberg, Germany
Monte Carlo modeling and in-vivo imaging to support high precision ion beam therapy

08.03.2012 **Prof. Dr. Wolfgang König,** House of Finance, Goethe University
Bridging barriers by negotiated culture – the case of IT offshoring in a bank

16.03.2012 **Dr. René Doursat,** Universidad de Malaga, Spain, Complex Systems Institute, Paris, and Ecole Polytechnique, France
Morphogenetic “neuron flocking”: dynamic self-organization of neural activity into mental shapes

26.03.2012 **Prof. Dr. Wolfgang Bauer,** Michigan State University, East Lansing, MI, USA
Energy – partial solutions for the biggest problem of our century

10.05.2012 **Prof. Dr. Joachim Denzler,** Friedrich Schiller University, Jena
Understanding aesthetic perception: ideas and first results from a computer vision perspective

16.05.2012 **Prof. Dr. Simon Connell,** Dept. of Physics, University of Johannesburg, South Africa
Some physics using near perfect diamond

24.05.2012 **Dr. Piero Nicolini,** FIAS/Goethe University, Frankfurt
The gravitational field at the shortest scales

21.06.2012 **Dr. Alexandre Gumberidze,** EMMI Fellow, Extreme Matter Institute, GSI, Darmstadt
Structure and dynamics of highly-charged ions: physics at extreme fields

28.06.2012 **Dr. Paul Neumayer,** EMMI Fellow, Extreme Matter Institute, GSI, Darmstadt
Studying matter at extreme astrophysical conditions in the laboratory

14.09.2012 **Prof. Dr. Bruno Olshausen,** University of California, Berkeley
20 years of learning about vision: questions answered, questions unanswered, and questions not yet asked

11.10.2012 **Prof. Dr. Réjean Plamondon,** École Polytechnique de Montréal
Emergence of four physical interactions

18.10.2012 **Prof. Dr. Elisabeth Gräb-Schmidt,** Eberhard-Karls-Universität Tübingen
Freedom explained: illusion or reality?

25.10.2012 **Prof. Dr. P. C. Mishra,** Banaras Hindu University, Varanasi, India
Molecular mechanism of DNA damage, repair and its prevention

15.11.2012 **Prof. Dr. Peter Hess,** Instituto de Ciencias Nucleares, UNAM, Mexico
A new theory of gravitation: experimental verifications

22.11.2012 **Prof. Dr. Mark Strikman,** Penn State University
Colorful physics of hadrons in high-energy (anti)proton-nucleus collisions

FIGSS Seminar

09.01.2012 **Hendrik von Hees**
Heavy-quark diffusion in the Quark Gluon Plasma

16.01.2012 **Claudio Ebel**
Calculation of realistic electrostatic potentials in star crusts

23.01.2012 **Marc Henniges**
Probabilistic generative models for component extraction from visual data

30.01.2012 **Alexander Yakubovich**
Thermomechanical mechanism of radiation biodamage by ions

06.02.2012 **Christoph Herold**
Nonequilibrium phenomena near the QCD phase transition

16.04.2012 **Viola Priesemann**
Self-organized criticality as a universal brain state in humans across all vigilance states

23.04.2012 **Carl Svensson**
A generative model of circulating tumor cells

30.04.2012 **Catalin Rusu**
ZAP or: How I learned to stop worrying and love magnetic stimulation

07.05.2012 **Daniela Pamplona**
Deriving retinal ganglion cell properties from the natural input to the visual system

14.05.2012 **Sarah Becker**
Fundamental properties of an increasingly renewable European electricity system

21.05.2012 **Lucas Burigo**
Monte Carlo simulations in heavy-ion cancer therapy

04.06.2012 **Quan Wang**
Infants in control: rapid anticipation of action outcomes in a gaze-contingent paradigm

11.06.2012 **Matthias Rupp,** ETH Zurich
Machine learning for quantum mechanics: density functionals and energy estimates

18.06.2012 **Alessandro Brillante**
Transition from neutron stars to quark stars

02.07.2012 **Matthias Hanauske**
Evolutionary quantum game theory in the context of socio-economic networks

15.10.2012 **Dmitry Tsigankov**
Non-equilibrium molecular transport in spiny dendrites and its role in synaptic plasticity

22.10.2012 **Zhenwen Dai**
Unsupervised learning of translation invariant occlusive components in visual scenes

29.10.2012 **Alexey Verkhovtsev**
Study of collective electron excitations in fullerenes by inelastic scattering of fast electrons

04.11.2012 **Yury Malyshkin**
Modeling of accelerator driven systems for transmutation of nuclear waste

12.11.2012 **Rudy Marty**
Simulation of the expansion and the phase transition of a quark/antiquark plasma

19.11.2012 **Hamza Berrehrah**
Study of heavy quark bound states ''Travel'' and the associated collective phenomena in a thermalized quarks gluons soup

26.11.2012 **Alexander Yakubovich**
Kinetics of liquid-solid phase transition in large nickel clusters as seen via calculations with graphics processing units

10.12.2012 **Vitalii Ozvenchuk**
Dynamical equilibration and transport coefficients of strongly-interacting parton matter

17.12.2012 **Luca Lonini**
Learning to see with two eyes

Conferences and meetings (co)organized by FIAS in the year 2012

▷ **Kyutech-FIAS Joint Workshop on** ***Brain Systems Technology,***
Kitakyushu, Japan, January 8, 2012

▷ **3rd International Workshop** ***"Future Challenges in Tracking and Trigger Concepts",***
Frankfurt, February 27 - 29, 2012

▷ **NICA/JINR-FAIR Bilateral Workshop** ***"Matter at highest baryon densities in the laboratory and in space",*** Frankfurt, April 2 - 4, 2012
`theor.jinr.ru/~nica_fair/`

▷ **Ernst Strüngmann Forum,** ***"Cultural Evolution",***
Frankfurt, May 27 - June 1, 2012
`www.esforum.de/forums/esf12_cultural_evolution.html`

▷ **ICIS 2012,** ***Preconference Workshop on Developmental Robotics***,
Minneapolis MN, USA, June 6, 2012
`www.frontiersin.org/events/ICIS_2012_Preconference_Workshop_on_Developmental_Robotics/1663`

▷ ***"Identifying the Self: Delusions, Full-Body Illusions, and Perceptual Unity",*** 16. Meeting of the Junior Research Group "Philosophy of Mind", Frankfurt, June 21 - 24, 2012
`fias.uni-frankfurt.de/mindgroup/index.php/meeting-16.html`

▷ **Ernst Strüngmann Forum,** ***"Schizophrenia",***
Frankfurt, July 22 - 27, 2012
http://www.esforum.de/forums/esf13_schizophrenia.html

▷ **FAIRNESS 2012,** ***Workshop for young scientists with research interests focused on physics of FAIR,*** Hersonissos, Greece, September 3-8, 2012
`fias.uni-frankfurt.de/de/fairness/`

▷ ***"Formal Phenomenology and the Self-Representational Structure of Consciousness",*** 17. Meeting of the Junior Research Group "Philosophy of Mind", Mainz, September 5 - 6, 2012
`http://fias.uni-frankfurt.de/mindgroup/index.php/meeting-17-46.html`

WPCF 2012, ***VIII Workshop on Particle Correlations and Femtoscopy ,***
Frankfurt, September 10-14, 2012
`fias.uni-frankfurt.de/de/wpcf/`

▹ **Joint Workshop *“Systemic Risk: Economists Meet Neuroscientists”,***
Frankfurt, September 17-18, 2012
`www.hof.uni-frankfurt.de/de/Systemic-Risk.html`

▹ **Ernst Strüngmann Forum, *"Rethinking Global Land Use in an Urban Era",***
Frankfurt , September 23 - 29, 2012
`www.esforum.de/forums/esf14_global_land_use.html`

▹ **DySoN 2012, International Conference *"Dynamics of Systems on the Nanoscale",***
Sankt Petersburg, Russia, September 30 - October 4, 2012
`fias.uni-frankfurt.de/dyson/home/`

▹ ***"Delusions and the Sense of Agency",*** 18. Meeting of the Junior Research Group "Philosophy of Mind", Mainz, October 17, 2012
`http://fias.uni-frankfurt.de/mindgroup/index.php/meeting-18-48.html`

▹ **NEOS 2012, *"Nuclear Equation of State for Compact Stars and Supernovae",***
Frankfurt, November 28 - 30, 2012
`fias.uni-frankfurt.de/~neos2012/`

▹ **IM-CLeVeR, *FIAS winter school "Intrinsic Motivations: From Brains to Robots",***
Frankfurt, December 3 - 8, 2012
`http://www.im-clever.eu/announcements/events/fias-winter-school`

In addition, members of FIAS were involved in the organization of various other conferences and workshops.

Talks at the FIAS Forum in the year 2012

The FIAS Forum was initiated in the year 2009. It provides a framework for a series of public evening lectures on scientific topics addressed to a broader audience of interested citizens of Frankfurt and the surrounding region.The speakers are mostly, but not exclusively, senior members of FIAS or scientists related to them. As a public-outreach activity, the FIAS forum strives to strengthen the understanding of scientific issues in the general public and at the same time to raise the awareness level of the Institute in Frankfurt and the Rhein-Main area. The events of the FIAS Forum have attracted a considerable number of participants, often filling the FIAS lecturing hall to its capacity, and also regularly generate a press echo in the local media.

19.01.2012 **Prof. Dr. Jochen Triesch,** Johanna-Quandt-Forschungsprofessor am FIAS, Frankfurt am Main
Säuglinge übernehmen die Kontrolle - Neue Erkenntnisse über die frühkindliche Hirnentwicklung

01.03.2012 **Prof. Dr. Anna Starzinski-Powitz,** Dekanin Fachbereich Biowissenschaften, Goethe-Universität Frankfurt
Pommes, Koks und Co - Wie unser Lebensstil die Ausprägung unserer Gene beeinflussen kann

26.04.2012 **Prof. Dr. Hermann Requardt,** Vorstandsmitglied der Siemens AG, München
Patente – eine Notwendigkeit in Forschung und Industrie

23.05.2012 **Prof. Dr. Eberhard Umbach,** Karlsruher Institut für Technologie (KIT)
Energie und Klima - Wie bewältigen wir die Herausforderungen?

05.07.2012 **Prof. Dr. Dr. h.c. mult Walter Greiner,** Goethe-Universität Frankfurt
Antimaterie: Was ist sie? – Gibt es sie im Weltall? Gefahren und Chancen

25.10.2012 **Prof. Dr. Gheorghe Stratan,** Joint Institute for Nuclear Research, Dubna and Horia Hulubei Institute of Physics and Nuclear Engineering, Bucharest
How did Galileo's and Kepler's astronomic discoveries impact our world? Scientific, philosophic and religious reactions

29.11.2012 **Prof. Dr. Jan Pieter Krahnen,** House of Finance, Lehrstuhl Kreditwirtschaft und Finanzierung, Goethe Universität Frankfurt am Main
Europas Banken in der Systemkrise - Re-Regulierung und Forschungsbedarf

4. Research Reports

4.1 Nuclear Physics, Particle Physics, Astrophysics

Evolution of antibaryon abundances in the early universe and in heavy-ion collisions

Collaborators: I. N. Mishustin[1,2], L. M. Satarov[1,2], W. Greiner[1]

[1] Frankfurt Institute for Advanced Studies, [2] National Research Center "Kurchatov Institute", Moscow, Russia

Standard thermal model calculations (A. Andronic et al., Phys. Lett. B 673 (2009) 142) overestimate noticeably the proton- and antiproton-to-pion ratios observed in central Pb+Pb collisions at LAC bombarding energies. According to UrQMD calculations (J. Steinheimer et al., Phys. Rev. Lett. 110 (2013) 042501) this may be a consequence of annihilation processes at late stages of a heavy-ion collision. In the present work we have studied the dynamics of production and annihilation of (anti) baryons in nuclear collisions at SPA, RICH and LAC energies. We have simplified the set of rate equations for (anti)baryon multiplicities (J.I. Kapusta et al., Phys. Rev. C 68 (2002) 014901), by assuming that all $\overline{B}B$ annihilation cross sections are approximately equal to the $\overline{N}N$ annihilation cross section taken at the same relative velocity.

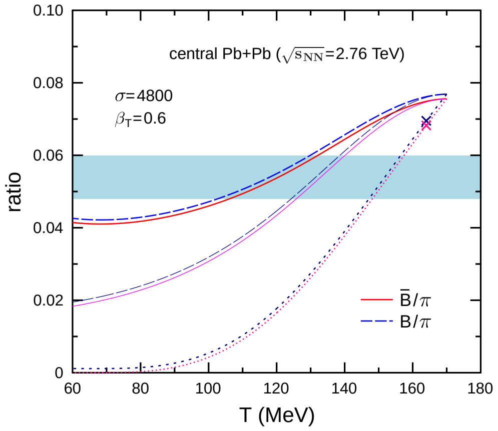


Figure: (Anti)baryon-to-pion ratios as functions of temperature in central Pb+Pb collisions at $\sqrt{s_{NN}} = 2.76$ TeV. Thick (thin) solid and dashed lines show the results with (without) transverse fireball expansion. Dotted lines represent these ratios in chemically equilibrium. Shading shows experimental bounds for B/π and $\overline{B}/\pi$ ratios obtained from ALICE midrapidity data. The predictions of thermal model are shown by the cross.

In our study we consider a homogeneous hadronic fireball, produced after hadronization of quark–gluon plasma and expanding adiabatically in longitudinal and transverse directions. It is assumed that initially the fireball is in the chemical and thermal equilibrium at the temperature $T = 170$ MeV. The temperature dependence of equilibrium chemical potentials along the adiabate $\sigma = S/B =$ const is calculated by using the ideal gas equation of state with excluded volume corrections. At given bombarding energy we choose the parameter σ equal to its "chemical freeze-out" value found in the thermal model. This in turn leads to a good agreement with observed ratios of meson multiplicities.

The expansion effects are taken into account by introducing a time-dependent volume of the fireball, $V = V(t)$. The 1D–Bjorken expansion corresponds to the case when $V(t)$ is proportional to t. To study the sensitivity to the choice of $V(t)$, we use a parametrization including the transverse expansion characterized by a transverse collective velocity β_T. The time-dependence of temperature $T(t)$ is found from the condition of total entropy conservation. The figure shows the results of calculations for Pb+Pb central collisions at the LAC energy. One can see that the annihilation of B-Bbar pairs continues even below the chemical freeze-out temperature of 165 MeV. The observed ratios can be reproduced only if the temperature is dropped to 120 MeV. Additionally about 30% of B-Bbar pairs have chance to annihilate when the system cools down from 165 to 120 Mev. According to our calculations, the assumption of common chemical freeze-out postulated in thermal models is not valid at least for antibaryons at SPS, RHIC and LHC collision energies.

We performed analogous calculation to study the evolution of antibaryon abundances in the early universe. As compared to heavy–ion collisions, deviations from chemically equilibrium for (anti)nucleons take place much later in this case. No clear signs of chemical freeze-out are noticed until the temperatures drops to $T \sim 1$ MeV. This explains extremely low primordial antinucleon-to-photon ratio observed in the present universe.

Related publication:

I.N. Mishustin, L.M. Satarov and W. Greiner, *Evolution of antibaryon abundances in the early universe and in heavy-ion collisions*, paper in preparation

The effects of medium on nuclear properties in multifragmentation

Collaborators: J. N. De[1], S. K. Samaddar[1], X. Viñas[2], M. Centelles[2], I. N. Mishustin[3], W. Greiner[3]

[1]Saha Institute of Nuclear Physics, 1/AF Bidhannagar, Kolkata, India, [2]Departament d'Estructura i Constituents de la Matèria, Facultat de Física and Institut de Ciències del Cosmos, Universitat de Barcelona, Spain, [3]Frankfurt Institute for Advanced Studies

In multifragmentation of hot nuclear matter, properties of fragments embedded in a soup of nucleonic gas and other fragments should be modified as compared with isolated nuclei. Such modifications are studied within a simple model where only nucleons and one kind of heavy nuclei are considered. The interaction between different species is described with a momentum-dependent two-body potential whose parameters are fitted to reproduce properties of cold isolated nuclei. The internal energy of heavy fragments is parametrized according to a liquid-drop model with density and temperature dependent parameters. Calculations are carried out for several subnuclear densities and moderate temperatures, for isospin-symmetric and asymmetric systems. We find that the fragments get stretched due to interactions with the medium and their binding energies decrease with increasing temperature and density of nuclear matter.

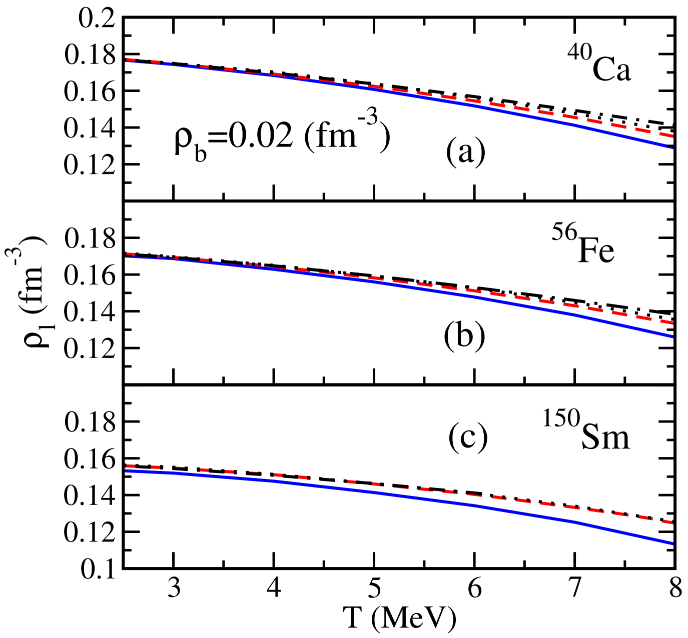


Figure: The nucleon number density in the nuclei (^{40}Ca, ^{56}Fe or ^{150}Sm) shown as a function of temperature, for baryon density $\rho_b = 0.02$ fm^{-3}. The red line corresponds to calculations when all interactions, (AA), (AN) and (NN), are included, The blue line shows the results when (AN) interaction is neglected, while the green line shows the results when both (AN) and (AA) interactions are neglected.

Questions may arise on the justification of the choice of only one kind of species in the calculations. Close examination of the results shows that in the medium, the interaction of the nuclei with surrounding nucleons plays the dominant role in bringing modifications in their properties. The nucleus-nucleus interaction has a negligible role. These results allow us to conclude that heavy nuclei embedded in the medium are affected mostly by the nucleons (and perhaps light clusters) surrounding them. This means that the description of the multicomponent nuclear system can be simplified by subdividing it into noninteracting cells containing one heavy nucleus and a proportional amount of the medium (Wigner-Seitz approximation). These results might be of significant relevance in the context of nuclear astrophysics and needs further exploration.

Related publications in 2012:

1) J. N. De, S. K. Samaddar, X. Viñas, M. Centelles, I. N. Mishustin, W. Greiner, *Effects of medium on nuclear properties in multifragmentation*, Phys. Rev. C 86, 024606 (2012)

Production of exotic projectile hypernuclei in collisions of relativistic ions

Collaborators: A. S. Botvina[1,2], I. N. Mishustin[1,3], J. Pochodzalla[4]

[1] Frankfurt Institute for Advanced Studies, [2] Institute for Nuclear Research, Moscow, Russia, [3] Kurchatov Institute, Moscow, Russia, [4] Institut für Kernphysik, J. Gutenberg-Universität Mainz

The investigation of hypernuclei allows to answer many fundamental questions of nuclear physics. In particular, discovery of new hypernuclei leads to extension of the nuclear chart into the strangeness sector. Studying properties of hypernuclei helps to understand the structure of conventional nuclei too. Hypernuclei provide a bridge between traditional nuclear physics (dealing with protons and neutrons) and hadron physics. Strangeness is an important degree of freedom for the construction of QCD motivated models of strong interactions. Also, hyperons should be abundant in nuclear matter at high baryon densities, which are realized in cores of neutron stars and in relativistic heavy-ion collisions . It has been realized long ago that the absorption of hyperons in spectator regions of peripheral relativistic ion collisions is a promising tool for producing hypernuclei. However, only recently the reliable experiments were conducted by HypHI collaboration at GSI Darmstadt, and the realistic calculations of these processes based on microscopic transport and statistical models were performed.

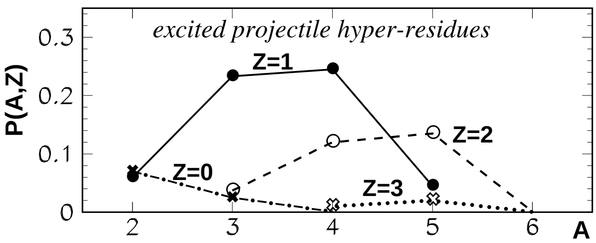


Figure: The relative probability to produce projectile residues with one absorbed Λ, mass A and charge Z as predicted by calculations for ^{6}Li (2 AGeV) + ^{12}C reaction. The dot-dashed, solid, dashed, and dotted lines correspond to residues with Z=0, 1, 2, and 3.

The HypHI collaboration has reported on the production of light hypernuclei in the disintegration of 2 GeV per nucleon ^{6}Li projectiles impinging on a ^{12}C target. In particular, $^{3}_{\Lambda}$H and $^{4}_{\Lambda}$H were identified, as well as bumps in the π^{-}-deuteron and π^{-}-triton invariant mass distributions. The latter may be interpreted as an evidence for production of bound Λ-neutron systems.

We have developed a combined approach where the first dynamical stage of this collision process is described within the Dubna cascade model (DCM), which can calculate production of Λ hyperons and their absorption in spectators. Then, the statistical disintegration of the spectator matter is considered within the Fermi break-up model generalized for excited hypernuclei. The DCM calculations of ^{6}Li (2 A GeV) + ^{12}C collisions predict formation of a broad ensemble of projectile residues with captured Λ hyperons shown in the figure. The following evolution depends on excitation energy of these residues: Their baryon content will not change significantly if the excitations are low. In the case of high excitations the residues will loose some nucleons, but small final hypernuclei will be produced abundantly, including exotic Λ-neutron (Λ*n* and Λ*nn*) hyper-systems. These results are consistent with the HypHI observations. The crucial component of this two-stage mechanism is formation of an intermediate moderately-excited hypernuclear system, which later on breaks up into normal fragments and hypernuclei. Obviously, similar processes can be realized in many nuclear reactions induced by high energy particles.

Related publications in 2012:

1) A.S. Botvina, I.N. Mishustin, J. Pochodzalla, *Production of exotic hypernuclei from excited nuclear systems*, Phys. Rev. C 86, 011601 (2012)
2) A.S. Botvina, K.K. Gudima, J. Steinheimer, I.N. Mishustin, J. Pochodzalla, A. Sanchez-Lorente, M. Bleicher, H. Stöcker, *Production of hyper-nuclei in peripheral collisions of relativistic ions.* Nucl. Phys. A 881, 228 (2012)

A comparative study of statistical models for nuclear equation of state of stellar matter

Collaborators: N. Buyukcizmeci[1,2], A. S. Botvina[1,3], I.N. Mishustin[1,4], R. Ogul[1], M. Hempel[5], J. Schaffner-Bielich[6], F.-K. Thielemann[5], S. Furusawa[7], K. Sumiyoshi[8,9], S. Yamada[8,10], H. Suzuki[11]

[1] Frankfurt Institute for Advanced Studies, Frankfurt, Germany, [2] Selcuk University, Konya, Turkey, [3] Institute of Nuclear Research, Moscow, Russia, [4]Kurchatov Institute, Moscow, Russia, [5]Universität Basel, Basel, Switzerland, [6]Institute for Theoretical Physics, Frankfurt am Main, Germany, [7]Waseda University, Tokyo, Japan, [8]Numazu College of Technology, Japan, [9]Theory Center, KEK, Japan, [10]ARISE, Waseda University, Japan, [11]Tokyo University of Science, Japan

In this collaborative project we study the equation of state (EOS) and nuclear composition of stellar matter at subnuclear densities and temperatures (0.5-10 MeV) expected to occur during the collapse of massive stars and supernova explosions. We compare the predictions of three different statistical models: the Statistical Model for Supernova Matter (SMSM) [1], the statistical model of M. Hempel and J.Schaffner-Bielich (HS) [2] and the statistical model of S. Furusawa, S.Yamada, K. Sumiyoshi and H.Suzuki (FYSS) [3] are compared. Calculations are done for two electron fractions, 0.4 and 0.2. Detailed results are presented in ref. [4]. It is demonstrated that the basic thermodynamic quantities e.g. pressure (see figure), entropy, chemical potentials of stellar matter under these conditions are similar in these three models, except in the region of high densities and low temperatures.

However, the mass and isotopic distributions have considerable differences related to the different assumptions of the models on properties of nuclei at these stellar conditions. Overall, the three models give similar trends, but the details reflect the uncertainties related to the modelling of medium effects, such as the temperature and density dependence of surface, bulk and symmetry energies of heavy nuclei, and the nuclear shell structure effects. We discuss similarities and differences between supernova matter and matter produced in heavy-ion collisions to emphasize the relationship between astrophysical conditions and nuclear experimental data. This comparison is especially useful in the region of the liquid-gas phase transition where the mass distributions of nuclei are especially broad. We hope that our analysis will help to develop more realistic models for nuclear composition and EOS of stellar matter. This work is relevant to the planned studies of exotic nuclei in future FAIR experiments.

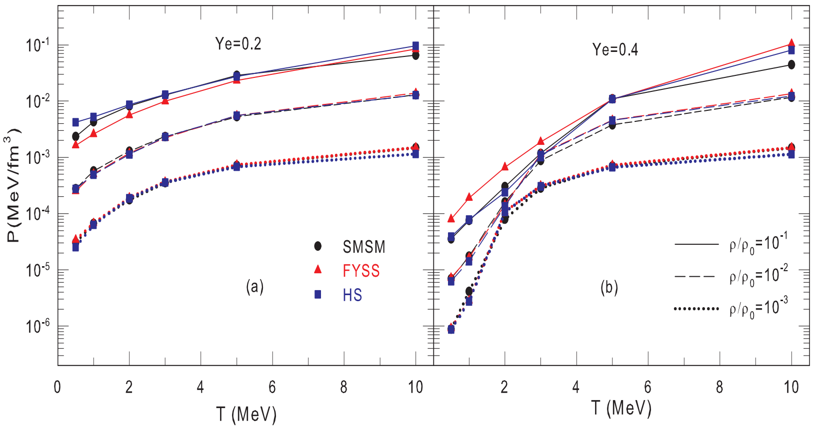


Figure: Comparison of SMSM, HS, and FYSS model results for the pure nuclear pressure as a function of temperature.

References:

1) A.S. Botvina, I.N. Mishustin, Phys. Lett. B 584, 233 (2004); Nucl. Phys. A 843, 98 (2010)
2) M. Hempel and J. Schaffner-Bielich, Nucl. Phys. A 837, 210 (2010)
3) S. Furusawa, S. Yamada, K. Sumiyoshi, H. Suzuki, Astrophys. Journal 738, 178 (2011)
4) N. Buyukcizmeci, A.S. Botvina, I.N. Mishustin, R. Ogul, M. Hempel, J. Schaffner-Bielich, F.-K. Thielemann, S. Furusawa, K. Sumiyoshi, S. Yamada, H. Suzuki, submitted to Nucl. Phys. A (2012), arXiv:1211.5990 [nucl-th]

Realistic electrostatic potentials in a neutron star crust

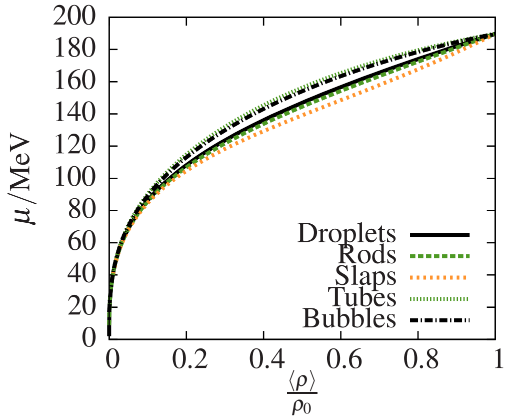
Collaborators: Claudio Ebel[1], Igor N. Mishustin[1,2], Thomas J. Bürvenich[1], Walter Greiner[1]

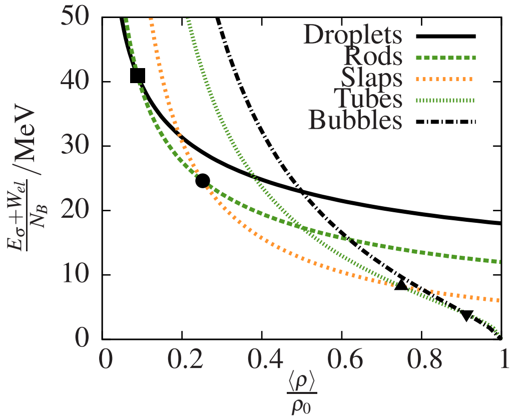
[1] Frankfurt Institute for Advanced Studies, [2] Kurchatov Institute, Moscow

Our goal is it to study the geometrical structure of nuclear matter in the crusts of neutron stars or in supernovae explosions. Such matter is composed of nuclei, free neutrons and electrons under the condition of electrical neutrality. Our calculations are performed within the Wigner-Seitz approximation, where the whole system is divided into electro-neutral cells, each containing one nucleus and a corresponding number of electrons. The calculations are done for spherical, cylindrical and Cartesian geometries. Generally, these geometrical configurations are called “pasta phases”.

Cells with five different geometrical shapes were filled with nuclear matter according to the average baryon density and electron-to-baryon ratio. The nuclear matter is assumed to occupy only a fraction of the cell with density equal to the normal nuclear density $\rho_0 = 0.15$ fm^{-3}. The electron distributions are calculated self-consistently in every configuration using Thomas-Fermi approximation. Then we obtain corresponding electron chemical potentials (left figure) and electrostatic energies (right figure). Since the bulk nuclear energy is independent of geometry, a most favourable phase is determined by the sum of the surface energy and the electrostatic energy. As our calculations show, with increasing average baryon density the favourable phases go in the following sequence: spherical nuclei, cylindrical rods, planar slobs, cylindrical tubes, spherical bubbles. It is interesting to note that pasta phases occupy a relatively narrow interval of baryon densities $(0.1 \div 0.9)\rho_0$.

Our results show that corrections due to non-uniform electron distributions grow with density and may reach 25%. They should be taken into account in realistic calculations of nuclear structure in dense stellar environments. The accurate evaluation of electron chemical potentials is needed in calculations of nuclear α- and β-stability and neutrino-induced reactions. As the next step we are going to perform self-consistent calculations of nuclear density profiles and electron distributions. The extension to finite temperatures is also planned.





Left figure: The chemical potential of electrons as function of avarage baryon density (in units of ρ_0=0.15 fm^{-3}) calculated for different geometrical shapes.

Right figure: The sum of Coulomb and surface energies for each geometrical shape as a function of avarage baryon density. The points where the geometry is changing are marked by symbols.

Related publications:

1) C. Ebel, I. N. Mishustin, W. Greiner, *Realistic electrostatic potentials in a neutron star crust*, to be published
2) I. N. Mishustin, T. J. Bürvenich, C. Ebel, W. Greiner, *Nuclei embedded in a neutron gas*, paper in preparation

Modeling Cosmic Phase Transitions in Dynamical Environments

Collaborators: D. Yueker[1], C. Ebel[1,2], I. N. Mishustin[1,2], M. Bleicher[1,3]

[1] Frankfurt Institute for Advanced Studies, [2] Kurchatov Institute, Russian Research Center, Moscow, Russia
[3] Institute for Theoretical Physics, Goethe University, Frankfurt, Germany

The investigation of phase transitions in the early universe is an important testing ground for the standard model of particle physics. Particularly interesting in this context are the electroweak and the QCD phase transitions. Our calculations were done for the deconfinement transition where the high-temperature phase of quarks and gluons transforms to the hadronic matter. The critical temperature for this phase transition is about 170 MeV which is reached at a time $t = 10^{-5}$s after the big bang. We have designed a simple field-theoretical model to investigate the role played in this phase transition by the background dynamics . Although the deconfinement phase transition at small baryon densities is expected to be of a crossover type, we have also considered a hypothetical possibility of a 1-st order phase transition. In this case one should expect a supercooling effect due to the trapping of the order-parameter field in a metastable state. Such a situation should lead to a mini-inflation scenario, which has been discussed by some authors.

We elaborated cosmological and thermodynamic conditions in the early universe at a QCD phase transition. Then we applied a dilaton-type field-theoretical model for a cosmic phase transition and discussed the characteristic time scales associated with possible supercooling and reheating. The dynamics of a delayed phase transition and its impact on the cosmological evolution were described self-consistently. In the course of this project we have found an exact analytic solution of Friedman's equations for a universe composed of radiation and vacuum energy density. Its graphical representation is shown in the left figure below.

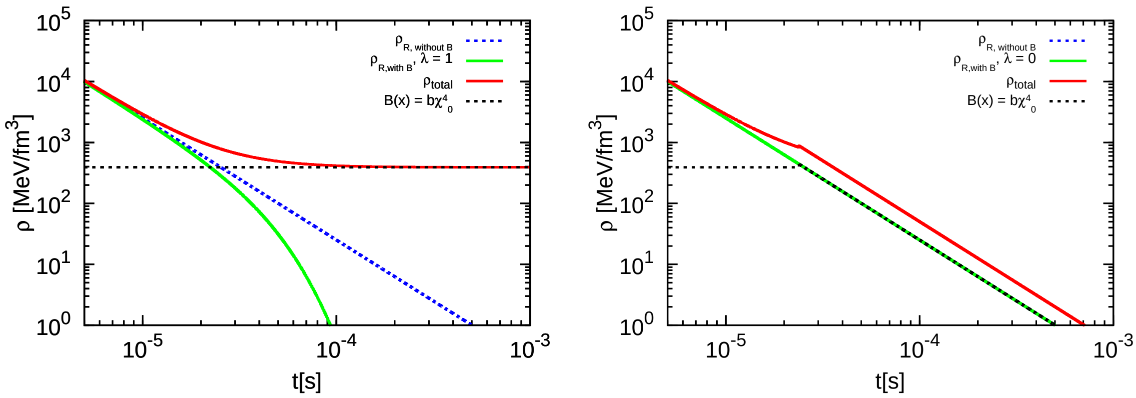


Figure: Logscale plots of different components of energy density for two scenarios: no phase transition (left) and first order phase transition with delay time of 10 $10\mu s$. The dashed blue line shows the evolution of ρ_R in a standard radiation dominated universe, the green line displays the same for a universe with an additional vacuum energy density $B = b\chi_0^4$ (black dotted line). The total energy density is reprreesented by red line.

From our analysis we conclude that trapping of the order-parameter field in the maetastable state might cause a mini-iinflation behaviour like in a very early universe. However, for this to happen the delay time must be comparable with the time scale of the universe expansion at this epoch. This is very unlikely for QCD-related phase transitions. The electroweak phase transition, associated with the Higgs mechanism, will be a good candidate for further investigations in that direction.

Related publications:

D. Yueker, C. Ebel, I.N. Mishustin and M. Bleicher, *Delayed phase transitions in early universe*, paper in preparation

Radial oscillations of compact stars in General Relativity

Collaborators: A. Brillante[1,2], I. N. Mishustin[1,3]

[1] FIAS, Frankfurt am Main, [2] Goethe University, Frankfurt am Main [3] Kurchatov Institute, Moscow

We review the equations governing adiabatic, small radial oscillations of compact stars within the framework of general relativity. We apply these equations to modern realistic equations of state and compute oscillation frequencies for hadronic stars, strange quark stars and hybrid stars. The solution of these equations allow to distinguish dynamically stable equilibria from those which are unstable.

We start with the spherically symmetric line element $ds^2 = -e^{2\Phi}dt^2 + e^{2\Lambda}dr^2 + r^2(d\theta^2 + sin^2\theta d\phi^2)$ and the energy-momentum tensor for a perfect fluid $T^{\mu\nu} = (\rho + P)u^\mu u^\nu + Pg^{\mu\nu}$. To derive the oscillation equation Einstein's equation $G^{\mu\nu} = 8\pi T^{\mu\nu}$ is perturbed in such a way, as to preserve spherical symmetry. This is done by expressing all time tependent quantities as a sum of a time independent part and a time dependent perturbation. Omitting all nonlinear terms in the amplitude and velocity one can obtain the following equation, first derived by Chandrasekhar in 1964:

$$0 = \frac{d}{dr}\left[P\frac{d\zeta}{dr}\right] + \left[Q + \omega^2 W\right]\zeta$$

where P, Q and W are functions of the equilibrium quantities of the star. Here ζ denotes the renormalized Lagrangian displacement of a fluid element due to the oscillation. All perturbed quantities are assumed to have a harmonic time dependence.

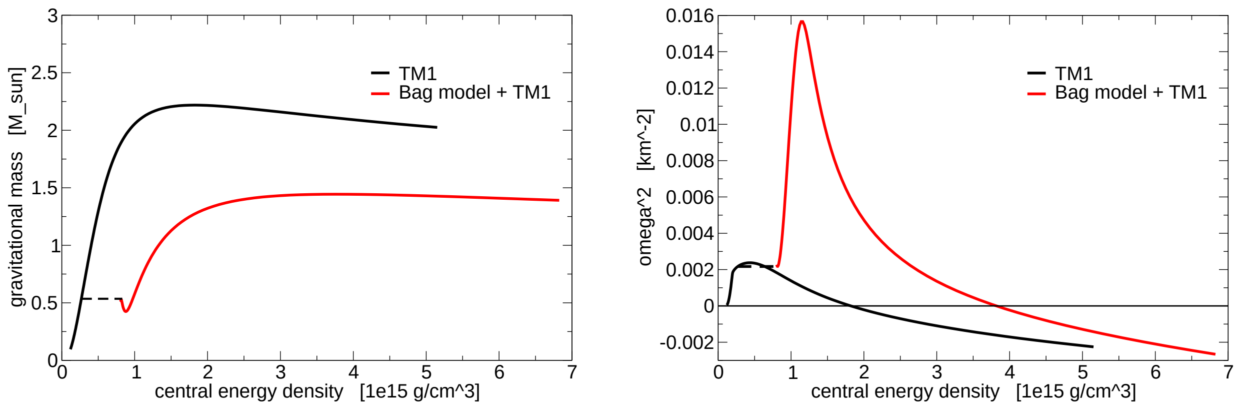


Figure: Calculated gravitational masses (left) and squared oscillation frequencies (right) of hadron stars (black lines) and hybrid stars (red lines) as functions of central energy density. The dashed horizontal lines show the discontinuity in the central density for hybrid stars. Crossing zero frequency line corresponds to the maximum mass of the atar sequence (turning point criterion).

For the hadronic phase we employ the relativistic mean field model with the parameter set TM1, which is fitted to the properties of heavy nuclei. The quark matter phase is modelled using an effective MIT bag like model. Our general conclusion is that the quark matter stars have a higher oscillation frequemces then hadron-matter stars of similar mass. We have also compared purely hadronic stars with hybrid stars containg a quark core. The results are presented in the figures above. The softening of the equation of state associated with the phase transition to deconfined quark matter leads to an initial decrease in the gravitational mass as function of central energy density (left figure). According to the turning point criterion this should lead to instability with respect to small radial perturbations. However, our calculation of the eigenmode frequencies shown in the right figure do not support this criterion. Instead, we observe an increase in the oscillation frequency of the fundamental mode after the onset of the phase transition.

Related publications:

1) A. Brillante, I. N. Mishustin, *Radial oscillations of compact stars in General Relativity*, paper in preparation

Monte Carlo modeling of neutron production and transport in uranium and americium spallation targets

Collaborators: I. Mishustin[1,2], I. Pshenichnov[1,3], Yu. Malyshkin[1], W. Greiner[1]

[1] Frankfurt Institute for Advanced Studies, [2] “Kurchatov Institute”, National Research Center, Russia, [3] Institute for Nuclear Research, Russian Academy of Science, Russia

A promising way of utilization of Minor Actinides (MA) from spent nuclear fuel is to burn them directly in a spallation target. Use of fissile targets allows to obtain higher neutron fluxes and, as a result, higher burning rates of MA in comparison with ordinary non-fissile targets. For our simulation we created a special Geant4-based software called MCADS. The Geant4 toolkit is widely employed in basic physics research to simulate the propagation and interaction of particles and nuclei in extended media. In the ptrevious works [1,2] several benchmark tests of the model were presented. The possibility of MA burning in different targets was discussed and burning rates were estimated.

At the next stage of our studies we hae extended the functionality of MCADS to use it with MA containing targets. Benchmark tests with ^{241,243}Am isotopes and critical mass calculations for U and several transuranic elements were performed. The results show that MCADS provides good agreement with existing experimental data in the important for our study proton and neutron energy ranges.

We modeled irradiation of spallation targets made of U, Am, their mixes and Am_2O_3 by 600 MeV proton beam. It was obtained that pure Am and Am_2O_3 targets allow to get higher burning rate in comparison with U and mixed (U+Am) targets. Up to 4 kg/year of americium can be burned in one target irradiated by a 10 mA proton beam. We discuss various scenarios of MA incineration in ADS-based spallation targets.

These results as well as results of MCADS benchmark tests and criticality simulations will be submitted for publication soon.

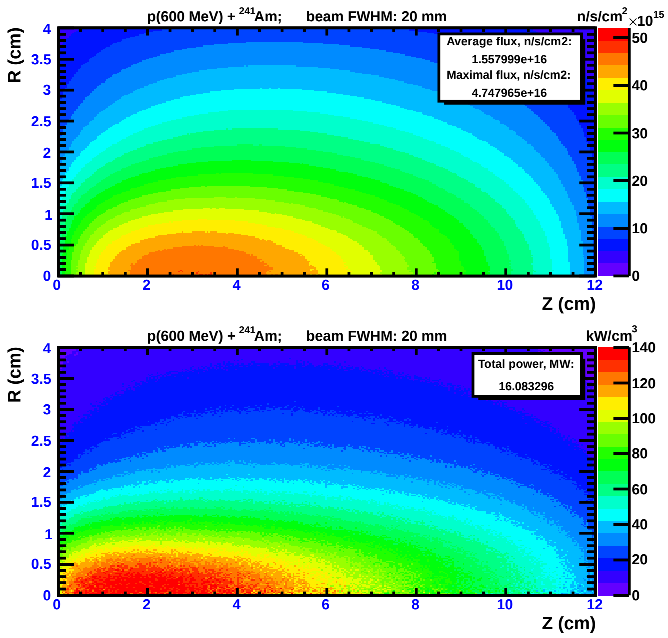


Figure: Spatial distribution of nuetron flux and heat deposition inside ^{241}Am cylindrical target irradiated by 600 MeV proton beam with current of 10 mA.

Related publications in 2012:

1) Yu. Malyshkin, I. Pshenichnov, I. Mishustin, T. Hughes, O. Heid, W. Greiner *Neutron production and energy deposition in fissile spallation targets studied with Geant4 toolkit*, Nucl. Instr. and Meth. 289, 79-90(2012)

2) Yu. Malyshkin, I. Pshenichnov, I. Mishustin, W. Greiner, *Modeling spallation reactions in tungsten and uranium targets with the Geant4 toolkit*, Poster at 3rd International Workshop on Compound Nuclear Reactions and Related Topics, published on-line: EPJ Web of Conferences 21, 10006 (2012)

Domain formation and fluctuations in Polyakov-chiral fluid dynamics

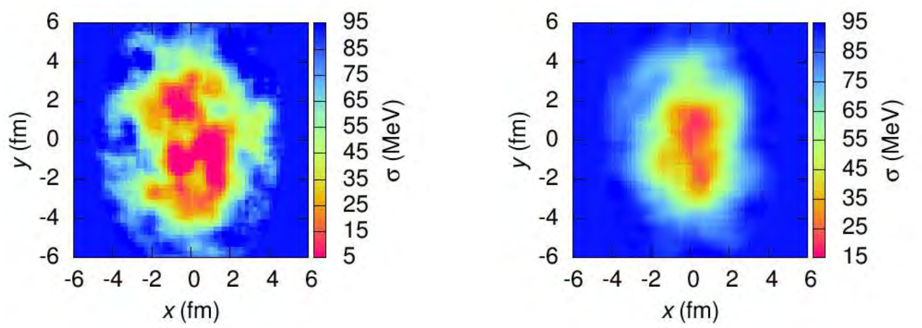
Collaborators: C. Herold [1,2], M. Nahrgang [2,3], I. N. Mishustin [1,4], M. Bleicher [1,2]

[1] Institut für theoretische Physik, Goethe Universität Frankfurt, [2] Frankfurt Institute for Advanced Studies, [3] SUBATECH, Université de Nantes, [4] Kurchatov Institute, National Research Center Moscow

The possibility of a critical point (CP) in QCD is under intensive theoretical and experimental investigation. For thermalized systems, fluctuations of conserved quantities may serve as a probe for the CP. However, it is not yet clear if and how these signals can survive the impact of nonequilibrium effects, which may become dominant in heavy ion collisions. On the other hand, for the same reason, effects at a first-order (FO) phase transition are enhanced. Here phenomena like nucleation or spinodal decomposition may lead to characteristic signals like the formation of disoriented chiral condensates or non-monotonic hadron multiplicity fluctuations.

With the use of the Polyakov loop extended chiral fluid dynamics model (PχFD) we study these effects for a FO and a CP scenario at vanishing baryochemical potential. A heat bath of quarks and antiquarks provides the fluid dynamically expanding background on which the relevant order parameters are propagated. These are the sigma field for the chiral and the Polyakov loop for the deconfinement phase transition. For the latter one we deploy its explicit propagation via a relaxation equation including stochastic noise.

If we allow the system to thermalize we observe critical slowing down and an enhancement of soft modes at the CP compared with the FO scenario. During the expansion of a hot plasma, supercooling and reheating significantly delay the relaxation process in the FO scenario. Correlating the stochastic fluctuations over spatial areas of volume $(1/m_\sigma)^3$ gives us the possibility to study qualitative differences in the two transition processes. While through the CP it proceeds smooth and homogeneous, we observe coexisting domains of the high- and low-temperature phases near the FO transition temperature, cf. Fig. 1. We expect this behavior to create clusters of high baryon density in systems of finite chemical potential, an excellent probe for the QCD phase transition in upcoming experiments at FAIR.



(a) (b)

Figure 1: (a) Sigma field for $z = 0$ at $t = 4$ fm at the FO phase transition. (b) Sigma field for $z = 0$ at $t = 3.2$ fm near the CP.

This work was supported by the Hessian LOEWE initiative Helmholtz International Center for FAIR.

Related publications in 2012:

1) C. Herold, M. Bleicher and M. Nahrgang, *Fluctuations and correlations in Polyakov loop extended chiral fluid dynamics*, Acta Phys. Polon. Supp. **5**, 529 (2012).

2) C. Herold, M. Nahrgang, I. Mishustin and M. Bleicher, *Chiral fluid dynamics with explicit propagation of the Polyakov loop*, accepted to Phys. Rev. C, arXiv:1301.1214 [nucl-th].

Chart of superheavy cluster emitters

Collaborators: D. N. Poenaru[1,2], R. A. Gherghescu[1,2], W. Greiner[1]

[1] Frankfurt Institute for Advanced Studies, [2] National Institute of Physics and Nuclear Engineering, Bucharest, Romania

We continue to investigate the cluster decay (CD) and α decay of superheavy nuclei (SH) with $Z = 104$-124. For many of them ($Z = 104$-$112, 114, 116$) there are already symbols available: Rf, Db, Sg, Bh, Hs, Mt, Ds, Rg, Cn, Fl, and Lv, respectively. Both kinds of disintegrations take place by quantum mechanical tunneling on which is based our analytical superasymetric fission (ASAF) model. To calculate α decay half-lives we use alternatively the semi-empirical fission (semFIS) model. As expected, the table of measured masses AME11 (G. Audi and W. Meng, private communication, 2011), is incomplete since we are concerned not only with the few known nuclides but also with heavier SHs. Consequently the theoretical mass models KTUY05 (H. Koura et al. Prog. Theor. Phys. 113 (2005) 305) and FRDM95 (P. Müller et al. Atomic Data Nucl. Data Tables 59 (1995) 185) are used to determine Q-value. The chart of cluster emitters from the Figure 1 is obtained by associating to each parent only the most probable emitted cluster in a systematic search based on FRDM95 masses.

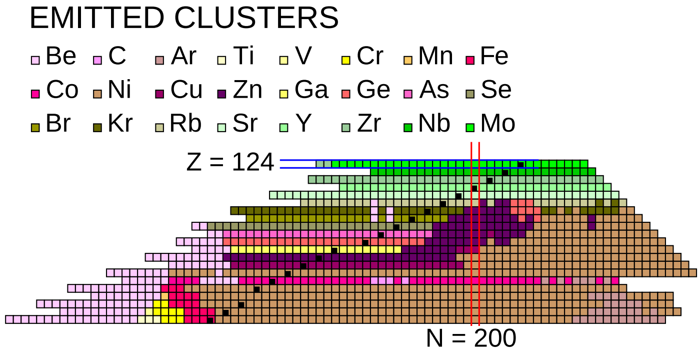


Figure 1: Chart of superheavy cluster emitters with atomic numbers $Z = 104124$. The Q values are calculated using the FRDM95 mass tables. Black squares mark the Green approximation of the line of beta stability.

Besides emitted clusters with $Z_e \leq 28$ (Be, C, Ar, Ti, V, Cr, Mn, Fe, Co, and Ni), many types of new CD modes with $Z_e > 28$ are present on this chart: Cu, Zn, Ga, Ge, As, Se, Br, Kr, Rb, Sr, Y, Zr, Nb, and Mo. Most frequently occurs the doubly magic ^{78}Ni radioactivity. We took only one color for every atomic number Z_e, despite the fact that one has various isotopes, as e.g. $A_e = 66, 68, 70$-78 for $Z_e = 28$.

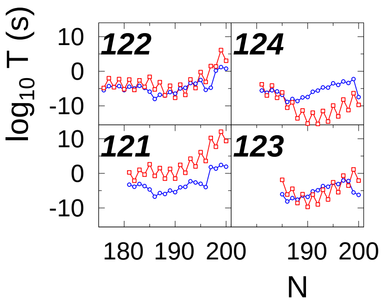


Figure 2: Decimal logarithm of the half-lives of superheavy nuclei with atomic numbers $121-124$ against α decay (blue circles) and CD (red squares) versus the neutron number of the parent nucleus. Q values are calculated using the KTUY05 mass table.

The trend toward shorter half-lives for heavier SHs is illustrated in Figure 2. By increasing the atomic number from 121 to 124 one has a transition from the "normal" case with $T_\alpha < T_c$ to the surprising result $T_\alpha > T_c$.

Related publications in 2012:

1) D. N. Poenaru, R. A. Gherghescu, W. Greiner, *Cluster decay of superheavy nuclei*, Phys. Rev. C85, 034615 (2012)

2) D. N. Poenaru, R. A. Gherghescu, W. Greiner, *Competition of α decay and heavy particle decay in superheavy nuclei*, Int. J. Mod. Phys. E21, 1250022 (2011)

3)D. N. Poenaru, R. A. Gherghescu, W. Greiner, *Simple relationships for α decay half-lives*, J. Phys. G: Nucl. Part. Phys. 39 (2012) 015105.

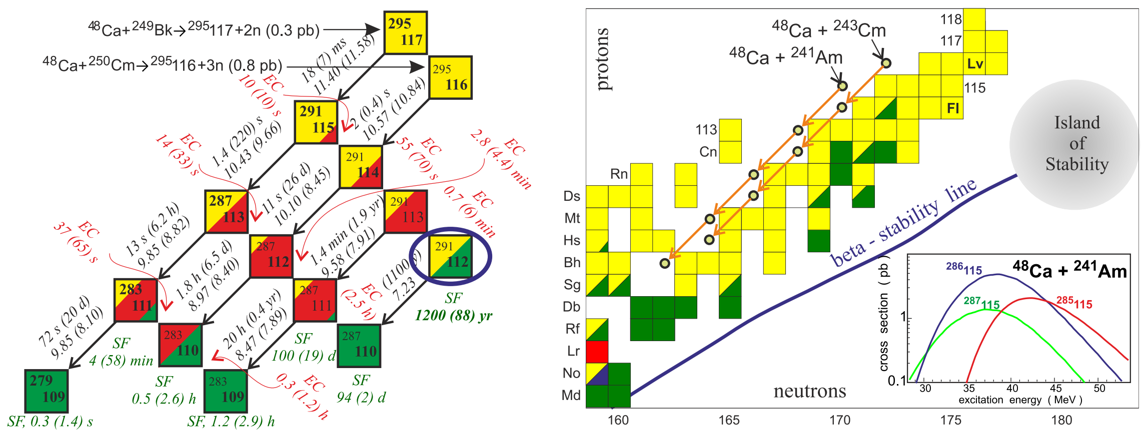
Possibilities for synthesis of new isotopes of superheavy elements in fusion reactions

Collaborators: V.I. Zagrebaev[1,2], A.V. Karpov[1,2], W. Greiner[1]

[1] Frankfurt Institute for Advances Studies, [2] Flerov Laboratory of Nuclear Reactions, Dubna, Russia

In the "cold" fusion reactions based on the use of lead and bismuth targets, the proton rich isotopes of superheavy (SH) elements up to $Z = 113$ have been produced. More neutron rich isotopes of SH elements (up to $Z = 118$) have been synthesized in "hotter" fusion reactions of ^{48}Ca with actinide targets. One might think that the epoch of ^{48}Ca in the production of SH nuclei was finished by the synthesis of element 118 in the ^{48}Ca+^{249}Cf fusion reaction [Yu. Oganessian et al., Phys. Rev. C 74, 044602 (2006)]. However this projectile still could be successfully used for the production of new isotopes of SH elements.

Alpha–decay half-lives of different isotopes of the same SH elements (for example, 112) were found to vary by several orders of magnitude. This indicates about strong shell effects in this area of the nuclear map. Understanding of these effects and other properties of SH nuclei is strongly impeded by the absence of experimental data on decay properties of the not-yet-synthesized isotopes of SH elements located between those produced in the "cold" and "hot" fusion reactions and also by the yet missing neutron-enriched isotopes of these elements. We found that the ordinary fusion reactions could be still useful for the production of new isotopes of SH elements. In particular, the gap of unknown SH nuclei could be filled in fusion reactions of ^{48}Ca with available lighter isotopes of Pu, Am and Cm (see the figure). The neutron-enriched isotopes of SH elements may be also produced with the use of ^{48}Ca beam if a ^{250}Cm target would be prepared. In this case we get a real chance to reach the island of stability due to a possible β^+ decay of ^{291}114 and ^{287}112 nuclei formed in the 3n evaporation channel of this reaction with cross section of about 0.8 pb (see the figure). The same path to the island of stability is opened also in the 2n evaporation channel of the ^{48}Ca+^{249}Bk fusion reaction ($\sigma^{2n}_{\mathrm{EvR}} \sim 0.3$ pb) leading to the isotope ^{291}115 having a chance for β^+ decay. Thus, for the first time a "narrow pathway" to the middle of the island of stability is found at last. All the proposed fusion reactions (having rather large EvR cross sections at the level of one picobarn) can be performed at existing experimental facilities in contrast with the widely discussed multi-nucleon transfer reactions which require design and construction of new experimental setups.



Left panel: The pathway to the middle of the island of stability via a possible β^+ decay of the isotopes ^{291}115 and ^{291}114. The first isotope may be formed after α decay of ^{295}117 (2n evaporation channel of the ^{48}Ca+^{249}Bk fusion reaction, cross section is 0.3 pb). The second one, ^{291}114, is formed after α decay of ^{295}116 in the 3n evaporation channel of the ^{48}Ca+^{250}Cm fusion reaction with cross section of about 0.8 pb. Decay half-lives and Q_α values (in MeV) are also shown calculated with nuclear masses of A. Sobizcewski et al. and of P. Möller et al. (in brackets). Right panel: Filling the gap of the nuclear map between SH nuclei synthesized in "cold" and "hot" fusion reactions. The use of ^{48}Ca beam and lighter actinide targets (^{239}Pu, ^{241}Am, ^{243}Cm) is most appropriate for this purpose. In the inset the corresponding cross sections are shown for the case of ^{48}Ca+^{241}Am fusion reaction.

Related publications in 2012:

1) V.I. Zagrebaev, A.V. Karpov, and Walter Greiner, *Possibilities for synthesis of new isotopes of superheavy elements in fusion reactions*, Physical Review C85, 014608 (2012)

Hadron formation: the QCD phase diagram substantiated by relativistic nuclear collision data

Collaborators: R. Stock[1,2], M. Bleicher[2], Th. Kollegger[2], with F. Becattini[3] and J. Steinheimer[4]

[1] Institute for Nuclear Physics, Frankfurt University, [2] FIAS, Frankfurt University, [3] Universita di Firenze and INFN, [4] Nuclear Science Division, Lawrence Berkeley Laboratory

Our group investigates the QCD process of hadron formation that occured in the course of the cosmological evolution at about 3 microseconds "big bang time". In the laboratory one recreates the parton to hadron phase transformation by means of central collisions of heavy nuclei at relativistic energies. In such collisions the initial kinetic projectile energy gets transformed into internal heating and compression of a "fireball" of strongly interacting matter, that traverses the QCD phase boundary entering a state of deconfined partons: the so-called "Quark-Gluon Plasma". It decays backwards, by expansion and cooling, into a multitude of hadronic species. Experimentally, the production rates of all species can be recorded and analysed, not only at the big bang conditions of approximate particle-antiparticle equipartition (at maximum collider energies such as provided by the CERN LHC), but also at lower energies of fireball formation which contain a varying density fraction of the initial "valence" quarks. The density ratio of newly formed fireball quarks and gluons to the input density of initial valence quarks is cast into the variable "hadro-chemical potential μ_B". The *phase diagram of QCD matter* is then given in the plane of temperature versus chemical potential.

In our study we aim at determining the position of the parton-hadron phase boundary line between deconfined partons, and confined hadrons, in the (T,μ_B) plane. From multihadron production data sets, gathered from top LHC energy (where μ_B is near zero) in the ALICE experiment, downwards to several, lower CERN SPS energies covered in the NA49 experiment (where μ_B reaches up to about 400 MeV) we determine the so-called "freeze-out" temperatures of the observed hadronic population. By means of analysis within the Gibbs grandcanonical ensemble (which has the principal variables T and μ_B), as implemented in the Statistical Hadronization Model (SHM), we have obtained a sequence of four such hadronization points in the (T,μ_B) phase diagram [1,2]. They are shown in the Figure, confronting predictions of recent lattice QCD calculations [3] at finite baryochemical potential, for the parton-hadron boundary line. Remarkably, the semi-empirical freeze-out points fully substantiate the QCD prediction. Hadronic freeze-out thus appears to coincide with hadron formation at the phase boundary.

These results thus resolve a long-standing discussion concerning the site of hadronic freeze-out in central A+A collisions, rendering hadron multiplicity data a unique signal of the QCD phase boundary. Our analysis was based, first, on final comprehensive data sets, and second upon the assessment of certain final-state reshuffling effects, occuring in the course of the final hadron-resonance cascade expansion phase. Whereas mesons freeze out directly at hadronization, the baryons and antibaryons are subject to annihilation and regeneration processes which distort the initially created Gibbs equilibrium yield distributions. We have quantified these effects employing a microscopic hadron transport model of the final cascade dynamics, the UrQMD model. From it we derived "survival factors" for each baryon/antibaryon species, which were then used as correction factors in the SHM analysis of the data. The results are quite remarkable because they appear to locate the QCD phase boundary at large values of the chemical potential.

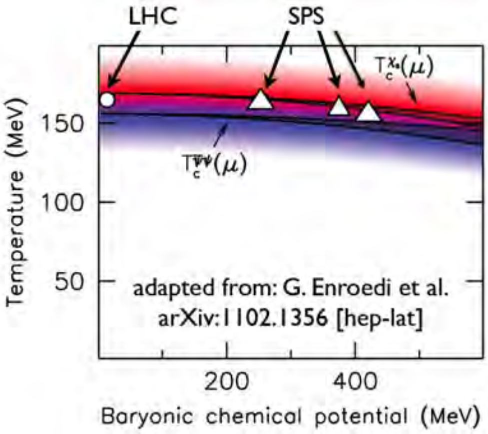


Figure: The QCD phase diagram as obtained from lattice QCD [3] at finite baryochemical potential, and hadronic freeze-out points from combined UrQMD and SHM analysis of ALICE data at top LHC energy, and of NA49 data at three SPS energies.

Related publications

1) F. Becattini, M. Bleicher, Th. Kollegger, M. Mitrovski, T. Schuster and R. Stock, Phys. Rev. C85, 044921 (2012), and J. Phys. G38, 124075 (2011)

2) F. Becattini, M. Bleicher, Th. Kollegger, T. Schuster, J. Steinheimer and R. Stock, arXiv: 1212.2431 submitted to Phys. Rev. Lett.

3) G. Enroedi et al., arXiv: 1102.1356 (hep-lat)

Studies of dilepton production at SIS energies within the UrQMD approach

Collaborators: Stephan Endres[1,2], Hendrik van Hees[1,2], Marcus Bleicher[1,2]

[1] Frankfurt Institute for Advanced Studies, [2] Institut für Theoretische Physik, Universität Frankfurt

Dileptons are interesting probes for physics at high baryon densities and high temperatures. As they do not interact with hadronic matter after their production, it is possible to deduce information concerning the in-medium properties of vector mesons from the measured dilepton spectra. In spite of several experimental and theoretical studies concerning this issue, it is still not clear how exactly the vector meson mass or width may change in nuclear matter. The experimental measurements could not completely be explained by theory so far.

In our investigations, the production of lepton pairs in elementary and nucleus-nucleus collisions at SIS energies is studied within the Ultra-relativistic Quantum Molecular Dynamics transport approach. Fot this we use the time integration method and assume that a resonance can continuously emit dileptons over its whole lifetime. Several channels for dilepton production are included in the calculations: Direct decays of vector mesons, Dalitz decays of pseudoscalar mesons and the ω vector meson. Also the Δ_{1232} resonance contributes via Dalitz decay, for which we now included an improved treatment. The previously used mass-independent lifetime of the resonance leads to the problem of overestimating the dilepton spectra at high masses and transverse momenta. In the Δ_{1232} case, we therefore now employ a mass-dependent lifetime for masses higher than the pole mass.

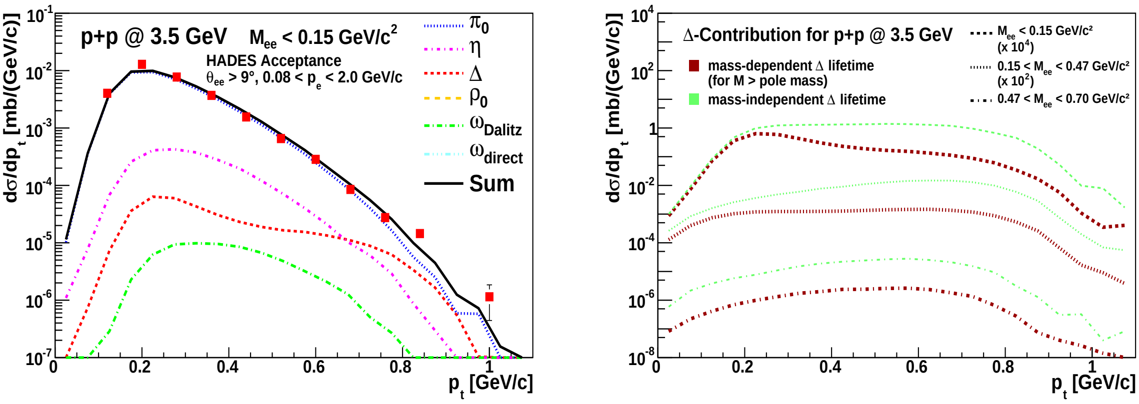


Figure: (Left) Low mass p_t spectrum for p+p at E_{lab}=3.5 GeV. (Right) Comparison of the Δ_{1232} contribution between previous UrQMD calculations with mass-independent lifetime and our present results.

In general we achieve a good description of the experimental results for invariant mass and transverse momentum spectra in elementary as well as heavy-ion collisions (see Figure for p+p results at 3.5GeV). Particularly the changed treatment of the Δ_{1232} resonance lifetime leads to an improved description of the p_t distribution. While the Delta contribution overshot the data significantly in previous calculations, it is signifacntly lower now and fits the data very well (see Figure, right).

However, recent experimental data from the HADES Collaboration show that the production cross-section especially of the ρ close to the threshold is not matched correctly in our model. This problem is related to the lack of experimental data for cross-sections and branching ratios of intermediate baryonic resonances, which are crucial for the ρ production. For an accurate study of in-medium modifictions, further and more detailed investigations of the elementary reactions as a baseline are necessary.

This work is supported by BMBF and the Hessian LOEWE initiative through the Helmholtz International Center for FAIR.

Related publication in 2012:

1) Stephan Endres, Marcus Bleicher, *Dilepton production at SIS energies with the UrQMD model*, accepted for publication in Journal of Physics Conference Series, in the FAIRNESS 2012 proceedings edition

Direct Photons in Heavy-Ion collisions

Collaborators: B. Bäuchle, A. Grimm, M. Bleicher

Frankfurt Institute for Advanced Studies

In our work, direct photon spectra from uranium-uranium collisions at FAIR energies (E_{lab} = 35 AGeV) are calculated within the hadronic Ultra-relativistic Quantum Molecular Dynamics transport model. In this microscopic model, one can optionally include a macroscopic intermediate hydrodynamic phase. The hot and dense stage of the collision is then modeled by a hydrodynamical calculation. Photon emission from transport-hydro hybrid calculations is examined for purely hadronic matter and matter that has a cross-over phase transition and a critical end point to deconfined and chirally restored matter at high temperatures. We find the photon spectra in both scenarios to be dominated by Bremsstrahlung. Comparing flow of photons in both cases suggests a way to distinguish these two scenarios.

Emission from Bremsstrahlung is the largest contribution to the total spectra in both cases. In calculations with a phase transition to deconfined matter, the amount of photons from Bremsstrahlung is reduced, since a sizeable portion of the system is in the deconfined state and therefore does not emit photons from hadronic processes. Emission from the QGP, however, makes up for the loss almost exactly, so that the total direct photon spectra from both calculations are very similar.

The elliptic flow v_2 from other hadronic channels is large compared to the flow from Bremsstrahlung and QGP in both the purely hadronic scenario and in the scenario with a cross-over phase transition. In both scenarios, elliptic flow is dominated by the largest contributions. The magnitude of flow from these contributions shows the space of time in which emission from these channels happens: QGP emission (cross-over calculations only) happens in the early stages of the collision, in which the underlying hadronic medium has not yet built up strong elliptic flow. Thus, photons emitted from this stage carry only little elliptic flow themselves.

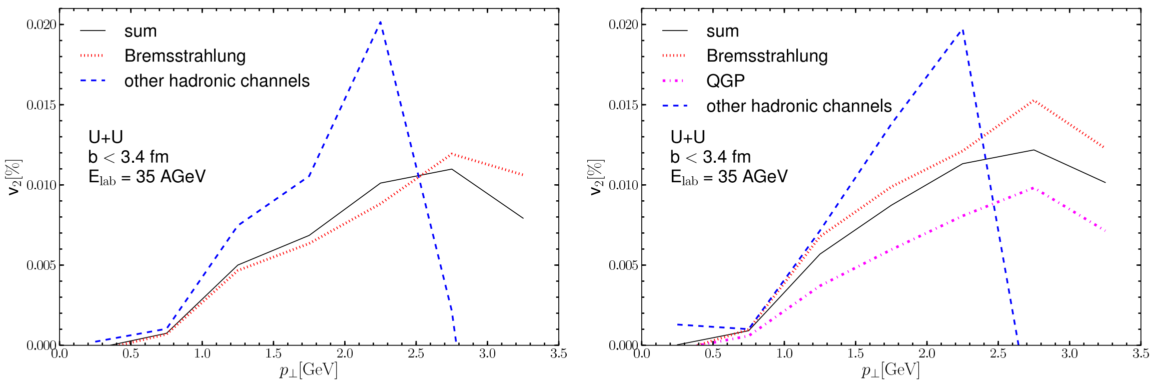


Figure: Elliptic flow of direct photons at FAIR calculated without (left) and with cross-over phase transition to deconfined matter.

Photons from processes that dominate in the late part of the fireball evolution, however, have a large hadronic flow present at their emission time imprinted in their elliptic flow pattern. Comparing flow results from both scenarios, we conclude that QGP emission in the cross-over scenario calculations basically substitutes Bremsstrahlung emission from Hadron Gas calculations in the early stages. Indeed, we see a larger elliptic flow from Bremsstrahlung in the cross-over scenario calculations than in the purely hadronic calculations, pointing to a later average emission time.

This work has been supported by the Frankfurt Center for Scientific Computing (CSC), the GSI and the BMBF. We would also like to thank for the support of the Hessian LOEWE initiative through the Helmholtz International Center for FAIR.

Related publication in 2012:

1) A. Grimm, B. Bäuchle, *Soft photons from transport and hydrodynamics at FAIR energies*, accepted to J. Phys. Conf. Ser. (FAIRNESS 2012), [arXiv:1211.2401 [nucl-th]]

UrQMD calculations of two-pion HBT correlations in central Pb-Pb collisions at $\sqrt{s_{NN}} = 2.76$ TeV

Collaborators: Qingfeng Li[1,2,4], Gunnar Gräf[2,3] and Marcus Bleicher[2,3]

[1] School of Science, Huzhou Teachers College, Huzhou 313000, P. R. China,
[2] Frankfurt Institute for Advanced Studies (FIAS), Ruth-Moufang-Str. 1, D-60438 Frankfurt am Main, Germany,
[3] Institut für Theoretische Physik, Goethe-Universität, Max-von-Laue-Str. 1, D-60438 Frankfurt am Main, Germany,
[4] Institute of Theoretical Physics, Chinese Academy of Sciences, Beijing 100080, P. R. China

In the current work we used the Ultra-relativistic Quantum Molecular Dynamics (UrQMD) to calculate heavy ion collisions at RHIC and LHC energies. We use $\pi\pi$ HBT correlations to compute correlation functions and to extract the HBT radii R_{out}, R_{side} and R_{long}. The longitudinal size of the pion emitting source is characterized by R_{long}, the transverse size by R_{out} and R_{side}. R_{out} has additional contributions from the source lifetime and space-momentum correlations. It increases with the lifetime and decreases with increasing correlation strength.

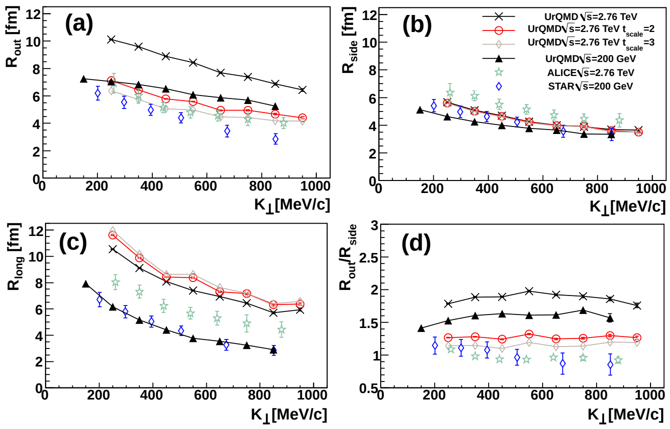


Figure 1: Pion pair momentum $K_\perp$ dependence of the HBT radii at RHIC and LHC energies. Green stars are experimental results from ALICE blue diamonds are experimental results from STAR. Black triangles and black crosses are UrQMD results for $\sqrt{s} = 2.76$ TeV and $\sqrt{s} = 200$ GeV. Red circles and beige diamonds are UrQMD results for $\sqrt{s} = 2.76$ TeV with source lifetimes artificially reduced by a factor of two and three respectively.

Figure 1 shows the HBT radii as well as the R_{out}/R_{side} ratio. It can be seen that R_{out} is overestimated by UrQMD at RHIC and more so at LHC. At LHC also R_{long} is overestimated. If we artificially decrease the source lifetime by a factor of three in the calculation of the correlation function we can reproduce the data in R_{out}. At the same time R_{side} and R_{long} remain basically unchanged as expected. We argue that the discrepancy between model and experiment is due to the absence of a partonic phase in UrQMD. As reasoned in other publications (S. Pratt, Nucl. Phys. A830 51C-57C (2009)), a partonic phase would lead to a more explosive expansion in the early stage, leading to an earlier decoupling of the system and increased flow. Both effects would reduce R_{out} while the earlier decoupling would also reduce R_{long}. We thus conclude that the partonic phase becomes very important at LHC energies.

Related publications in 2012:

1) G. Graef, Q. Li and M. Bleicher, *Formation time dependence of femtoscopic $\pi\pi$ correlations in p+p collisions at $\sqrt{s_{NN}} = 7$ TeV*, J. Phys. G 39, 065101 (2012)
2) Q. Li, G. Graef, M. Bleicher, *UrQMD calculations of two-pion HBT correlations in central Pb-Pb collisions at $\sqrt{s_{NN}} = 2.76$ TeV*, Phys. Rev. C 85 034908 (2012)
3) G. Graef, M. Bleicher and Q. Li, *Examination of scaling of Hanbury-Brown–Twiss radii with charged particle multiplicity*, Phys. Rev. C 85 044901 (2012)
4) Q. Li, G. Graef and M. Bleicher, *UrQMD calculations of two-pion HBT correlations in p+p and Pb+Pb collisions at LHC energies*, arXiv:1209.0042

Jets, Bulk Matter, and their Interaction in Heavy Ion Collisions at Several TeV

Collaborators: K. Werner[3], Iu. Karpenko[1,2], M. Bleicher[1], T. Pierog[4], S. Porteboeuf-Houssais[5]

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Traditionally the physics of ultrarelativistc heavy ion collisions is discussed in terms of different categories like collective dynamics, parton-jet physics, and fluctuation-correlation studies, although these different topics are highly correlated. In our studies, a complete dynamical picture of particle production in ultra-relativistic heavy ion collisions at all p_t scales is presented, which accounts for the production and evolution of bulk matter and jets, and theinteraction between the two components (which is not only the well known parton energy loss).

In our approach, initial hard scatterings result in mainly longitudinal flux tubes, with transversely moving pieces carrying the p_t of the partons from hard scatterings. These flux tubes constitute eventually both bulk matter (which thermalizes, flows, and finally hadronizes) and jets: a string segment will contribute to the bulk, when its energy loss is bigger than its energy, $\Delta E \geq E$. The hadrons still interact via cascade after hydrodynamic freezeout, the latter happens at the constant temperature of 165 MeV. High energy flux tube segments will leave the fluid, providing jet hadrons via the Schwinger mechanism of flux-tube breaking caused by quark-antiquark production. However, there are the segments which are formed inside but still escape, because they have $E > \Delta E$. Such segments leave "matter" at the hadronization surface at a particular space-time point x, which is characterized by some collective flow velocity $\vec{v}(x)$. We assume that the string breaking in this case is modified such that the quark and antiquark (or diquark) necessary for the string breaking are taken from the flowing fluid rather than being produced via the Schwinger mechanism.

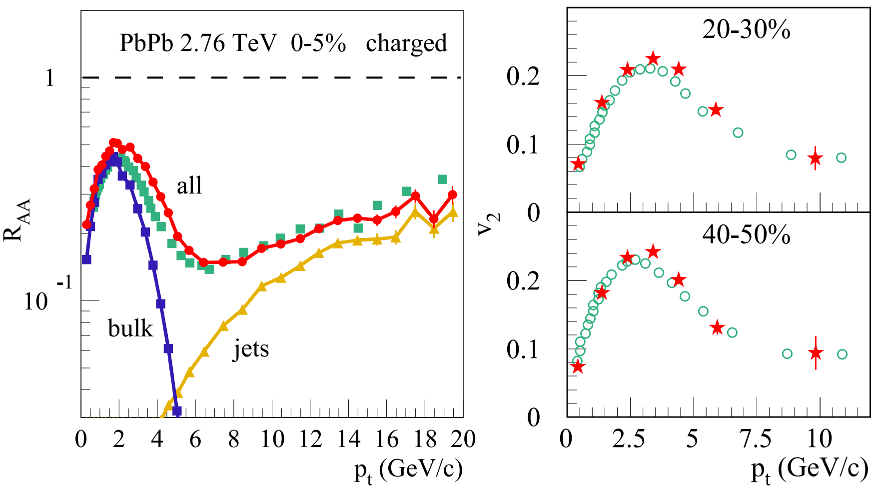

Figure: Left: the nuclear modification factor in Pb-Pb at 2.76 TeV LHC energy vs p_t, exp. data (ALICE collaboration, squares), full calculation in EPOS 2.17 model (red line + circles) and its jet contribution (yellow line + triangles), as well as the bulk (hydro) contribution of a calculation without hadronic cascade (blue line + squares). Right: v_2 vs p_t, data from ALICE (red stars) compared to the model (green circles).

Our prescription for bulk-jet separation and interaction strongly affect dihadron correlations. First of all, we compute dihadron correlation functions for different $(\Delta\eta, \Delta\phi)$ and observe ridge structure in 0-10% central collisions even for relatively high $p_t^{trigg} = 5.5 - 8.0$ GeV and beyond, due to abovementioned mechanism. Finally, we calculate $R(\Delta\phi) = 1 + \sum_{n=1}^{5} 2V_{n\Delta}\cos(n\Delta\phi)$ and compare the coefficients $V_{n\Delta}$ as a function of p_t^{trigg} (upto $p_t^{\mathrm{trigg}} = 10$ GeV) for different intervals of p_t^{assoc} with the results from ALICE detector at LHC. We observe a good quantitative agreement with the data, in particular, $V_{2\Delta}$does not at all drop to zero at high p_t because here the correlations between soft and jet particles come into play – the jet particles which suffered a push by the fluid. The same effects can interpret the behavior of the elliptic flow at high p_t.

We acknowledge the financial support by the ExtreMe Matter Institute EMMI and Hessian LOEWE initiative.

Related publication in 2012:

1) K. Werner, Iu. Karpenko, M. Bleicher, T. Pierog, S. Porteboeuf-Houssais, *Jets, Bulk Matter, and their Interaction in Heavy Ion Collisions at Several TeV*, Phys. Rev. C 85, 064907 (2012)

Heavy quark transport in heavy ion collisions at RHIC within the UrQMD transport model

Collaborators: T. Lang[1], H. van Hees[1], J. Steinheimer[2], M. Bleicher[1]

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Heavy quarks are an ideal probe for the Quark Gluon Plasma (QGP). They are produced in the beginning of the collision in hard processes and therefore probe the created medium during its entire evolution. When the system cools down they hadronize. The decay electrons of these heavy flavor hadrons can be measured experimentally. By investigating heavy-quark observables we can thus explore the interaction processes within the hot and dense medium. Two of the most interesting observables are the nuclear modification factor, R_{AA}, and the elliptic flow, v_2.
We explore the medium modification of heavy-flavor p_T spectra in Au+Au collisions at RHIC energies, using a hybrid model, consisting of the Ultra-relativistic Quantum Molecular Dynamics (UrQMD) model and a full (3+1)-dimensional ideal hydrodynamical model to simulate the bulk medium. The heavy-quark propagation in the medium is described by a relativistic Langevin approach.
The aim of this study is to find a consistent description of the experimental measurements for both the elliptic flow, v_2, and the nuclear modification factor, R_{AA}, with a realistic dynamical description of the background medium. To compare our calculations to data, we perform a hadronization to D-mesons and B-mesons using a coalescence approach as soon as the heavy quarks decouple from the hot medium and a sub-following decay to electrons.
To perform the calculations we used two different sets of drag and diffusion coefficients for the Langevin simulation, based on a T-Matrix approach and a resonance-scattering model for the elastic scattering of heavy quarks with light quarks and antiquarks. Both sets of coefficients lead to similar results for the heavy-flavor observables. Additionally we assumed different decoupling temperatures of the heavy quarks from the medium, and found that the late phase of the collision can have a considerable effect on the heavy-quark observables. Within our study we find the best agreement to experimental data using a low decoupling temperature of 130 MeV as can be seen in the figures.

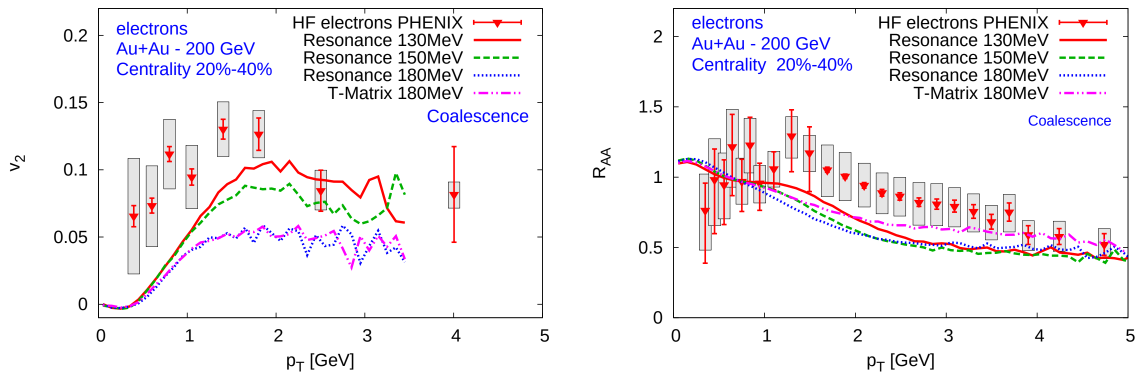


Figure 1: Elliptic flow v_2 (left) and nuclear modification factor R_{AA} (right) of electrons from heavy quark decays in Au+Au collisions at $\sqrt{s_{NN}} = 200\,\text{GeV}$. We use a rapidity cut of $|y| < 0.35$. For a decoupling temperature of 130 MeV we get a reasonable agreement to data (Adare et al., 2010).

Related publications in 2012:

1) T. Lang, H. van Hees, J. Steinheimer, M. Bleicher, *Heavy quark transport in heavy ion collisions at RHIC and LHC within the UrQMD transport model*, arXiv:1211.6912
2) T. Lang, H. van Hees, J. Steinheimer, Y. Yan, M. Bleicher, *Heavy quark transport at RHIC and LHC*, arXiv:1212.0696

Heavy quark scattering and dynamics in vacuum and in the quark gluon plasma (QGP)

Collaborators: H. Berrehrah[1], E. Bratkovskaya[1], W. Cassing[2], P.B Gossiaux[3], J. Aichelin[3]

[1] Frankfurt Institute for Advanced Studies, [2] Institut für Theoretische Physik, Giessen, [3] Subatech, Nantes, France

Heavy quarks (Q) are produced in hard binary initial collisions between the incoming nucleons in relativistic heavy-ion reactions. They provide an important independent observable that can probe some proprieties of the quark-gluon plasma (QGP) produced in these collisions. To this aim, we study the heavy quarks dynamics from their production until hadronization and freeze-out.

Our study of the heavy quark propagation is realized within the microscopic Parton-Hadron-String-Dynamics (PHSD) transport approach [3], where hadronic and partonic interactions and the dynamics of heavy flavours degrees-of-freedom are included. The scattering of heavy quarks with the QGP particles represents the first step of this study. Therefore, we have determined the elastic scattering cross section (σ^{Q}_{elas}) of heavy quarks in vacuum and in the QGP medium. Indeed, the calculation of σ^{Q}_{elas} at finite temperature in the strongly interacting medium is considered for the first time.

Our determination of σ^{Q}_{elas} at finite temperature couples pQCD calculation with the dynamical Quasi-Particle Model (DQPM). The partons are considered as off-shell quasi-particles, their masses are described by DQPM spectral functions for different temperatures of the medium. Figure 1 (left) shows the gluon, light and heavy quark DQPM spectral functions at different temperatures. In Fig. 1 (right) we show the elastic scattering cross section of heavy quark on a light quark as a function of $\sqrt{s}$, the energy in the c.m of the collision for different temperatures. This figure shows clearly the effect of finite parton masses and widths on the perturbative elastic cross section.

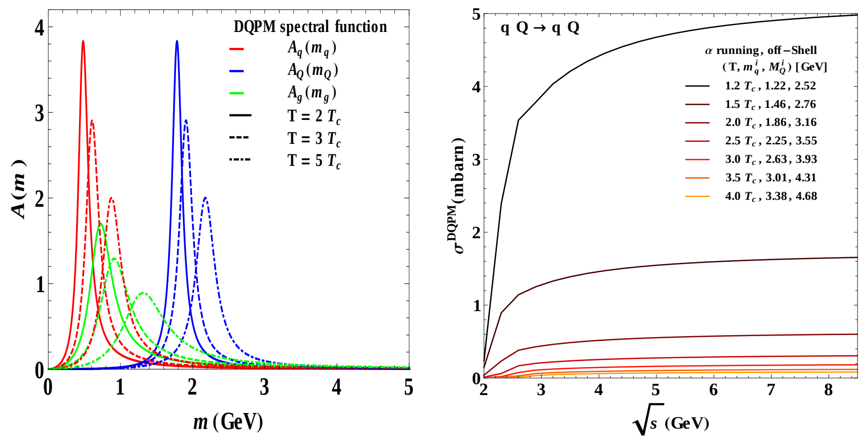


Figure 1: Left: DQPM spectral functions of the gluon ($A_g(m_g)$), light ($A_q(m_q)$) and heavy quarks ($A_Q(m_Q)$) for T = 2; 3; 5 Tc. Right: elastic scattering cross section of heavy quark on light quarks ($qQ \to qQ$) as a function of $\sqrt{s}$, the energy in the c.m of the collision for different temperatures.

The knowledge of elastic and inelastic scattering cross sections of heavy quarks in a finite temperature medium leads to the relevant evaluation of several physical quantities, the dynamical collisional and radiative energy loss of heavy quarks, their interaction rates, diffusion coefficients, viscosity, etc. Ultimately, the explicit microscopic dynamics of heavy flavours in the QGP and the hadronic phase can be performed within PHSD.

Related publications in 2012:

[1] H. Berrehrah, P.B. Gossiaux, J. Aichelin, E. Bratkovskaya, W. Cassing and M. Bleicher, *Collisional and radiative processes of heavy quarks in vaccum and in the QGP medium*, in preparation

[2] H. Berrehrah, P.B. Gossiaux, J. Aichelin, *Perturbative elastic scattering cross section of quarkonia bound states*, to be submitted

[3] V. P. Konchakovski, E. L. Bratkovskaya, W. Cassing, V. D. Toneev, S. A. Voloshin, and V. Voronyuk, *Azimuthal anisotropies for Au+Au collisions in the parton-hadron transient energy range*, Phys. Rev. C 85, 044922 (2012)

Initial conditions, transport and hadronization in heavy-ion collisions

Collaborators: R. Marty[1], E. Bratkovskaya[1], W. Cassing[2], J. Aichelin[3]

[1] Frankfurt Institute for Advanced Studies, [2] Institut für Theoretische Physik, Giessen, [3] Subatech, Nantes, France

The study of the properties of the Quark-Gluon Plasma (QGP) - formed in heavy-ion collisons - requires to understand how initially nuclei convert to quarks and gluons and how the partonic matter hadronizes again.

We have developed a relativistic molecular dynamics approach based on the Nambu–Jona-Lasinio (NJL) Lagrangian [1] for the light u,d,s quarks in order to study the hadronization from an initial state of quarks and antiquarks while in NJL the gluonic degrees of freedom are integrated out and not considered explicitly but contained in an effective coupling constant for the interaction of quarks/antiquarks. As initial condition we use the energy density profile from an actual heavy-ion collision calculated within the Parton-Hadron-String-Dynamics (PHSD) transport approach [2]. In Fig. 1 (left) we show the slice of plasma during the beginning of a Au+Au collision at $\sqrt{s} = 200$ GeV in terms of the energy density in the local cells. In Fig. 1 (middle) we show an example of initial conditions using the PHSD energy density converted to NJL partons with the help of the NJL equation of state. Fluctuations in the energy density are clearly visible in the initial parton density. The microscopic study of the expansion and the hadronization through a cross over transition is possible within our transport model.

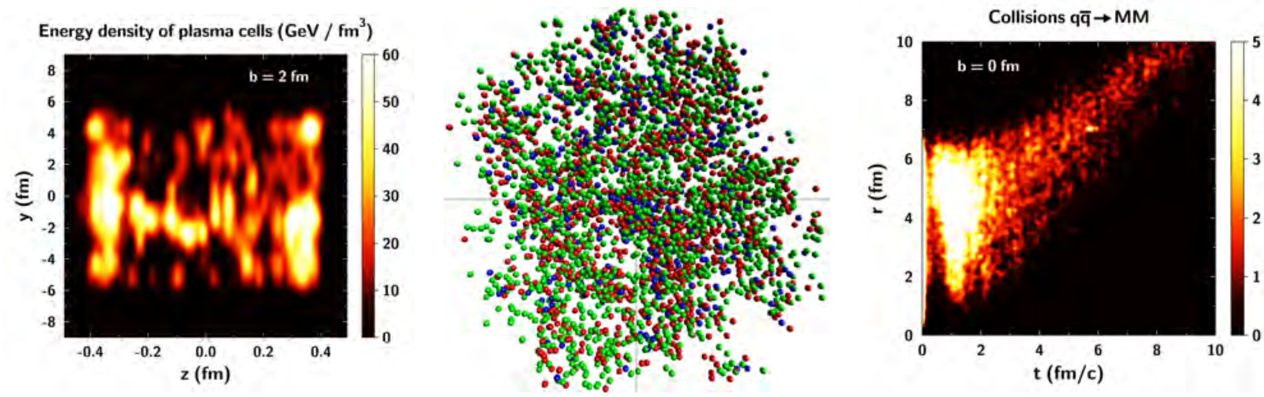


Figure 1: Left: initial energy density for cells in the local rest frame in the $y-z$ plane, Middle: initial geometry profile of quarks and antiquarks in the $x-y$ plane, Right: distribution of inelastic collisions $q\bar{q} \to MM$ in space $\vec{r}$ (distance from the center of the plasma) and time t from the molecular dynamics calculations.

The hadronization volume can be extracted from the r.h.s of Fig. 1 where we show the position in space and time of the inelastic collisions $q\bar{q} \to MM$ that lead to hadron production in the NJL. Since the full microscopic information is available we can also extract a variety of observables from such simulations as the transverse flow, the p_T-spectra and also study of the influence of the initial condition fluctuations on the final observables.

Related publications in 2012:

1) R. Marty, J. Aichelin, *Molecular dynamics description of an expanding $q/\bar{q}$ plasma with the Nambu-Jona-Lasinio model and applications to heavy ion collisions at RHIC and LHC energies*, arXiv:1210.3476 [hep-ph]

2) V. P. Konchakovski, E. L. Bratkovskaya, W. Cassing, V. D. Toneev, S. A. Voloshin, and V. Voronyuk, *Azimuthal anisotropies for Au+Au collisions in the parton-hadron transient energy range*, Phys. Rev. C 85, 044922 (2012), arXiv:1201.3320 [nucl-th]

Shear and bulk viscosities of strongly-interacting 'infinite' parton-hadron matter within the Parton-Hadron-String Dynamics (PHSD) transport approach

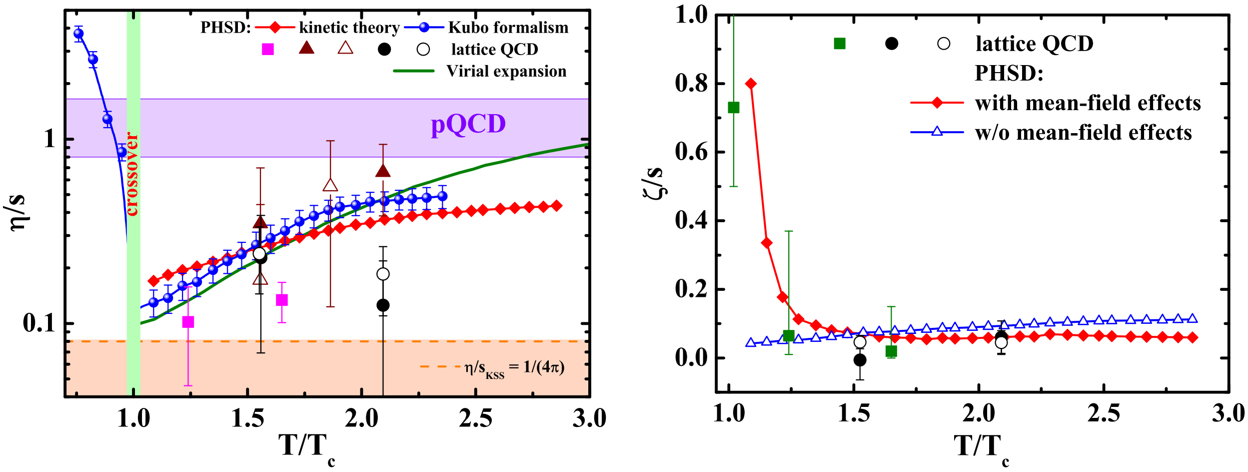
Collaborators: V. Ozvenchuk[1], O. Linnyk[2], M. I. Gorenstein[1,3], E. L. Bratkovskaya[1,4], W. Cassing[2]

[1] Frankfurt Institute for Advanced Studies, [2] Institut für Theoretische Physik, Universität Giessen, [3] Bogolyubov Institute for Theoretical Physics, Kiev, Ukraine, [4] Institut für Theoretische Physik, Goethe-Universität Frankfurt am Main.

We study the shear and bulk viscosities of 'infinite' partonic and hadronic matter as functions of temperature T within the Parton-Hadron-String Dynamics (PHSD) off-shell transport approach.

The 'infinite' matter is simulated within a cubic box with periodic boundary conditions initialized at various values for baryon density (or chemical potential) and energy density. The size of box is fixed to 9^3 fm^3. The initialization is done by populating the box with light (u, d) and strange (s) quarks, antiquarks and gluons with random space positions. The system initially is close to the thermal equilibrium with thermal distribution for the momenta of partons and far out from the chemical equilibrium due to the strangeness suppression by factor of 3 in comparison to the light quarks and antiquarks. The system approaches kinetic and chemical equilibrium at all energies densities during it's evolution within PHSD.

The ratio of the shear viscosity to entropy density $\eta(T)/s(T)$ extracted from the PHSD simulations in the box, which is presented in Fig. 1(a), shows a minimum (with a value of about 0.1) close to the critical temperature T_c, while it approaches the perturbative QCD (pQCD) limit at higher temperatures. For $T < T_c$, i.e. in the hadronic phase, the ratio η/s rises fast with decreasing temperature due to a lower interaction rate of the hadronic system and a significantly smaller number of degrees-of-freedom. We obtain practically the same results in the Kubo formalism and in the relaxation time approximation. Our results are also in almost quantitative agreement with the ratio $\eta(T)/s(T)$ from the virial expansion approach as well as with lQCD data for the pure gauge sector.



(a) (b)

Figure 1: The transport coefficients as a function of T/T_c extracted from the PHSD simulations in the box: (a) specific shear viscosity η/s; (b) specific bulk viscosity ζ/s.

The bulk viscosity $\zeta(T)$ evaluated in the relaxation time approach, which is shown in Fig. 1(b), is found to strongly depend on the effects of mean fields (or potentials) in the partonic phase. We find a significant rise of the ratio $\zeta(T)/s(T)$ in the vicinity of the critical temperature T_c, when consistently including the scalar mean-field from PHSD, which is also in agreement with that from lQCD calculations.

Related publications in 2012:

1) V. Ozvenchuk, O. Linnyk, M. I. Gorenstein, E. L. Bratkovskaya, W. Cassing, arXiv:1203.4734 [nucl-th]
2) V. Ozvenchuk, O. Linnyk, M. I. Gorenstein, E. L. Bratkovskaya, W. Cassing, arXiv:1212.5393 [nucl-th]

Dilepton production in proton-proton and Pb+Pb collisions at $\sqrt{s_{\rm NN}}$ = 2.76 TeV

Collaborators: J. Manninen[1], J. Aichelin[2], E. L. Bratkovskaya[1,3], W. Cassing[4], P. B. Gossiaux[2], C. M. Ko[5], O. Linnyk[3], T. Song[5]

[1] Frankfurt Institute for Advanced Studies, [2] SUBATECH/University of Nantes , [3] Johann Wolfgang Goethe Universität, [4] Justus Liebig Universität Giessen, [5] Texas A&M University

We study correlated e^+e^- pair production in proton-proton and central Pb+Pb collisions at $\sqrt{s_{\rm NN}} = 2.76$ TeV within two models: an extended statistical hadronization model (SHM) and the Parton-Hadron-String Dynamics (PHSD) transport approach. We find that the PHSD calculations roughly agree with the dilepton spectrum from hadronic sources with the 'cocktail' estimates from the SHM matched to available data at LHC energies.

We have modeled in great detail all relevant hadronic (see Table 1) and partonic dielectron sources in our analysis in order to estimate the relative importance of partonic processes in heavy-ion collisions. Indeed, pronounced traces of the partonic degrees of freedom are found in the PHSD results in the intermediate mass regime (see Figure 1). The dilepton production from the strongly interacting quark-gluon plasma (sQGP) exceeds that from the semi-leptonic decays of open charm and bottom mesons. Additionally, we observe that a transverse momentum cut of 1 GeV/c further suppresses the relative contribution of the heavy meson decays to the dilepton yield, such that the sQGP radiation strongly dominates the spectrum for masses from 1 to 3 GeV, allowing a closer look at the electromagnetic emissivity of the partonic plasma in the early phase of Pb+Pb collisions.

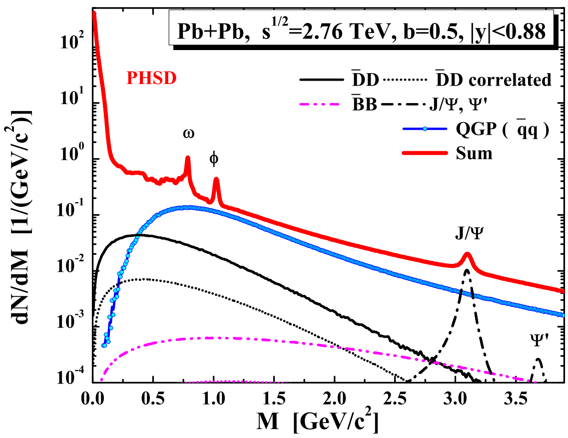


Figure 1: Correlated dielectron invariant mass spectrum in 10% most central central Pb+Pb collisions at $\sqrt{s_{\rm NN}}$=2.76 TeV.

	direct	Dalitz	other
π^0	-	$\pi^0 \to \gamma e^+e^-$	-
η^0	-	$\eta^0 \to \gamma e^+e^-$	$\eta^0 \to \pi^+\pi^-e^+e^-$
η'	-	$\eta^0 \to \gamma e^+e^-$	$\eta' \to \pi^+\pi^-e^+e^-$
ρ^0	$\rho^0 \to e^+e^-$	-	-
ω^0	$\omega^0 \to e^+e^-$	$\omega^0 \to \pi^0 e^+e^-$	-
ϕ^0	$\phi^0 \to e^+e^-$	$\phi^0 \to \eta\, e^+e^-$ (*)	-
J/ψ	$J/\psi \to e^+e^-$	$J/\psi \to \gamma e^+e^-$	-
ψ'	$\psi' \to e^+e^-$	$\psi' \to \gamma e^+e^-$	-
D	-	-	$D^\pm \to e^\pm \nu_e + X$
B	-	-	$B^\pm \to e^\pm \nu_e + X$

Table 1: List of the most important hadronic dielectron sources taken into account in the analyses.

Related publications in 2012:

1) E. L. Bratkovskaya, O. Linnyk, V. P. Konchakovski, W. Cassing, V. Ozvenchuk, J. Manninen and C. M. Ko, *Dilepton production from SIS to LHC energies*, J. Phys. Conf. Ser. 389, 012016 (2012)

2) O. Linnyk, W. Cassing, J. Manninen, E. L. Bratkovskaya and C. M. Ko, *Analysis of dilepton production in Au+Au collisions at* $\sqrt{s_{NN}} = 200$ *GeV within the Parton-Hadron-String Dynamics (PHSD) transport approach*, Phys. Rev. C 85, 024910 (2012)

Effective gluon potential and hybrid approach to Yang-Mills thermodynamics

Collaborators: C. Sasaki[1], K. Redlich[2]

[1] Frankfurt Institute for Advanced Studies, [2] Institute of Theoretical Physics, University of Wroclaw, Poland

The structure of the QCD phase diagram and thermodynamics at finite baryon density is of crucial importance in heavy-ion phenomenology. Due to a sign problem in lattice calculations, a major approach to the finite density QCD is based on effective chiral models. The important input in these models is a pure gluon potential $U(L)$ which is parameterized by the Polyakov loop L. Different parameterizations of $U(L)$ are possible, and have been proposed in literature, since the only constraints on their structure was to preserve a global $Z(N_c)$ symmetry.

In this work we have shown that the Polyakov-loop potential can be derived, using a field theoretical methods, directly from the SU(3) Yang-Mills theory. A class of the Polyakov-loop effective potentials used so far in literature appears as limiting cases of our potential. We deduce the correspondence of $U(L)$ to the strong-coupling expansion, of which the relevant coefficients of the gluon energy distribution are specified solely by characters of the SU(3) group.

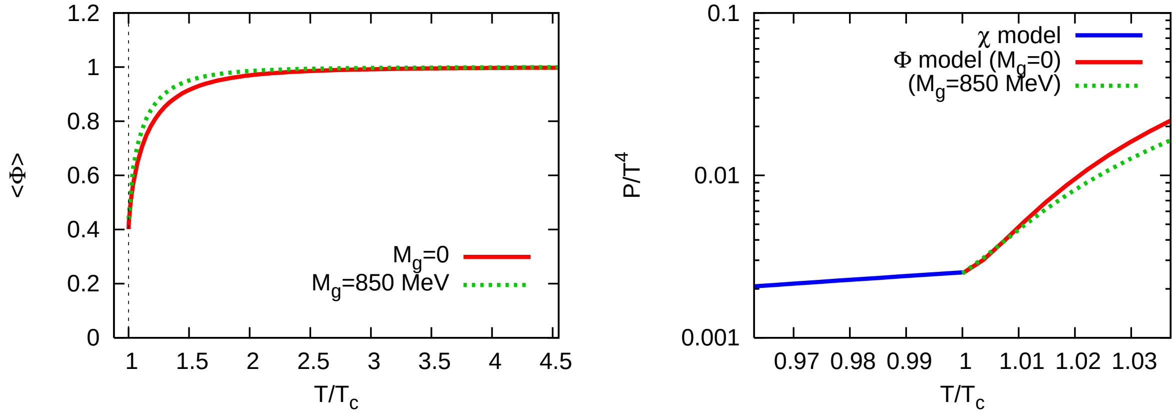


Figure 1: Thermal expectation value of the Polyakov loop (left-hand figure) and the normalized pressure (right-hand figure) calculated in the hybrid model for massless $M_g = 0$ and massive $M_g = 850$ MeV gluons.

At high temperatures the derived gluon potential exhibits the correct asymptotic behavior, whereas at low temperatures, it disfavors gluons as appropriate dynamical degrees of freedom since otherwise we are confronted with the *negative* entropy density. To avoid this drawback and to quantify the Yang-Mills thermodynamics in a confined phase, we propose a hybrid approach which matches the effective gluon potential to the one of glueballs constrained by the QCD trace anomaly in the context of dilaton fields.

C. S. acknowledges partial support by the Hessian LOEWE initiative through the Helmholtz International Center for FAIR (HIC for FAIR).

Related publication in 2012:

1) C. Sasaki and K. Redlich, *An Effective gluon potential and hybrid approach to Yang-Mills thermodynamics*, Phys. Rev. D 86, 014007 (2012) [arXiv:1204.4330 [hep-ph]]

Triangular Flow as a Measure of Initial State Granularity

Collaborators: H. Petersen[1], S. A. Bass[2]

[1] Frankfurt Institute for Advanced Studies, [2] Department of Physics, Duke University, Durham, NC, USA

Higher order flow coefficients have recently been recognized as new observables to gain information about the creation of the quark gluon plasma in relativistic heavy ion reactions and its properties. Pressure gradients translate the initial state coordinate space eccentricity to the final state momentum space ellipticity and this connection is affected by the viscosity and the equation of state. The higher odd anisotropic flow coefficients require the treatment of event-by-event fluctuations, since for smooth initial conditions they vanish by symmetry constraints. The ultimate goal is to understand the initial energy deposition which is related to the distributions of the nucleons/partons in the incoming nuclei and the interactions they are undergoing.

By using a hybrid transport approach that is based on the Ultra-relativistic Quantum Molecular Dynamics including an (3+1) dimensional ideal hydrodynamic expansion, we demonstrate that triangular flow is directly related to the amount of fluctuations in the initial state. In the figure below results for the averaged $v_{2,3}$ coefficients for charged particles calculated for different granularities ($n = 1,...,25$) via the event plane method are presented. The clear dependency of the mean values of triangular flow in non-central collisions on the number of events over which the initial average has been performed proves that one can constrain the granularity of the initial state by comparing flow coefficients of calculations to experimental data. The average elliptic flow stays constant since it is related to the overall geometry of the event.

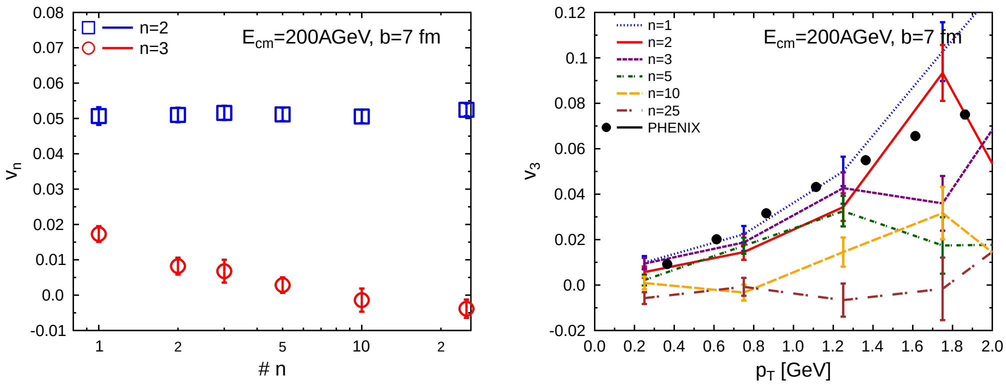


Figure 1: Anisotropic flow for different granularities in mid-central ($b = 7$ fm) Au+Au collisions at $\sqrt{s_{NN}} = 200$ GeV. Right: Triangular flow versus transverse momentum for different granularities mid-central ($b = 7$ fm) Au+Au collisions at $\sqrt{s_{NN}} = 200$ GeV compared to PHENIX data.

To get a first impression on the amount of fluctuations that is consistent with the PHENIX data on triangular flow, the transverse momentum dependence of triangular flow of charged particles has been calculated in the hybrid approach (see figure (right)). This first comparison to data indicates that the full single-event configuration is close to the amount of initial state fluctuations that is necessary. That indicates that a hadron-based initial state description with a particle size of the order of 1 fm generates the least amount of fluctuations that is needed. Since additional viscosity during the hydrodynamic evolution would dilute fluctuations faster this is a lower bound on the initial state granularity.

Related publications in 2012:

1) H. Petersen, R. La Placa, S. A. Bass, *A systematic study of the sensitivity of triangular flow to the initial state fluctuations in relativistic heavy-ion collisions*, J. Phys. G 39, 055102 (2012)

2) H. Petersen, *Event-by-Event Observables and Fluctuations*, arXiv:1211.5526 [nucl-th]

3) A. Adare, M. Luzum and H. Petersen, *Initial state fluctuations and final state correlations: Status and open questions*, arXiv:1212.5388 [nucl-th]

Event-by-event distributions of azimuthal asymmetries in ultrarelativistic heavy-ion collisions

Collaborators: G. S. Denicol[1,2], H. Holopainen[3], P. Huovinen[3], H. Niemi[4]

[1] Department of Physics, McGill University, Montreal, Canada, [2] Institut für Theoretische Physik, Johann Wolfgang Goethe-Universität, [3] Frankfurt Institute for Advanced Studies, [4] Department of Physics, University of Jyväskylä, Finland

One of the goals of the present heavy-ion physics is to experimentally determine the shear viscosity coefficient over entropy density ratio, η/s, of the strongly interacting deconfined matter formed in ultrarelativistic heavy-ion collisions. The effect of shear viscosity is manifested in the azimuthal anisotropy of the observed particles. The anisotropy is measured in terms of the Fourier coefficients, v_n, of the azimuthal distribution. Unfortunately the extraction of the value of η/s from the measured v_n is hampered by our ignorance of the shape of the droplet of deconfined matter at the beginning of the expansion. This shape is characterised by anisotropy coefficients ε_n, and the rule of thumb, especially for the lowest order coefficients $n = 2, 3$ is that the larger the ε_n, the larger the v_n. As well, the larger the η/s, the smaller the v_n.

We have found that the event-by-event fluctuations of these anisotropies behave differently. It is practical to study these fluctuations using the scaled variables $\delta v_n = (v_n - \langle v_n \rangle)/\langle v_n \rangle$ and $\delta\varepsilon_n = (\varepsilon_n - \langle \varepsilon_n \rangle)/\langle \varepsilon_n \rangle$, where the average has been removed. The probability distributions for δv_n and $\delta\varepsilon_n$, $n = 2, 3, 4$, in $Au+Au$ collisions at $\sqrt{s_{\rm NN}} = 200$ GeV were calculated using a hydrodynamical model. As seen in the figure, the value of the shear viscosity over entropy ratio η/s does not affect the distribution of δv_n. As well, the distributions of the scaled spatial anisotropy coefficients $\delta\varepsilon_n$ are practically equal to the scaled Fourier coefficients δv_n.

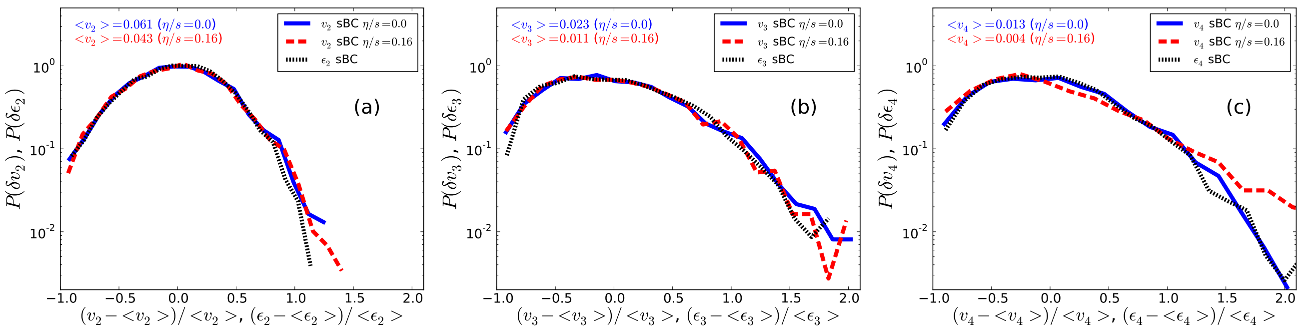


Figure 1: Probability distributions: a) $P(\delta v_2)$ and $P(\delta\varepsilon_2)$, b) $P(\delta v_3)$ and $P(\delta\varepsilon_3)$, and c) $P(\delta v_4)$ and $P(\delta\varepsilon_4)$, of the scaled Fourier coefficients δv_n of the particle distributions, and the scaled anisotropy coefficients $\delta\varepsilon_n$ of the initial state. The calculations are done for collisions in the $20-30\%$ centrality class using two different values of η/s, $\eta/s = 0$ and $\eta/s = 0.16$. As seen the distributions of δv_n are independent of the viscosity and equal to the distributions of $\delta\varepsilon_n$.

This means that the relative fluctuations of the shape of the produced matter can be measured experimentally. The model describing the matter production in the nucleus-nucleus collision can be constrained by experimental data to reproduce the observed fluctuations. Once they are known, the shear viscosity coefficient over entropy density ratio η/s can be evaluated by requiring the calculation to reproduce the observed average v_n.

Related publication in 2012:

1) H. Niemi, G. S. Denicol, H. Holopainen and P. Huovinen, *Event-by-event distributions of azimuthal asymmetries in ultrarelativistic heavy-ion collisions*, arXiv:1212.1008 [nucl-th]

Centrality dependence of the emission of thermal photons from fluctuating initial conditions

Collaborators: H. Holopainen[1], R. Chatterjee[2], T. Renk[2,3], K. J. Eskola[2,3]

[1] Frankfurt Institute for Advanced Studies, [2] University of Jyväskylä, Jyväskylä, Finland, [3] Helsinki Institute of Physics, Helsinki, Finland

Event-by-event fluctuations in the initial density profile in the hydrodynamical modeling of ultrarelativistic heavy ion collisions have been shown to enhance the production of thermal photons compared to a smooth initial profiles (R. Chatterjee et al. Phys.Rev. C83, (2011) 054908). This enhancement is originating from the fact that hot spots in the fluctuating initial conditions produce much more photons with transverse momenta $p_T > 1$ GeV due to strong temperature dependence of the photon emission rates.

In this work the initial states are obtained from Monte Carlo Glauber model and density is distributed around the positions of the wounded nucleons using 2-dimensional Gaussians with width σ. These initial states are then evolved with (2+1)-dimensional ideal hydrodynamics and thermal photon emission is obtained by integrating over the whole medium using thermal emission rates (P. Arnold et al. JHEP 0112 (2001) 009; S. Turbide et al. Phys. Rev. C69 (2004) 014903).

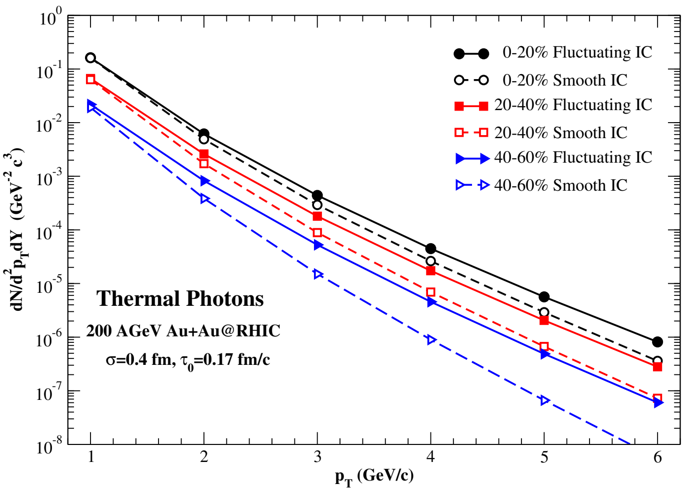


Figure: Transverse momentum spectra of thermal photons from smooth and fluctuating initial conditions at RHIC for different collision centralities.

In the figure we have plotted the p_T-spectra of thermal photons in Au+Au collisions at $\sqrt{s_{NN}} = 200$ GeV for different centralities. We can see from the figure that the enhancement is more prominent in the peripheral collisions: the exponential slope of the spectra in the region $2 < p_T < 4$ GeV is 10%, 12% and 16% flatter for fluctuating initial conditions at 0–20%, 20–40% and 40–60% centrality bins respectively. This shows that the relative importance of the hot spots increases towards peripheral collisions, where the number of sources, *i.e.* the number of participants, is smaller. We also showed that the effect of fluctuations in the initial density distribution is smaller for thermal photon production at LHC energies than for RHIC energies.

Related publications in 2012:

1) R. Chatterjee, H. Holopainen, T. Renk, K. J. Eskola, *Collision centrality and τ_0 dependence of the emission of thermal photons from fluctuating initial state in ideal hydrodynamic calculation*, Phys. Rev. C85, 064910 (2012)
2) R. Chatterjee, H. Holopainen, T. Renk, K. J. Eskola, *Centrality and initial formation time dependence of the emission of thermal photons from fluctuating initial conditions at RHIC and LHC*, arXiv:1207.6917 [nucl-th]
3) R. Chatterjee, H. Holopainen, T. Renk, K. J. Eskola, *Influence of initial state fluctuations on the production of thermal photons*, arXiv:1210.3517 [hep-ph]

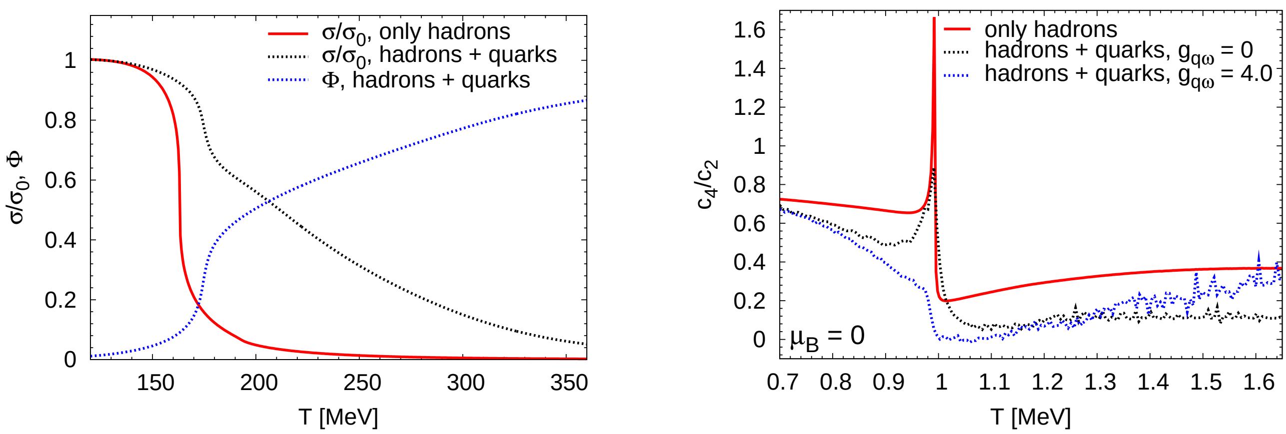
Quark and Hadron Degrees of Freedom in a Chiral Hadronic Model

Collaborators: Philip Rau[1,2], Jan Steinheimer[3], Stefan Schramm[1], Horst Stöcker[1,4]

[1] FIAS, [2] Institut für Theoretische Physik, Goethe Universität Frankfurt, [3] Lawrence Berkeley National Laboratory, USA,[4] GSI – Helmholtzzentrum für Schwerionenforschung, Darmstadt

We developed an effective model for the equation of state (EoS) of strongly interacting matter that incorporates the presumably correct degrees of freedom in wide range of temperatures and densities. This unified model is conceptually based on combining a chiral hadronic mean field model with a phenomenological quark model. The quarks in this approach are introduced in a way similar to a well tested Polyakov loop extended Nambu-Jona-Lasinio (PNJL) model. Therefore, the model is applicable in the hadronic sector at low energies and densities as well as in the partonic sector at high temperatures and densities. Order parameters for both the chiral and the deconfinement transition as well as thermodynamic properties and different particle abundancies can be studied.

At vanishing baryochemical potential, we observe a smooth cross over for both order parameters at the same critical temperature (cf. Fig. 1(a)) which is in good agreement with newest results from lattice QCD. We find, that the coupling of particles to the repulsive vector meson fields has a major impact on the resulting phase diagram. With increasing coupling, a first order phase transition at non-zero baryochemical potentials ceases to exits in favor of a broad cross over transition. Furthermore, fluctuations of conserved charges, which occur in the transition region, are significantly suppressed when increasing the vector coupling of the quarks (cf. Fig. 1(b)). Realistic equations of state from this model can for example be used to study neutron star formation or the dynamics in heavy ion collisions.



(a) (b)

Figure 1: a): Order parameter for the chiral transition σ/σ_0 as a function of the temperature T in the pure hadron model (red solid line) and with additional quarks (black dashed line). The order parameter for deconfinement Φ is also shown for the model including quarks (blue dashed line). Both transition happen at the same critical temperature. b): Ratio of fourth to second order quark number fluctuations c_4/c_2 as a function of T. Results for the purely hadronic model (red solid line) as well as the quark hadron model with two different vector coupling strengths $g_{g\omega}$ (black and blue dashed lines) are shown. Fluctuations are substantially suppressed by larger vector couplings.

Related publications in 2012:

1) P. Rau, J. Steinheimer, S. Schramm, and H. Stöcker, *Baryon Resonances in a Chiral Hadronic Model for the QCD EoS*, Phys. Rev. C 85, 025204 (2012) [arXiv:1109.3621 [hep-ph]]

2) P. Rau, J. Steinheimer, S. Schramm, and H. Stöcker, *Resonance States in an Effective Chiral Hadronic Model*, Central Eur. J. Phys. 10, 1302 (2012) [arXiv:1201.3834 [hep-ph]]

Quark Coalescence at lower energies

Collaborators: Giorgio Torrieri[1], Michael Mitrovski[1,2], Vincenzo Greco[3]

[1] Frankfurt Institute for Advanced Studies, [2] Brookhaven National Laboratory, Upton, New York, USA, [3] INFN Laboratori Nazionali del Sud, Catania, Italy

We examine whether the breakdown in elliptic flow quark number scaling observed at the Relativistic Heavy Ion Collider (RHIC) energy scan is related to the turning off of deconfinement by testing the hypothesis that hydrodynamics and parton coalescence always apply, but are obscured, at lower energies, by variations in the widths of quark and anti-quark rapidity distribution.

In [1] we have explored the observable signal from a coalescence of a fluid of quarks and antiquarks on elliptic flow at lower energies, where one cannot guarantee a "large" rapidity plateau and balance between quarks and antiquarks. We find that these two conditions are enough to break the "number of constituent quarks scaling" even if coalescence also occurs at lower energies (See Figure), but the expected systematics is opposite to that observed: antiquarks should have more flow than quarks, just as in a hadronic system. These considerations make it somewhat non-trivial to understand when does the onset of quark coalescence occur. We plan to explore this issue in subsequent work.

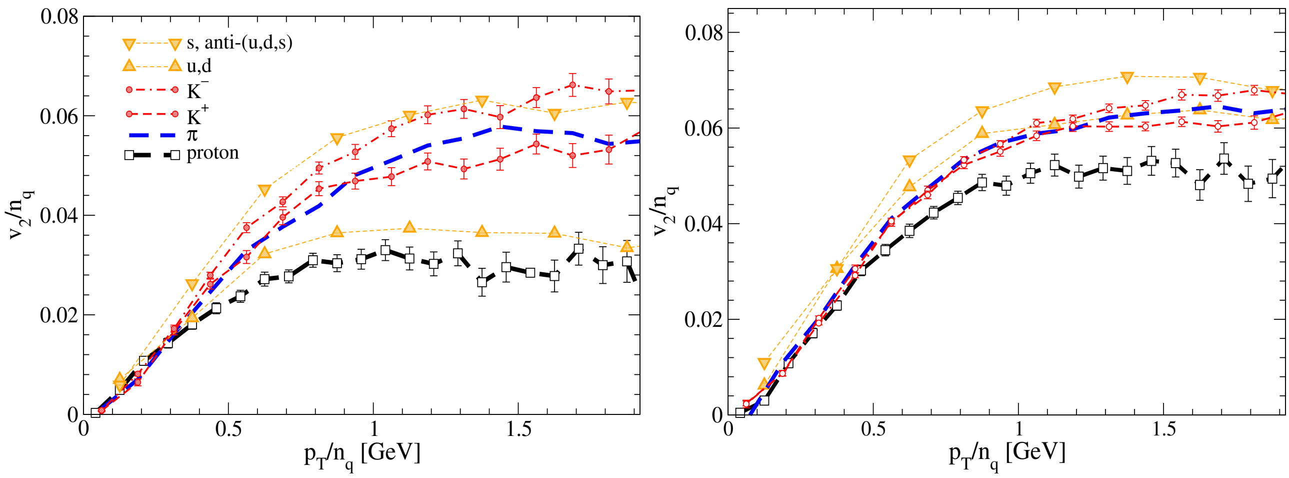


Figure: v_2/n_q vs p_T/n_q of quarks, mesons baryons and anti-baryons in the $|y| \leq 0.5$ rapidity window and for two different σ values: Left panel assumes $\sigma_y = 0.25$ and right panel has $\sigma_y = 0.5$. See [1] for details.

Related publication in 2012:

1) V. Greco, M. Mitrovski and G. Torrieri, *Elliptic flow in heavy ion collisions at varying energies: Partonic versus hadronic dynamics*, Phys. Rev. C 86, 044905 (2012) [arXiv:1201.4800 [nucl-th]]

Theory and phenomenology of quarkyonic percolation

Collaborators: Giorgio Torrieri[1], Stefano Lottini[2]

[1] Frankfurt Institute for Advanced Studies, [2] Institute for Theoretical Physics, Goethe University Frankfurt

We have extended our earlier work on percolation to consider varying density as well as number of colors, and to try to estimate if a percolating but confined phase is possible in our $N_c = 3$ world [1-3]. We find that this is indeed possible, but at chemical potentials significantly higher than those originally indicated for quarkyonic matter $\mu_B/N_c \simeq \Lambda_{QCD}$. The biggest uncertainity here is whether deconfinement occurs before or after this phase transition.

We have also tried to develop a phenomenology of percolating quarkyonic matter, to try to see if it can be detected in forthcoming experiments such as FAIR. Experimental signatures, based around electromagnetic signals (photons and dileptons) are expected to be the focus of our activity in this area for 2013. Some qualitative signatures (the equivalent of energy gaps in QED conductors) have alread been indicated (see Figure).

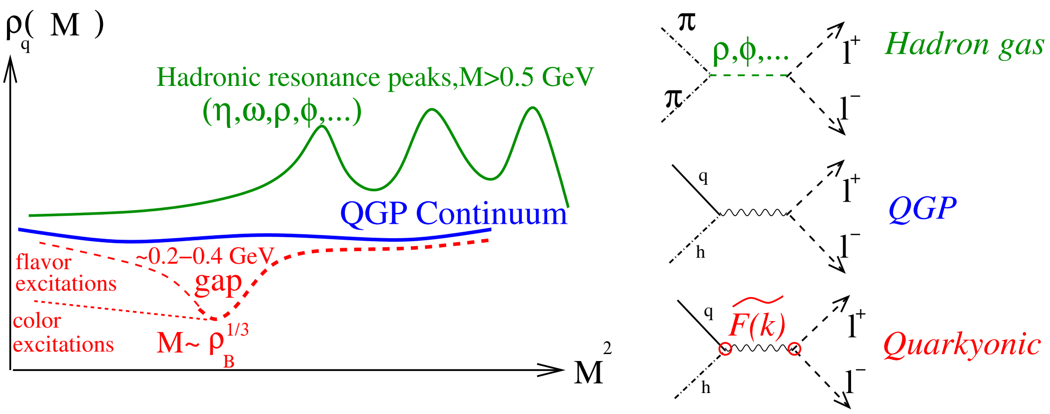


Figure: Spectral function of dileptons in a hadron gas, in a pQCD, and in quarkyonic matter. See [1] for details.

Related publications in 2012:

1) G. Torrieri and S. Lottini, *Phenomenology of quarkyonic percolation at FAIR*, arXiv:1211.2433 [nucl-th]

2) S. Lottini and G. Torrieri, *Quarkyonic percolation in dense nuclear matter*, Acta Phys. Polon. Supp. 5, 1089 (2012), arXiv:1206.6663 [hep-ph]

3) S. Lottini and G. Torrieri, *Quarkyonic Percolation and deconfinement at finite density and number of colors*, arXiv:1204.3272 [nucl-th]

Jet-Medium Coupling at the Large Hadron Collider

Collaborators: B. Betz[1,2], M. Gyulassy[3]

[1] Institute for Theoretical Physics, Johann Wolfgang Goethe-University, 60438 Frankfurt am Main, Germany, [2] Frankfurt Institute for Advanced Studies, [3] Department of Physics, Columbia University, New York, 10027, USA

During the last years, we developed a generic energy-loss model in collaboration with the nuclear theory group at Columbia University, New York, USA to investigate different jet-energy loss scenarios and different prescriptions of the fluctuating initial conditions proposed for heavy-ion collisions. Using this algorithm, we studied both the nuclear modification factor R_{AA}, quantifying the jet queching in a heavy-ion collisions, and the elliptic flow v_2 at collisional energies reached at Relativistic Heavy Ion Collider (RHIC) and at the Large Hadron Collider (LHC).

Recent results on this nuclear modification factor R_{AA} measured at the LHC indicate that the medium created in such a heavy-ion collision is much more transparent to jets than expected from direct extrapolations based on the RHIC measurements.

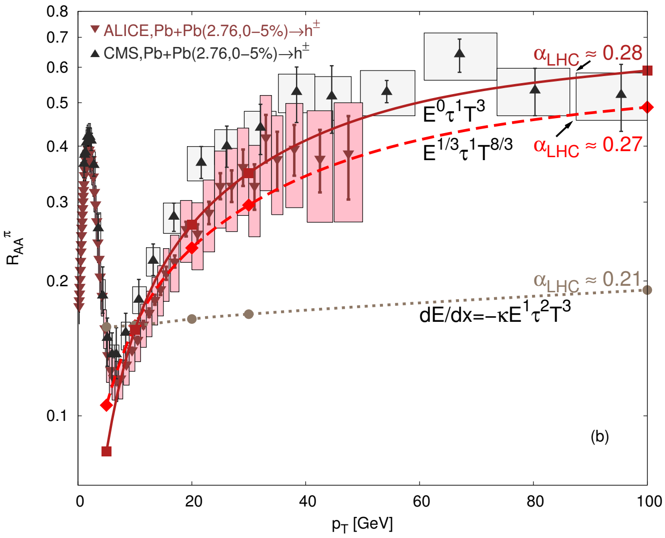


Figure: The nuclear modification factor R_{AA} as a function of transverse momenta p_T measured at LHC energies and compared to model calculations for different jet-energy loss scenarios $dE/dx = -\kappa E^a x^z T^c$.

We quantified the reduction factor between RHIC and LHC from a combined fit to the available data on the nuclear modification factor R_{AA} and the elliptic flow v_2 over a transverse momentum range $p_T \sim 10-300$ GeV and a broad impact parameter, b, range.

We used a simple analytic model ($dE/dx = -\kappa E^a x^z T^c$) to additionally investigate the dynamical jet-energy loss model dependence. Here, varying $a = 0-1$ interpolates between weakly-coupled and strongly-coupled models of jet-energy dependence while $z = 0-2$ covers a wide range of possible jet-path dependencies from elastic and radiative to holographic string mechanisms.

Our fit to LHC data indicates an approximate 40% reduction of the coupling κ and excludes energy-loss models characterized by a jet-energy exponent with $a > 1/3$ (see Fig. 1). In particular, the rapid rise of R_{AA} with $p_T \geq$ 10 GeV combined with the slow variation of the asymptotic $v_2(p_T)$ at the LHC rules out popular exponential geometric optics models ($a = 1$). The LHC data are compatible with $0 \leq a \leq 1/3$ pQCD-like energy-loss models where the jet-medium coupling is reduced by approximately 10% between RHIC and LHC .

Related publications in 2011:

1) B. Betz and M. Gyulassy, *Examining a reduced jet-medium coupling in Pb+Pb collisions at the Large Hadron Collider*, Phys. Rev. C 86, 024903 (2012)
2) B. Betz and M. Gyulassy, *Quantifying a Possibly Reduced Jet-Medium Coupling of the sQGP at the LHC*, accepted for publication in Nuclear Physics A, arXiv:1211.0804 [nucl-th]

SU(2) 3d Yang-Mills-Vlasov Hard-Expanding-Loop simulations

Collaborators: M. Attems[1,2], A. Rebhan[2], M. Strickland[1,3]

[1] Frankfurt Institute for Advanced Studies, Germany, [2] Institut für Theoretische Physik, Technische Universität Wien, Austria [3] Department of Physics, Kent State University, USA

The Chromo-Weibel instabilities play a crucial role in the nonequilibrium dynamics of a weakly coupled non-Abelian plasma. They have been proposed as a possible mechanism for the fast apparent thermalization of the quark-gluon plasma. In a kinetic theory approach the Yang-Mills-Vlasov coupled equations can be applied to nonstationary, anisotropically expanding plasmas resulting in coupled equations of "hard" plasma quasi-particles with "soft" collective modes.

The *Hard Expanding Loop (HEL)* framework is a practicable discretization method for real-time simulations in comoving coordinates. These simulations provide a method to probe the frontiers of non-equilibrium gauge field theory. This report will discuss recent developments of the C++ HEL code that simulates non-Abelian plasma instabilities.

Ideally the simulations should have no infrared (IR) cutoff. HEL, being an effective field theory, the ultraviolet cutoff doesn't need to be sent to infinity. This means that in the longitudinal direction $\nu_{\min}$ should be as low as possible. On a lattice with periodic boundary conditions, the size of the lattice determines the infrared cutoff $\nu_{\min} = \frac{4\pi}{(N_\eta a_\eta)}$ in full wavelengths. Continuum extrapolation and detailed IR studies with fine spacings between the longitudinal mode numbers call for simulations with a big N_η number of longitudinal lattice sites.

In the present work we changed the way of parallelization in HEL. 10^{10} matrices of auxiliary fields result in a big memory pressure on each CPU per node. The efficient parallelization is the key in order to process them. The improved setup allows to split the matrices in smaller parts leading to a more efficient parallelization. The memory layout for the larger longitudinal grid, distributed on several nodes, got optimized by usage of longitudinal instead of previously transverse slices. Each slice runs per CPU on a node.

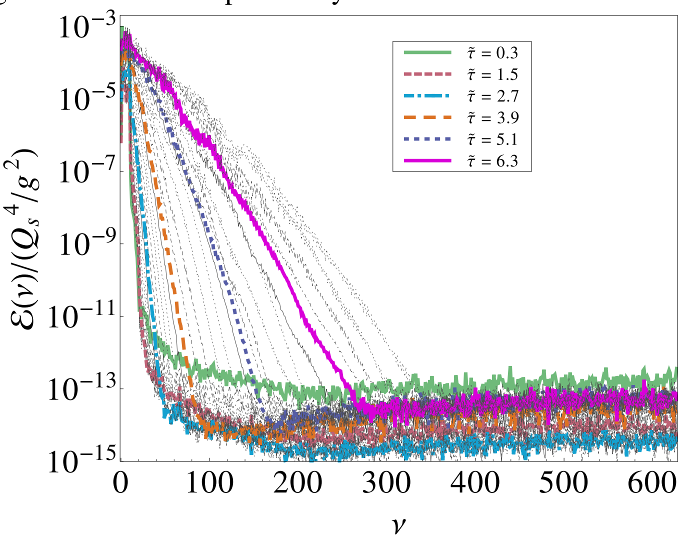


Figure: The longitudinal energy spectra at various proper times as a function of ν. The data taken from a single run with typical anisotropic parameter set and $N_\eta = 1024$. The initial mode number cut off in the seed modes is visible at start (green line). At later times one sees energy deposited into the higher modes (orange, blue, purple lines).

This results in a gain of speed by a factor 3 for the same lattice sizes or in the possibility of bigger lattice sizes in longitudinal direction by at least a factor 8 for the same overall time. This paves the way for efficient fine grained IR studies. We demonstrate rapid emergence of an exponential distribution of longitudinal energy.

Related publications in 2012:

1) M. Attems, A. Rebhan and M. Strickland, *Instabilities of an anisotropically expanding non-Abelian plasma: 3D+3V discretized hard-loop simulations*, Phys. Rev. D **87** (2013) 025010, [arXiv:1207.5795 [hep-ph]]
2) M. Attems, *Real-time evolution of a non-equilibrium non-Abelian plasma*, PhD thesis, Technische Universität Wien

Cooling of Rotating Neutron Stars

Collaborators: S. Schramm[1], R. Negreiros[1,2], F. Weber[3]

[1] Frankfurt Institute for Advances Studies, [2] Fluminense Federal University, Rio de Janeiro, Brazil [3] San Diego State University, USA

The investigation of the properties of neutron stars is the most important approach available to understand strongly interacting matter at extremely high densities. Thus, neutron star physics complements the heavy-ion physics program, which largely addresses hot matter. To deduce the properties of the star matter from observation as many different types of observational data as possible are needed. The most common ones are the mass and radius of the star (the latter one being notoriously difficult to determine). In addition there are especially the rotational frequency of the star as well as its temperature. Recently, for the first time, the actual cooling of a star over a period of 10 years has been measured. In order to combine these quantities we developed a 2-dimensional cooling simulation for neutron stars, which is necessary, as fast spinning stars are not spherical any more but are highly deformed. The simulation couples the solution of the Einstein equations with the heat transport equations.

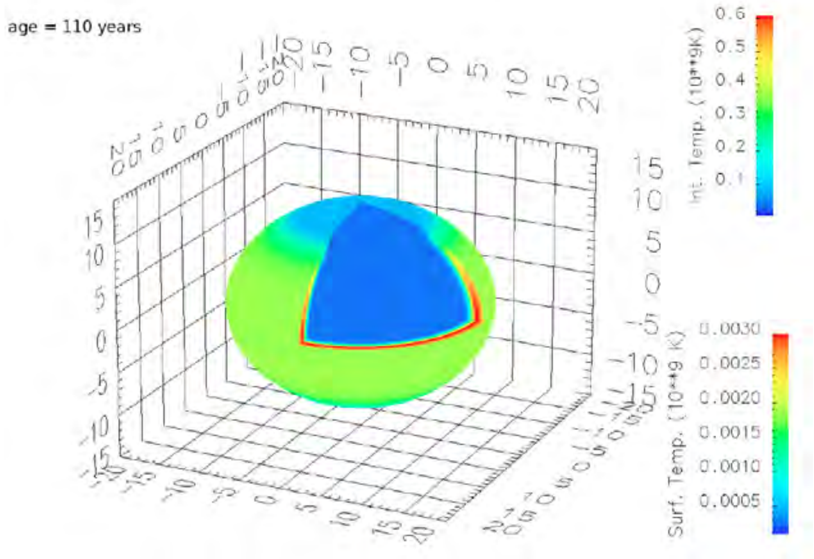


Figure 1: Snapshot of the temperature distribution for a deformed neutron star 100 years after the supernova. Note the different temperature scales for the interior and surface of the star.

A snapshot of such a cooling calculation of a rotating star can be seen in the figure. One an observe the temperature distribution with a cold area around the polar region, which could have observational consequences. The thermal evolution develops a time delay between various regions of the star. Therefore, especially for the important phase of fast cooling that occurs after about 100 years one can clearly be observe an offset in the temperature evolution between the polar and equatorial region.

The project has wide-ranging potential and is just at the beginning of exploiting the various codes that we developed. In the future we plan to investigate accreting spinning-up neutron stars with this approach and to study the influence of magnetic fields, as these in general break isotropy and therefore demand a higher-dimensional treatment as it is done here for the very first time in this field.

Related publications in 2012:

1) R. Negreiros, S. Schramm, F. Weber, *Thermal Evolution of Neutron Stars in 2 Dimensions*, Phys. Rev. D 85, 104019 (2012).

2) R. Negreiros, S. Schramm, F. Weber, *Impact of Rotation-Driven Particle Repopulation on the Thermal Evolution of Pulsars*, to be published in Phys. Lett. B.

Planck scale corrections to black holes production cross sections

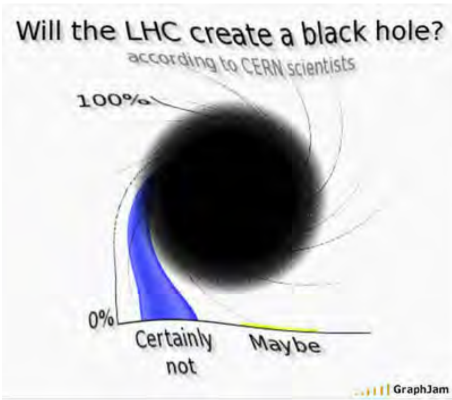
Collaborators: P. Nicolini[1], M. Bleicher[1,2], J.R. Mureika[3], E. Spallucci[4], M. Sprenger[1,2], E. Winstanley[5]

[1]Frankfurt Institute for Advanced Studies, [2]Institut für Theoretische Physik, Johann Wolfgang Goethe-Universität, [3]Loyola Marymount University, Los Angeles, USA, [4]University of Trieste, Italy. [5]University of Sheffield, UK.

Collisions of neutron stars (or massive objects like galaxies or clusters) may lead upon certain conditions to the formation of black holes. The mechanism which governs black formation is not known, but it is customary modelled via the Thorne's "Hoop conjecture": a black hole forms whenever the collision impact parameter b becomes smaller than the Schwarzschild radius, r_{H}, of the effective two-body matter system. While for astrophysical black holes such a conjecture consistently implies a black disk profile of the cross section σ_{BH}, in the case of particle collisions this is no longer acceptable. In hindsight, the black disk profile leads to the absurd result that roughly one black hole a day would have formed at the Super Proton Synchrotron (SPS) in 1985, provided additional spatial dimensions are assumed to overcome the hierarchy problem. Against this background, we need to recall that, within the paradigm of quantum gravity at the Terascale, the impact parameter cannot be smaller than a minimum resolution length $\ell \sim 10^{-19}$ m. On the ground of this line of reasoning, we analytically derived an improved version of the black hole cross section

$$\sigma_{\mathrm{BH}}(s) = \pi\ell^2\Gamma\left(-1;\ell^2/r_{\mathrm{H}}^2(s)\right), \quad \Gamma(\alpha;x) = \int_x^\infty dt\, t^{\alpha-1}e^{-t}.$$

The above formula smoothly interpolates the classical result in the trans-Planckian regime and the expected suppression of sub-Planckian black holes, without introducing, "by hand", any threshold function. With the current limits on the LHC luminosity, we have estimated the black hole production rate $\dot{N}$, which turns to be virtually vanishing for $\sqrt{s} \leq 14$. Only for M-theory inspired 11-dimensional spacetimes, the "new physics" might be just behind the corner, *i.e.*, roughly $\dot{N} \sim 3/\text{year}$ for $\sqrt{s} \sim 16$ TeV. As a result the number of extradimensions logically connects our findings with the observation of any physics beyond the standard model.

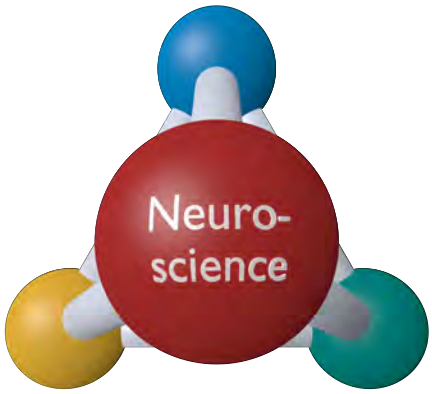


Expectations for black hole production are dropping.
Are we at the sunset of any "new physics" beyond the standard model?

Related publications in 2012:

1) J. R. Mureika, P. Nicolini and E. Spallucci, *Could any black holes be produced at the LHC?*, Phys. Rev. D 85, 106007 (2012)
2) M. Sprenger, P. Nicolini and M. Bleicher, *Physics on the Smallest Scales - An Introduction to Minimal Length Phenomenology*, Eur. J. Phys. 33, 853 (2012)
3) P. Nicolini, *Nonlocal and generalized uncertainty principle black holes*, arXiv:1202.2102 [hep-th]
4) J. Mureika and P. Nicolini, *Self-completeness and spontaneous dimensional reduction*, arXiv:1206.4696 [hep-th]
5) P. Nicolini and E. Spallucci, *Holographic screens in ultraviolet self-complete quantum gravity*, arXiv:1210.0015 [hep-th]

4.2 Neuroscience



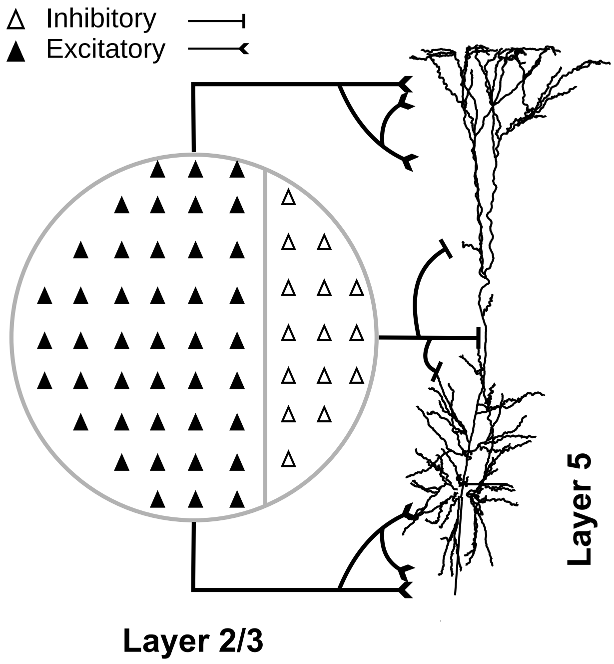
Modeling the Effect of Transcranial Magnetic Stimulation on Cortical Circuits

Collaborators: M. Murakami[1], C. Rusu[1,2], J. Triesch[1], U. Ziemann[3]

[1] Frankfurt Institute for Advanced Studies, [2] Romanian Institute of Science and Technology, Cluj-Napoca, Romania, [3] Dept. of Neurology, Universität Tübingen

Transcranial magnetic stimulation (TMS) allows to manipulate neural activity non-invasively. Much research is currently trying to exploit this ability in clinical and basic research settings. However, the details of how TMS induces neural activity patterns in cortical circuits remain poorly understood, which hampers targeted clinical application. In a standard TMS paradigm, single-pulse stimulation over motor cortex produces high-frequency repetitive responses of around 600 Hz in descending motor pathways called I-waves.

We have used computational modeling to shed light on the mechanism underlying I-wave generation. Our model consists of a detailed layer 5 (L5) pyramidal cell and a population of layer 2 and 3 (L2/3) neurons projecting onto it with synapses exhibiting short-term depression. Our model successfully explains all basic characteristics of I-waves observed in epidural responses during *in vivo* recordings of conscious humans. In addition, it shows how the complex anatomical structure of L5 neurons plays an important role in the generation of I-waves. We find that later I-waves are formed due to inputs to distal synapses, while earlier ones are driven by synapses closer to the soma. Finally, the model explains, inhibition and facilitation effects in paired-pulse stimulation protocols. In contrast to previous models which required either neural oscillators or chains of inhibitory interneurons acting upon L5 cells our model is fully feed-forward, without lateral connections or loops. It parsimoniously explains findings from a range of experiments and brings us one step closer to designing optimized stimulation protocols for specific clinical purposes.



The model we have developed includes a reconstructed dendritic tree of a L5 pyramidal cell. A total of 300 excitatory and inhibitory L2/3 cells (ratio 4:1) project synapses on to the L5 cell. Our model predicts that short-term synaptic depression of these synapses plays an important role in certain effects obverd in paired-pulse stimulation protocols.

Related publications in 2012:

1) C. Rusu, U. Ziemann, J. Triesch, *A Model of I-Wave Generation during Transcranial Magnetic Stimulation (TMS)*. COSYNE, February 23-26, 2012, Salt Lake City, Utah, USA
2) C. Rusu, M. Murakami, U. Ziemann, J. Triesch, *A Model of TMS-induced I-waves in Motor Cortex*, submitted

Learning and self-organization in neural network models of brain function

Collaborators: G. Deak[1], C. Dimitrakakis[2], D. Krieg[3], P. Sterne[3], J. Triesch[3], P. Zheng[3]

[1] UC San Diego, La Jolla, California, USA, [2] EPFL, Lausanne, Switzerland, [3] Frankfurt Institute for Advanced Studies

Understanding the learning and self-organization processes in the brain is of fundamental importance for understanding its function. A major activity of the Triesch lab is to study these issues with neural network models.

In a major line of research we have considered the self-organization of neural circuits through the interaction of different forms of neuronal plasticity. This allowed us to parsimoniously explain recent findings on the statistics and fluctuations of synaptic connection strengths. The distribution of synaptic strengths of local excitatory connections in the cortex is long-tailed (approximately lognormal), but individual synapses can undergo strong fluctuations from day to day. This raises the question how the brain can maintain stable long-term memories at all. Recent evidence has shown that very strong synapses are relatively more stable than weak ones and could thus be the physiological basis of long-lasting memories. We have shown that the distribution of synaptic strengths and their pattern of fluctuations are explained by self-organization in a recurrent spiking network model combining spike-timing-dependent plasticity, synaptic scaling, structural plasticity, and intrinsic plasticity. In this network, STDP induces a rich-get-richer mechanism for excitatory synapses, while synaptic scaling induces competition between them. The resulting dynamics produces lognormal-like weight distributions (see Figure) and patterns of synapse fluctuations closely matching experimental data. This process is robust to parameter changes in the network but critically depends on the presence of the different homeostatic plasticity mechanisms.

In a second line of research we have developed a neural network model of how infants learn an important social interaction skill. Gaze following is the skill of looking where somebody else is looking and it develops during the first 18 month of life. The model parsimoniously explains a large number of findings from different labs in a simple model based on reinforcement learning processes.

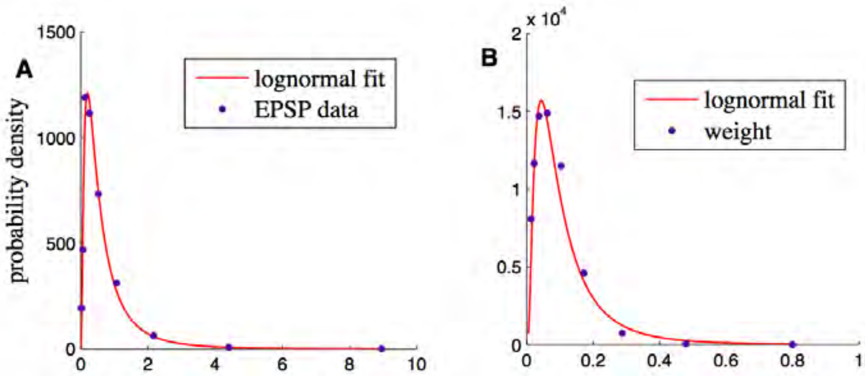


Figure: Distribution of synaptic weights in our model matches lognormal distribution of EPSPs in cortex. A: distribution of EPSP sizes from Song et al. (2005) and lognormal fit. B: distribution of weight strengths in our model and lognormal fit.

Related publications in 2012:

1) P. Zheng, C. Dimitrakakis, J. Triesch, *Network Self-organization Explains the Statistics and Dynamics of Synaptic Connection Strengths in Cortex*, PLoS Computational Biology 9(1), e1002848 (2012)
2) P. Sterne, *Efficient and robust associative memory from a generalized Bloom filter.* Biological Cybernetics 106(4-5), 271–281 (2012)
3) H. Jasso, J. Triesch, G. Deak, J. M. Lewis, *A Unified Account of Gaze Following.* IEEE Trans. on Autonomous Mental Development 4(4), 257–272 (2012)
4) D. Krieg, J. Triesch, *A unifying theory of synaptic long-term plasticity based on a sparse synaptic strength*, in preparation.

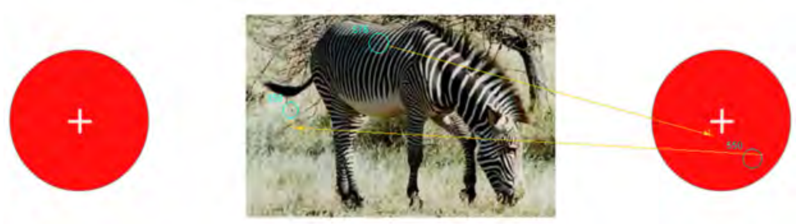
Studying infant cognitive development using gaze-contingency paradigms

Collaborators: J. Bolhuis[1], M. Knopf[1], T. Kolling[1], A. Romberg[2], C. Rothkopf[3], J. Triesch[3], Q. Wang[3], C. Yu[2]

[1] Dept. of Psychology, Goethe University Frankfurt, [2] Indiana University, Bloomington, USA, [3] Frankfurt Institute for Advanced Studies

Studying infant cognitive development is notoriously difficult due to infants' poorly developed motor abilities. Fortunately, however, infants reach accurate control over their eyes comparatively early, which is why many paradigms for studying infant cognition rely on their eye movements. With recent advances in remote eye tracking technology, the eye movements of infants can be measured accurately and non-invasively. We have developed gaze-contingent paradigms where infants can control some aspect of their environment through their eye movements. This allows studying infant cognition in the full perception action cycle.

In a first line of research, we have exploited gaze-contingency to study the discovery of agency. As an infant tries to make sense of the vast array of sensory signals and wins control over its body and physical environment, one of its most fundamental problems is to learn which sensory events are the consequence of its own motor actions and which ones are not. Using a newly-developed gaze-contingent (GC) paradigm employing automated eye-tracking, we have shown that 6 and 8-month-old infants readily look at targets to trigger certain sensory events and that they rapidly anticipate the outcomes of their actions. In contrast to previous paradigms for studying infant cognition based on looking behavior, our paradigm gives infants direct control over the physical environment, allowing them to change what is "out there" with their eye movements. The ability of infants to quickly discover new ways of controlling their environment that we have demonstrated, paves the way for truly interactive approaches to studying infant learning and cognition and may provide a basis for novel training and medical intervention strategies.



Example of a gaze-contingent paradigm: by looking at one of the two red buttons, infants can trigger the appearance of a new animal picture.

Along those lines, in collaboration with Chen Yu and his team at Indiana University, we have begun to investigate whether and how gaze-contingent paradigms can be used to study language development. An exciting possibility is that gaze-contingency could be exploited to teach the meaning of words to infants. In this way, it may be possible to start teaching them a second language very early on. Due to so-called critical periods in brain development, the experiences made during the first year of life are particularly important for language development. Gaze-contingent paradimgs could allow training infants on a second language when their brains are most receptive for it.

Related publication in 2012:

1) Q. Wang, J. Bolhuis, C. Rothkopf, T. Kolling, M. Knopf, J. Triesch, *Infants in Control: rapid anticipation of action outcomes in a gaze-contingent paradigm*. PLoS ONE 7(2): e30884. doi:10.1371/journal.pone.0030884.

Studying the interaction of perception and working memory

Collaborators: G. Cicchini[1], K. R. Gegenfurtner[2], L. Scocchia[3,2,4], J. Triesch[3], M. Valsecchi[2]

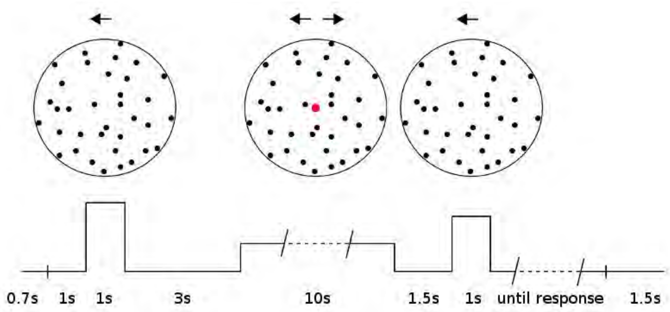
[1] Institute of Neuroscience, Pisa, Italy, [2] University of Giessen, Giessen, Germany, [3] Frankfurt Institute for Advanced Studies, [4] University of Milano-Bicocca, Milano, Italy

Visual working memory is the system that allows us to temporarily store and manipulate visual information. As such, it is fundamental for most activities requiring vision. While much research has focused on characterizing the capacity of visual working memory, little work has addressed how it interacts with ongoing perception. For example, does holding an object in visual working memory interfere with the perception of other stimuli? To address such questions we have been performing a number of experiments.

In a first study we have investigated whether holding the orientation of a simple bar in memory affects the perception of the orientation of other bars. Subjects first memorized the orientation of a white bar on black background. While they held it in memory they had to judge whether two subsequently presented bars were tilted clockwise or anticlockwise from the oblique 45° orientation. Interestingly, we found that holding in memory the first bar influenced how the two other bars were perceived. The memorized bar had a repulsive effect, *i.e.* the subsequently presented bars were perceived as rotated away from it. This effect is distinct from a simple adaptation effect as shown in a control experiment where subjects only attend to but do not memorize the initial bar.

In a second study we have investigated how holding an object in visual working memory influences the perception of ambiguous stimuli. For ambiguous stimuli such as the famous Necker cube, perception spontaneously alternates between the two different interpretations of the stimulus. In our experiment, subjects perceived an ambiguously rotating sphere, which can be perceived as rotating clockwise or anticlockwise. Subjects reported their percept (rotating clockwise or anticlockwise) on a moment to moment basis, while they held in memory the velocity of an unambiguously rotating sphere. Interestingly, the memory content systematically influenced their interpretation of the ambiguous sphere. Subjects were more likely to interpret the ambiguous sphere as rotating in the same direction as the sphere held in memory.

Together, both studies show how holding an item in visual working memory can alter ongoing perception. These results extend our previous finding that a visual working memory load can selectively slow down the perception of similar objects.



Trial structure in the experiment on ambiguous motion perception. The working memory load given at the beginning of the trial affects the perceived direction of motion of an ambiguously rotating sphere. At the end of the trial the memorized velocity has to be compared to a test stimulus.

Related publications in 2012:

1) L. Scocchia, G. Cicchini, J. Triesch, *What's "up"? Working memory contents can bias orientation processing*. Vision Research 18(15):46–55, 2013

2) L. Scocchia, M. Valsecchi, K. R. Gegenfurtner, J. Triesch, *Visual working memory contents bias ambiguous structure from motion perception*, PLoS One, accepted

Quantifying human behavioral goals with inverse optimal control

Collaborators: C. A. Rothkopf[1], C. Dimitrakakis[2], D. H. Ballard[3]

[1] Frankfurt Institute for Advanced Studies, [2] Ecole Polytechnique Federale de Lausanne, Lausanne, Switzerland [3] Department of Computer Science, University of Texas at Austin, Austin, Texas, USA

In a large variety of situations one would like to have an expressive and accurate model of observed animal or human behavior. While general purpose mathematical models may capture successfully properties of observed behavior, it is desirable to root models in biological facts. Because of ample empirical evidence for reward-based learning in visuomotor tasks we use a computational model based on the assumption that the observed agent is balancing the costs and benefits of its behavior to meet its goals. This leads to using the framework of Reinforcement Learning, which additionally provides well-established algorithms for learning of visuomotor task solutions.

To quantify the agent's goals as rewards implicit in the observed behavior we propose to use inverse reinforcement learning, which quantifies the agent's goals as rewards implicit in the observed behavior. Based on the assumption of a modular cognitive architecture, we introduce a modular inverse reinforcement learning algorithm that estimates the relative reward contributions of the component tasks in navigation, consisting of following a path while avoiding obstacles and approaching targets. It is shown how to recover the component reward weights for individual tasks and that variability in observed trajectories can be explained succinctly through behavioral goals. It is demonstrated through simulations that good estimates can be obtained already with modest amounts of observation data, which in turn allows the prediction of behavior in novel configurations.

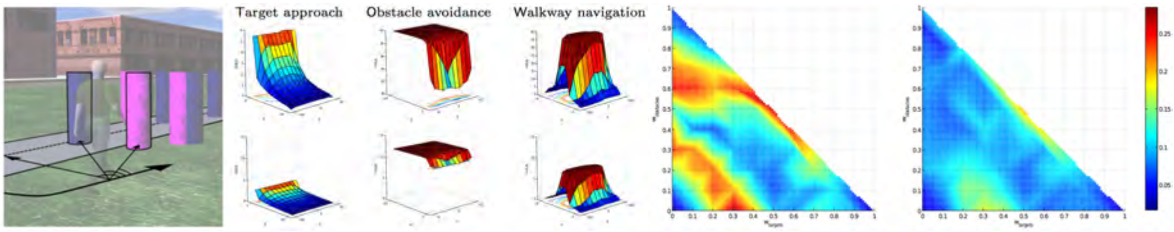


Figure: *Left:* Overview of ego-centric polar coordinate reference frame of navigation problem formulation. *Center:* Value functions quantifying the expected total discounted reward obtainable in the component tasks of target approach, obstacle avoidance, and path following. *Right:* RMS error in estimation of the true reward weights given observation data using the proposed maximum likelihood algorithm and the proposed regularized estimation technique.

Related publications in 2012:

1) C. A. Rothkopf, D. H. Ballard, *Modular inverse reinforcement learning for visuomotor behavior*, (submitted)
2) C. A. Rothkopf, *Inferring human intrinsic rewards through inverse reinforcement learning*, Bernstein Conference, September 12-14, Munich, Germany, (2012)

Human gaze allocation in naturalistic tasks

Collaborators: C. A. Rothkopf[1], B. T. Sullivan[2], D. H. Ballard[3], G. Diaz[4], M. M. Hayhoe[4]

[1] Frankfurt Institute for Advanced Studies, [2] Smith-Kettlewell Eye Research Institute, San Francisco, CA, USA [3] Department of Computer Science, University of Texas at Austin, Austin, Texas, USA [4] Center for Perceptual Systems, University of Texas at Austin, Austin, Texas, USA

Despite general agreement that prediction is a central aspect of perception, there is relatively little evidence concerning the basis on which visual predictions are made. Although both saccadic and pursuit eye-movements reveal knowledge of the future position of a moving visual target, in many of these studies targets move along simple trajectories through a fronto-parallel plane. Here, using a naturalistic and racquet-based interception task in a virtual environment, we demonstrate that subjects make accurate predictions of visual target motion, even when targets follow trajectories determined by the complex dynamics of physical interactions and the head and body are unrestrained. Furthermore, we found that, following a change in ball elasticity, subjects were able to accurately adjust their prebounce predictions of the ball's post-bounce trajectory. This suggests that prediction is guided by experience-based models of how information in the visual image will change over time.

Similarly, eye movements during natural tasks are well coordinated with ongoing task demands and many variables could influence gaze strategies. Previous models have proposed a gaze-scheduling mechanism that uses a utility-weighted uncertainty metric to prioritize fixations on task-relevant objects and predicted that human gaze should be influenced by both reward structure and task-relevant uncertainties. To test this conjecture, we tracked the eye movements of participants in a simulated driving task where uncertainty and implicit reward (via task priority) were varied. Participants were instructed to simultaneously perform a Follow Task where they followed a lead car at a specific distance and a Speed Task where they drove at an exact speed. We varied implicit reward by instructing the participants to emphasize one task over the other and varied uncertainty in the Speed Task with the presence or absence of uniform noise added to the car's velocity. Subjects' gaze data were classified for the image content near fixation and segmented into looks. Gaze measures, including look proportion, duration and interlook interval, showed that drivers more closely monitor the speedometer if it had a high level of uncertainty, but only if it was also associated with high task priority or implicit reward. The interaction observed appears to be an example of a simple mechanism whereby the reduction of visual uncertainty is gated by behavioral relevance.

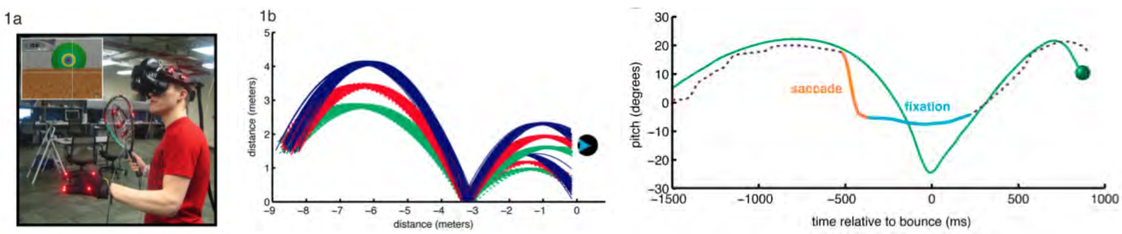


Figure: *Left:* Setup of the virtual ball hitting task in virtual reality. *Center:* Ball trajectories in different task conditions. *Right:* Gaze and ball trajectory in one particular experimental trial.

Related publications in 2012:

1) G. J. Diaz, J. Cooper, C. A. Rothkopf, M. M. Hayhoe, *Saccades to future ball location reveal memory-based prediction in a natural interception task*, Journal of Vision, 13(1):1, 1-14 (2013)
2) B. T. Sullivan, L. Johnson, C. A. Rothkopf, D. H. Ballard, M. Hayhoe, *The role of uncertainty and reward on eye movements in a virtual driving task*, Journal of Vision, 12(13):19, 1-16 (2012)

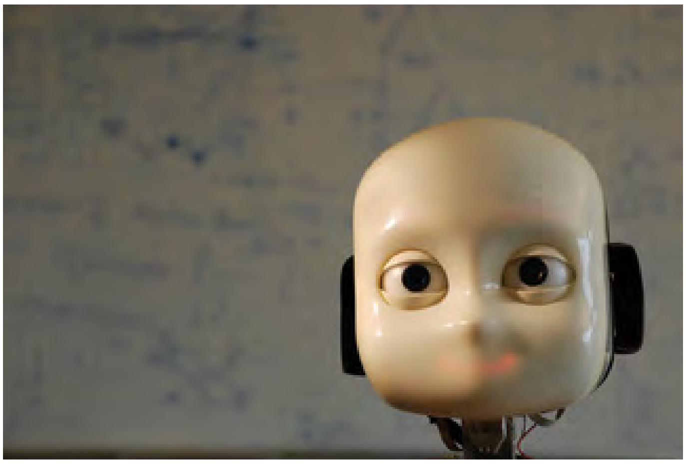
Autonomous Learning in a Humanoid Robot

Collaborators: P. Chandrashekhariah[1], L. Lonini[1], C. Rothkopf[1], B. Shi[2], J. Triesch[1], Y. Zhao[2]

[1] Frankfurt Institute for Advanced Studies, [2] Hong Kong University of Science and Technology, Hong Kong, China

How can the principles of learning and development from biological organisms be exploited to build autonomously learning robots? Our focus is on active visual perception and learning. The fundamental question is how effective representations of visual input can be learned in an autonomous fashion and how intelligent behavior can be acquired on the basis of the learned representations. Along these lines we have developed a "curious" active vision system that autonomously explores its environment and learns object representations without any human assistance. Similar to an infant, who is intrinsically motivated to seek out new information, our system is endowed with an attention and learning mechanism designed to search for new information that has not been learned yet. Our method can deal with dynamic changes of object appearance which are incorporated into the object models.

In a second line of research in collaboration with researchers at the Hong Kong University of Science and Technology we are working on methods for efficient coding of sensory information in the perception action cycle. We have been developing a new way to combine unsupervised learning of generative models with reinforcement learning and apply this to the development of disparity tuning in visual cortex and vergence eye movements. Concretely, a generative model is learning to jointly encode patches of the left eye and right eye images. At the same time, the system is generating vergence movements of the eyes. Crucially, it is receiving internal reward signals for generating eye movements that make the left and right images easier to encode for the generative model. This way it learns to perform vergence eye movements that align the left and right images making them maximally redundant. Our approach explains how the ability to properly align the two eyes and the ability to learn a representation of binocular disparity can develop and self-calibrate completely autonomously on the basis of efficient coding principles.



The iCub robot head used in our studies. Its degrees of freedom and appearance are modeled after a 2-year-old child.

Related publications in 2012:

1) P. Chandrashekhariah, G. Spina, J. Triesch, *Let it Learn: A Curious Vision System for Autonomous Object Learning*, International Conference on Computer Vision Theory and Applications, 21-24 February, 2013, Barcelona, Spain

2) Y. Zhao, C. A. Rothkopf, J. Triesch, B. Shi, *A unified model of the joint development of disparity selectivity and vergence control*, IEEE 8th International Conference on Development and Learning, November 7-9, 2012 (Paper of Excellence award)

Statistics of the natural input to the visual system

Collaborators: D. Pamplona[1], J. Triesch[1], C. A. Rothkopf[1]

[1] Frankfurt Institute for Advanced Studies

The efficient coding hypothesis posits that sensory systems are adapted to the regularities of their signal input so as to reduce redundancy in the resulting representations. It is therefore important to characterize the regularities of natural signals to gain insight into the processing of natural stimuli. While measurements of statistical regularity in vision have focused on photographic images of natural environments it has been much less investigated, how the specific imaging process embodied by the organism's eye induces statistical dependencies on the natural input to the visual system. This has allowed using the convenient assumption that natural image data are homogeneous across the visual field. Extensive previous researlch of the autocorrelation function and the power spectrum of natural images has shown that for large image ensembles the average power spectrum falls off with radial frequency as $1/f_r^{\alpha}$ where the value for α is empirically estimated to be close to 2.

Here we give up on this assumption and show how the imaging process in a human model eye influences the local statistics of the natural input to the visual system across the entire visual field. Artificial scenes with three-dimensional edge elements were generated and the influence of the imaging projection onto the back of a spherical model eye were quantified. These distributions show a strong radial influence of the imaging process on the resulting edge statistics with increasing eccentricity from the model fovea. This influence is further quantified through computation of the second order intensity statistics as a function of eccentricity from the center of projection using samples from the dead leaves image model. Using data from a naturalistic virtual environment, which allows generation of correctly projected images onto the model eye across the entire field of view, we quantified the second order dependencies as function of the position in the visual field using a new generalized parameterization of the power spectra. Finally, we compared this analysis with a commonly used natural image database, the van Hateren database, and show good agreement within the small field of view available in these photographic images. We conclude by providing a detailed quantitative analysis of the second order statistical dependencies of the natural input to the visual system across the visual field and demonstrating the importance of considering the influence of the sensory system on the statistical regularities of the input to the visual system.

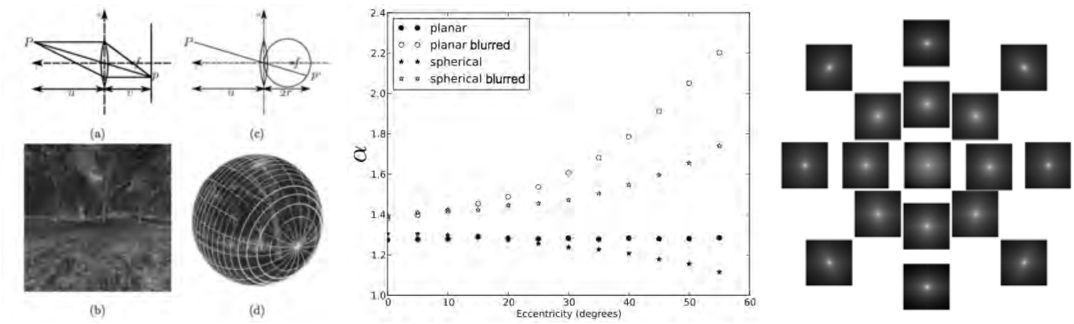


Figure: *Left:* Differences of the image formation process between photographic images and images projected into a model eye. *Center:* Dependence of the parameter α describing the power spectra in the above equation across the visual field as a function of eccentricity. *Right:* Local power spectra across 17 position in the visual field.

Related publications in 2012:

1) D. Pamplona, J. Triesch, C. A. Rothkopf, *Power spectra of the natural input to the visual system*, Vision research, (in press)
2) D. Pamplona, J. Triesch, C. A. Rothkopf, *The statistics of looking: Deriving properties of retinal ganglion cells across the visual field*, 12th annual meeting of the Vision Science Society, May 11-16, 2012, Naples, Florida, USA (2012)

Common design of orientation columns in the visual cortex

Collaborators: Fred Wolf[1], Siegrid Löwel[2], Zoltan F. Kisvarday[3], David M. Coppola[4], Leonard White[5], Matthias Kaschube[6]

[1]MPI for Dynamics and Self-Organization, Göttingen, Germany, [2]Göttingen University, Germany. [3]University of Debrecen, Hungary, [4]Randolph-Macon College, Ashland VA, USA. [5]Duke University, Durham NC, USA. [6]FIAS, Goethe University, Frankfurt

In primates and carnivores, detectors for different visual features are not randomly distributed across the visual cortex, but form spatially well organized maps. For instance, in the orientation preference map, neurons are tuned to a particular location in the visual world and to the orientation of an edge like stimulus at that location and both tuning properties vary mostly smoothly across the cortical surface (Fig. 1). An exception to this are the so-called pinwheels, point like topological defects, in the vicinity of which all orientations are represented (white dots in Fig. 1B). By quantitatively analyzing large sets of brain imaging data, we previously found that the layout of the orientation preference map precisely follows a single common design in different species separated since the basal radiation of placental mammals (Kaschube et al., Science, 2010). These findings indicated that the evolution of visual cortical circuitry is much more constrained than previously anticipated. Recently, by extending the repertoire of analyzed species to cover a 40-fold difference in body weight, we could show that this constraint appears to be invariant against brain and body size (Fig. 1; Keil et al, 2012). Moreover, numerical studies and a symmetry-based analysis of a cortical network self-organization model revealed that the observed common design cannot be explained by a coupling to the development of other cortical maps. The analyses, instead, indicate that cortical long-ranging interactions have constrained the evolution of visual cortical circuitry much more than previously anticipated (Reichl et al, 2012a, 2012b).

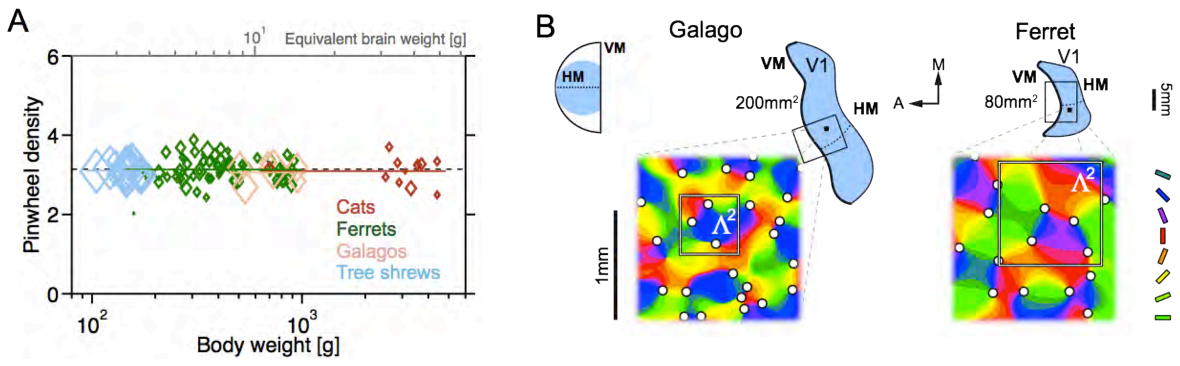


Figure 1: (A) Pinwheel density (i.e. the number of pinwheels per 'hypercolumn' size Λ^2 (see B)) against body size in four mammalian species. Each symbol corresponds to one brain hemisphere (size is proportional to measured area in units of Λ^2). Solid lines indicate species averages. (B) (Top) V1 surface area and representation of the visual hemifield in galago (left) and ferret (right). Blue area, V1; HM, horizontal meridian. (Bottom) Typical orientation map insets in galago (left) and ferret (right). White dots, pinwheels; white square, area of $1\Lambda^2$. Galago V1 contains more than 400 Λ^2, ferret V1 only about 100. Reproduced from Keil et al. (2012).

Related publications in 2012:

1. W. Keil, M. Kaschube, M. Schnabe, Z.F. Kisvarday, S. Löwel, D.M. Coppola, L.E. White, F. Wolf, *Response to Comment on "Universality in the Evolution of Orientation Columns in the Visual Cortex"*, Science 336:413 (2012)
2. L. Reichl, D. Heide, S. Löwel, J.C. Crowley, M. Kaschube, F. Wolf, *Coordinated Optimization of Visual Cortical Maps (II) Numerical Studies.* PLoS Comput Biol. 8(11):e1002756 (2012)
3. L. Reichl, D. Heide, S. Löwel, J.C. Crowley, M. Kaschube, F. Wolf, *Optimization of Visual Cortical Maps (I) Symmetry-based Analysis*. PLoS Comput Biol. 8(11):e1002466 (2012)

Generating a rich repertoire of visual feature detectors with minimal training

Collaborators: Dmitry Tsigankov[1], Audrey Sederberg[2], Matthias Kaschube[1]

[1]FIAS and Goethe University, Frankfurt, [2]University of Chicago, Chicago IL, USA

Learning to represent complex sensory input with limited training data is a challenging problem. In this project as part of the Bernstein-Focus: Neurotechnology Frankfurt we explore the possibility to prime neuronal circuits in order to reduce the training necessary to learn a broad range of tasks. Here we make use of the intrinsic capability of neuronal circuits to spontaneously generate a wealth of dynamical structures. Specifically, we have studied the diverse set of feature selectivities arising in recurrent networks of firing rate neurons as models of cortical circuits involved in tasks such as object recognition (Fig. 1A). As a simple example, we have analyzed the selectivity of neurons in these networks for stimulus motion, probed by driving the network with a moving grating stimulus. We found that for increasingly heterogeneous connections, increasingly strong levels of selectivity arise spontaneously in the network (Fig. 1C). Furthermore, we have started computing explicitly the structure of receptive fields of neurons in recurrent networks and found many features of receptive fields in the visual cortex (see e.g. Fig. 1B). Thus, our work shows that detectors for important visual feature can arise spontaneously in networks of neurons if recurrent connections have a significant impact on their responses to stimuli. This suggests that a limited amount of training is necessary to adjust these circuits to solve more complex detection problems.

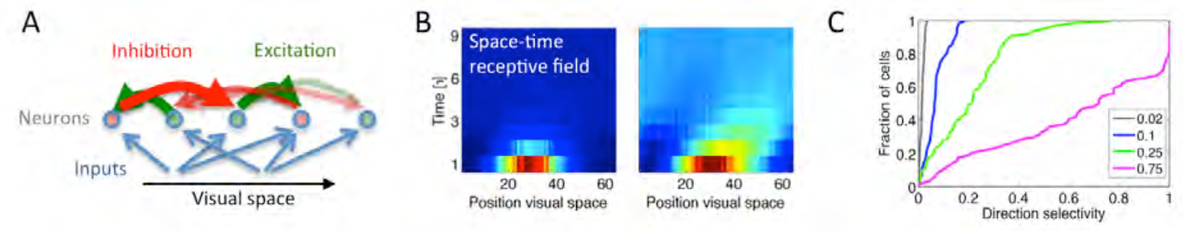


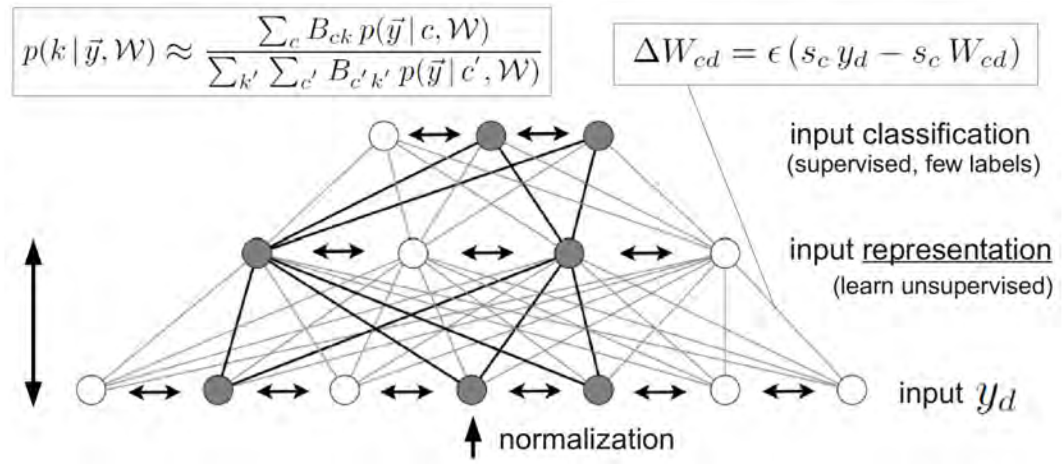
Figure 1: Receptive fields in recurrent networks: emergence of direction selectivity. (**A**) A simple V1 Model: random recurrent network of firing-rate neurons. Each neuron receives afferent inputs from a confined region of visual space centered at a random position. This input is not selective for the direction of motion of a stimulus. (**B**) Receptive field of a neuron, i.e. the structure of visual stimulus (orange bright; blue, dark), which elicits the maximal response at time t=0. Time is backwards and in units of the time constant τ of the neuron. Left: For weak recurrent connections, only stimuli immediately before t=0 are effective in driving the cell. Right: For stronger inhibitory connections, a space-time slant emerges and the neuron becomes direction selective. (**C**) Cumulative distribution of direction selectivity in the network for various strengths of recurrent connections (in units of the critical connection strength). Direction selectivity was assessed based on the response to a moving grating of optimal spatiotemporal frequency. Since the feed-forward input is non-selective, levels of selectivity are small for weak recurrent connections (gray curve). However, for strong connections (pink curve) the distribution becomes similar to those observed in the visual cortex of ferrets (Li et al., Nature, 2008) or mice (Rochefort et al., Neuron, 2011).

Neurally Plausible and Statistically Optimal Approaches to Learning

Collaborators: J. Lücke[1], J. A. Shelton[1], A. S. Sheikh[1], J. Bornschein[1], Z. Dai[1], P. Sterne[1], C. Savin[2]

[1] Frankfurt Institute for Advanced Studies, [2] Computational and Biological Learning Lab, University of Cambridge, UK

The brain's ability to recognize and interpret images, sounds and other sensory data is unmatched by any artificial system, so far. Much or most of this ability is acquire by neural through a long process of small improvements while being exposed to sensory stimuli. This process we call 'learning', and it has been recognized as the key to build intelligent systems. In our studies we bring together the information theoretic foundations of learning and learning in neural circuits. Our results help improve the understanding of brain functions and help building functional approaches for scientific data analysis and computer vision.



Hierarchical graphical memory model for pattern learning and classification. Representations for normalized patterns are learned in the first hierarchical stage. The representations can be learned via neurally plausible interaction and learning rules. A classifier is learned from few labeled data points in the second stage.

As part of the Bernstein Focus Neurotechnology Frankfurt and of the DFG project "Non-linear Generative Models for Representational Recognition and Unsupervised Learning in Vision" we study novel approaches for efficient and neurally plausible learning. We directly relate to recent experimental findings (Berkes et al., Science, 2011) which suggest that neural response variability and spontaneous activity are a consequence of a probabilistic neural code. Such a code stochastically activates neurons for the representation of all potential stimulus interpretations. We have used the newly developed approaches to train stimulus encoding models that are (A) consistent with the stochastic activation of neurons and (B) match the neural response properties in primary visual cortex well (Shelton et al., 2012).

In a related line of research we went one step further and studied neural interaction and learning rules resulting a convergence to theoretically optimal solutions for clustering (Keck et al., 2012). We investigated the pattern learning and classification capabilities of such optimal neural networks, and found competitive pattern classification performance for datasets with few labels.

Related publications in 2012:

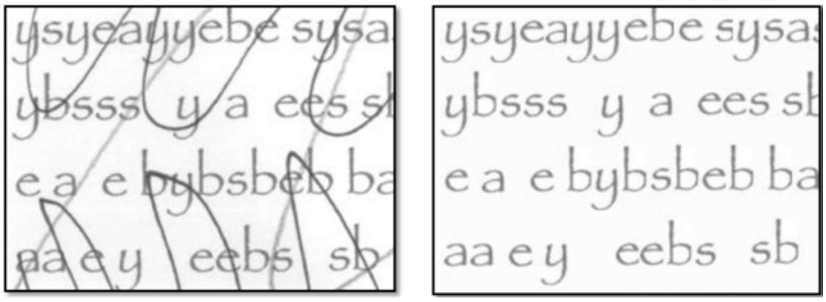
1) J.A. Shelton, P. Sterne, J. Bornschein, A.S. Sheikh, J. Lücke, *Why MCA? Nonlinear Sparse Coding with a Spike-and-slab Prior for Neurally Plausible Image Encoding*, Advances in Neural Information Processing Systems (NIPS) 25, 2285–2293 (2012)
2) C. Keck, C. Savin, J. Lücke, *Feedforward Inhibition and Synaptic Scaling – Two Sides of the Same Coin?*, PLoS Computational Biology 8(3), e1002432 (2012)

Non-linear Generative Models And Their Applications

Collaborators: J. Lücke[1], J. Eggert[2], M. Henniges[1], A. S. Sheikh[1], J. Bornschein[1], Z. Dai[1], J. Shelton[1], P. Sterne[1]

[1] Frankfurt Institute for Advanced Studies, [2] Honda Research Institute, Europe

The salient components of visual scenes are objects. While the visual system of humans and animals identifies visual objects with apparent ease, this task, in general, is still considered as one of the major unsolved problems in computer vision. Learning from visual data is challenging because visual data components combine non-linearly, are dependent, and their identities remain unchanged by position changes. In contrast, state-of-the-art approaches such as independent component analysis (ICA) assume linear component combination, independent components, and fixed component positions. In the DFG project "Non-linear Generative Models for Representational Recognition and Unsupervised Learning in Vision" we develop a new theoretical framework that allows for the development of approaches that go beyond the state-of-the-art in all these aspects. In 2012 we have demonstrated that our new training technology (Lücke, Eggert, 2010; Shelton et al., 2011; Lücke, Henniges, 2012) allows for the development of new algorithms for the non-linear domain (Dai, Lücke, 2012a; Dai, Lücke, 2012b; Shelton et al., 2012). Furthermore, we have shown that the same technology if applied to linear models results in competitive results on benchmarks (Lücke, Sheikh, 2012) and new models (Exarchakis et al., 2012).



Example application of a representational learning approach to autonomous document cleaning. The algorithm first learns characters as the statistically most regular patterns from the original document (left). Using the character representations it then reconstructs a cleaned version (right) of the corrupted document without any supervision (Dai, Lücke, CVPR 2012).

Related publications in 2012:

1) Z. Dai and J. Lücke, *Unsupervised Learning of Translation Invariant Occlusive Components*, IEEE Conference on Computer Vision and Pattern Recognition (CVPR), 2400-2407 (2012)
2) Z. Dai and J. Lücke, *Autonomous Cleaning of Corrupted Scanned Documents – A Generative Modeling Approach, IEEE Conference on Computer Vision and Pattern Recognition (CVPR)*, 3338–3345 (2012) Highest possible CVPR 2012 reviewer score, Google Travel Award and oral presentation.
3) J.A. Shelton, P. Sterne, J. Bornschein, A.S. Sheikh, J. Lücke, *Why MCA? Nonlinear Sparse Coding with a Spike-and-slab Prior for Neurally Plausible Image Encoding*, Advances in Neural Information Processing Systems (NIPS) 25, 2285–2293 (2012)
4) J. Lücke and M. Henniges, *Closed-Form Entropy Limits – A Tool to Monitor Likelihood Optimization of Probabilistic Generative Models*. Proceedings AI Stats, JMLR W&CP 22, 731–740 (2012)
5) G. Exarchakis, M. Henniges, J. Eggert, J. Lücke, *Ternary Sparse Coding*, Proceedings ICA/LVA, LNCS 7191, 204–212 (2012
6) J. Lücke and S. Sheikh, *A Closed-Form EM Algorithm for Sparse Coding and its Application to Source Separation*, Proceedings ICA/LVA, LNCS 7191, 213–221 (2012)

Membrane Resonance and Gamma Oscillations

Collaborators: V.V. Moca[1], D. Nikolić[2,3,4], W. Singer[2,3,4], R.C. Mureşan[1,2]

[1] Center for Cognitive and Neural Studies, Romanian Institute of Science and Technology, Cluj-Napoca, Romania, [2] Max Planck Institute for Brain Research, Frankfurt, [3] Frankfurt Institute for Advanced Studies, [4] Ernst Strüngmann Institute, Frankfurt

Neuronal mechanisms underlying beta/gamma oscillations (20-80 Hz) are not completely understood. We have shown that in vivo beta/gamma oscillations in the cat visual cortex exhibit remarkably stable frequency even when inputs fluctuate. Enhanced frequency stability is associated with stronger oscillations. Simulations of neuronal circuitry demonstrate that membrane properties of inhibitory interneurons strongly determine the characteristics of emergent oscillations. Exploration of networks containing either integrator or resonator inhibitory interneurons revealed that resonance, as opposed to integration, promotes robust oscillations with large power and stable frequency via a mechanism called RING (Resonance INduced Gamma). Stability of frequency and robustness of the oscillation also depend on the relative timing of excitatory and inhibitory volleys within the oscillation cycle; RING can reproduce characteristics of both Pyramidal INterneuron Gamma (PING) and INterneuron Gamma (ING), transcending such classifications. Results suggest that interneuronal membrane resonance can be an important ingredient for generation of robust gamma oscillations having stable frequency.

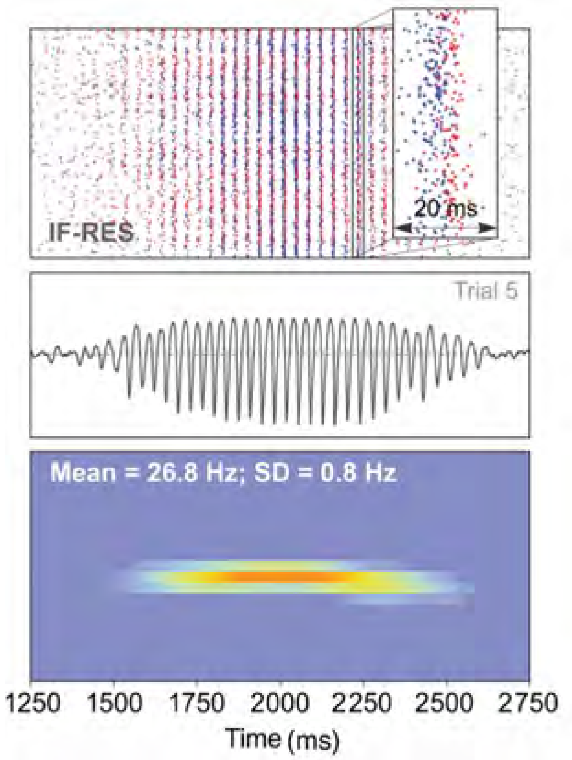


Figure: Gamma oscillations in simulated neuronal circuits of 625 neurons.
Top, zoomed in integrator-resonator (IF-RES) raster; middle, local field potential corresponding to spike raster above; bottom, time-resolved power spectrum of the local field potential averaged across 20 trials.

Related publication in 2012:

V. V. Moca, D. Nikolić, W. Singer, R.C. Mureşan, *Membrane resonance enables stable and robust gamma oscillations*, Cerebral Cortex, in press (2012), doi:10.1093/cercor/bhs293.

Scaled correlation analysis

Collaborators: Danko Nikolić[1,2], Raul C. Mureşan[1,3], Weijia Feng[1,2], Wolf Singer[1,2]

[1] Max Planck Institute for Brain Research, Frankfurt, [2] Frankfurt Institute for Advanced Studies, [3] Center for Cognitive and Neural Studies, Romanian Institute of Science and Technology, Cluj-Napoca, Romania

When computing a cross-correlation histogram, slower signal components can hinder the detection of faster components, which are often in the research focus. For example, precise neuronal synchronization often co-occurs with slow co-variation in neuronal rate responses. We invented a method - dubbed scaled correlation analysis - that enables the isolation of the cross-correlation histogram of fast signal components. The method computes correlations only on small temporal scales (i.e. on short segments of signals such as 25 ms), resulting in the removal of correlation components slower than those de?ned by the scale. Scaled correlation analysis has several advantages over traditional filtering approaches based on computations in the frequency domain. Among its other applications, as we show on data from cat visual cortex, the method can assist the studies of precise neuronal synchronization.

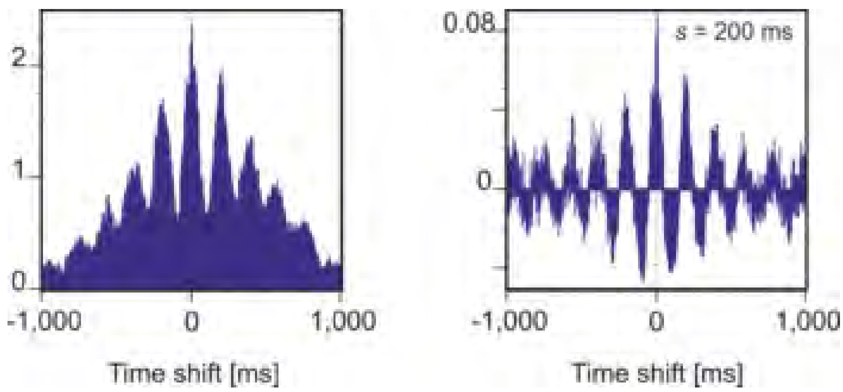


Figure: Example of a cross-correlogram between spike trains computed in a classical manner (left) and by using scaled correlation (right; $S = 200$ ms). Scaled correlation removes the slow component from the cross-correlogram.

Related publication in 2012:

D. Nikolić, R.C. Mureşan, W. Feng, W. Singer, *Scaled correlation analysis: A better way to compute a cross-correlogram*, European Journal of Neuroscience 35, 742–762 (2012), doi: 10.1111/j.1460-9568.2011.07987.x

Measuring information-transfer delays

Collaborators: Raul Vicente[3,8], Michael Wibral[1], Nicolae Pampu[2], Viola Priesemann[3], Felix Siebenhühner[1,4], Hannes Seiwert[1], Michael Lindner[5], Joseph T. Lizier[6,7]

[1] MEG Unit, Brain Imaging Center, Goethe University, Frankfurt, Germany, [2] Center for Cognitive and Neural Studies (Coneural), Cluj-Napoca, Romania, [3] Frankfurt Institute for Advanced Studies (FIAS), Goethe University, Frankfurt, Germany, [4] Department of Physics, University of California, Santa Barbara, CA, USA, [5] Center for Economics and Neuroscience, Friedrich-Wilhelms University, Bonn, Germany, [6] Max Planck Institute for Mathematics in the Sciences, Leipzig, Germany, [7] CSIRO Information and Communication Technologies Centre, Marsfield, NSW, Australia, [8] Max-Planck Institute for Brain Research, Frankfurt, Germany

In complex networks such as gene networks, traffic systems or brain circuits it is important to understand how long it takes for the different parts of the network to effectively inuence one another. In the brain, axonal delays between brain areas can amount to several tens of milliseconds, adding an intrinsic component to any timing-based processing of information. Inferring neural interaction delays is thus needed to interpret the information transfer revealed by any analysis of directed interactions across brain structures.

However, a robust estimation of interaction delays from neural activity faces several challenges if modeling assumptions on interaction mechanisms are wrong or cannot be made. During this year we have worked to propose a robust estimator for neuronal interaction delays rooted in an information-theoretic framework, which allows a model-free exploration of interactions. In particular, we have extended transfer entropy to account for delayed source-destination interactions, while crucially retaining the conditioning on the embedded destination state at the immediately previous time step. We have proved that this particular extension is indeed guaranteed to identify interaction delays between two coupled systems and is the only relevant option in keeping with Wiener's principle of causality. We have also demonstrated the performance of our approach in detecting interaction delays on finite data by numerical simulations of stochastic and deterministic processes, as well as on local field potential recordings. Importantly, we also showed the ability of the extended transfer entropy to detect the presence of multiple delays, as well as feedback loops. While evaluated on neuroscience data, we expect the estimator to be useful in other fields dealing with network dynamics.

Related publication in 2012:

1) *Measuring information-transfer delays*, accepted in PLoS One (to appear in 2013)

4.3 Biology, Chemistry, Molecules, Nanosystems

First high-energy proton tomography of a mouse

Collaborators: M. Durante[1,2], C. La Tessa[1], P. Lang[1], F. Merrill[3], M. Prall[1], H. Stöcker[1,2], L. Shestov[1], D. Varentsov[1]

[1] GSI, Darmstadt, Germany, [2] FIAS, Frankfurt, Germany, [3] Los Alamos National Laboratory, NM, USA,

Relativistic protons have been proposed as an alternative to low-energy ions in the treatment of cancer and non cancer diseases (M. Durante and H. Stöcker, J. Phys.: Conf. Ser. 373 012016 (2012)). The increase of the primary beam energy to the GeV region will overcome several limitations of Bragg-Peak therapy with protons, such as the broadening of the primary beam due to multiple scattering and uncertainties on the particle range and Relative Biological Effectiveness (RBE). These processes lead to a reduced dose gradient between the tumor volume and the surrounding tissue and thus to an increase of side effects. The main advantage of relativistic protons is that the beam crossing the patient can be exploited for imaging purposes. Proton radiography was investigated for many years because of its low radiation dose and high density resolution, but until recently the image blurring caused by scattering was limiting its practical applications in medicine. In the past years, the Los Alamos National Laboratory (LANL) system based on a magnetic lens after the object for imaging and chromatic aberration corrections pushed the technique to unprecedented time and spatial resolution (F. E. Merrill et al., Rev. Sci. Instr. 82 103709 (2011)). This technique exploits differences in the lateral scattering of the primary ions due to the material thickness and density they encounter. The application of this methodology to medical imagining has been tested at the pRad facility (LANL) in December 2012. The experiment was performed within the framework of the PANTERA (Proton Therapy and Radiography) project. Radiographies of simple (plastic tissue-equivalent targets) and complex (antropomorphic phantom, zebra fishes) geometries were acquired using 800 MeV protons. Furthermore, the first proton tomography of a formalin-preserved mouse was obtained. First preliminary results of the latter target are shown in this report. The mouse was placed with its main axis perpendicular to the beam direction. A rotational stage was used to allow a 360 degrees movement of the sample with a 0.5 degrees step. An example of the mouse profile acquired in the orthogonal direction with respect to the beam axis is reported in Figure below.

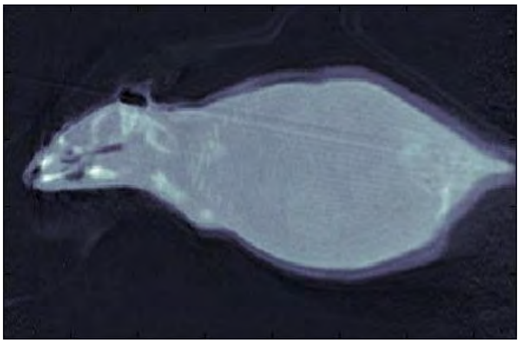


Figure: Profile of the mouse acquired in the direction orthogonal to the beam axis.

The shape of the mouse as well as some internal bony structures (mainly in the head) can be clearly distinguished. The application of relativistic protons to diagnostic has shown promising results. Further tests on live animals are planned at pRad in 2013 and at the proton microscope PRIOR located in the FAIR facility, where energies above 1 GeV will be available. The experiments will focus on optimizing the technique for the image of lesions implanted in the animals and couple the irradiation with standard radiotherapy.

Related publications in 2012:

1) M. Durante and H. Stöcker, *Relativistic protons for image-guided stereotactic radiosurgery*, J. Phys.: Conf. Ser. 373, 012016 (2012)
2) Z. Yu et al., *Biophysical characterization of a relativistic proton beam for image-guided radiosurgery*, J. Rad. Res. 53, 620 (2012)
3) D. Varentsov et al., *First biological images with high-energy proton microscopy*, Phys. Med. in press, http://dx.doi.org/10.1016/j.ejmp.2012.03.002 (2012)

Deceleration of Fusion-Fission Cycles Improves Mitochondrial Quality Control during Aging

Collaborators: Marc Thilo Figge[1,2,3], Andreas S. Reichert[4,5], Michael Meyer-Hermann[2,3], Heinz D. Osiewacz[6]

[1] Leibniz-Institute for Natural Product Research and Infection Biology and Friedrich Schiller University, Jena, [2] FIAS, [3] Department of Systems Immunology, Helmholtz Centre for Infection Research, Braunschweig, [4] Mitochondrial Biology, Medical School, Goethe University, [5] Mitochondrial Biology, Buchmann Institute for Molecular Life Sciences, Frankfurt, [6] Molecular Developmental Biology, Cluster of Excellence Macromolecular Complexes, Goethe University

Mitochondria are organelles that play a central role as "cellular power plants". The cellular organization of these organelles involves a dynamic spatial network where mitochondria constantly undergo fusion and fission associated with the mixing of their molecular content. Together with the processes of mitophagy and biogenesis of mitochondrial mass, this results into a cellular surveillance system for maintaining their bioenergetic quality. We applied a probabilistic modeling approach based on the master equation allowing us to simulate mitochondrial function and quality control during aging in silico.

We propose the "mitochondrial infectious damage adaptation" (MIDA) model of aging (see Figure). It reconciles a number of counterintuitive observations obtained during the last decade including infection-like processes of molecular damage spread, the reduction of fusion and fission rates during cellular aging, and observed life span extension for reduced mitochondrial fission. Interestingly, the MIDA model suggests that a reduction in mitochondrial dynamics rather than being merely a sign or even cause of aging, may actually reflect a systemic adaptation to prolong organismic life span.

In particular, we demonstrate that cycles of fusion and fission and mitophagy indeed are essential for ensuring a high average quality of mitochondria, even under conditions in which random molecular damage is present. Prompted by earlier observations that mitochondrial fission itself can cause a partial drop in mitochondrial membrane potential, we tested the consequences of mitochondrial dynamics being harmful on its own. Next to directly impairing mitochondrial function, pre-existing molecular damage may be propagated and enhanced across the mitochondrial population by content mixing. In this situation, such an infection-like phenomenon impairs mitochondrial quality control progressively. However, when imposing an age-dependent deceleration of cycles of fusion and fission, we observe a delay in the loss of average quality of mitochondria. This provides a rational why fusion and fission rates are reduced during aging and why loss of a mitochondrial fission factor can extend life span in fungi. Thus, according to the MIDA model, a deceleration of fusion-fission cycles reflects a systemic adaptation increasing life span.

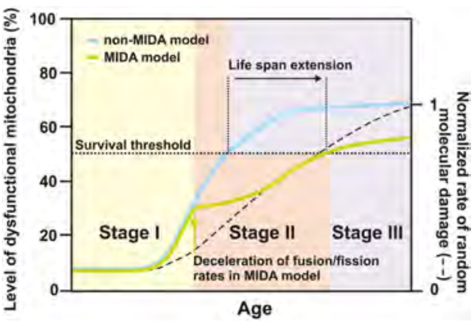


Figure: Mitochondrial infectious damage adaptation (MIDA) model. Schematic representation showing the loss of mitochondrial quality over the fictive life span of an organism according to the MIDA model (green) versus a non-MIDA model (blue). In the MIDA model fusion-fission rates are reduced when a certain degree of molecular damage has accumulated (green arrow). In the non-MIDA model this adaptation was omitted. Stage I is characterized by high fusion-fission rates, low levels of accumulated random molecular damage, yet a high removal rate of those few dysfunctional mitochondria. Stage II represents the time/age when already a significant amount of molecular damage has accumulated. This damage is propagated and enhanced by ongoing fusion and fission cycles, representing "infectious molecular damage". At some time point the latter outweighs the benefit of mitochondrial dynamics and mitophagy in removing dysfunctional mitochondria. Decelerating mitochondrial dynamics (green arrow), in the MIDA model, slows down the accumulation of dysfunctional mitochondria compared to the situation in the non-MIDA model. Still, this adaptation in the MIDA model renders the system less capable of dealing with additional random molecular damage. Assuming a certain survival threshold (dotted line) this results in a net life span extension. Reaching this threshold marks stage III and cell death.

Work supported by BMBF ("GerontoMitoSys" project), Deutsche Forschungsgemeinschaft (DFG project RE-1575/1-1), the European Commision (Contract 512020, "MiMage"), and the Cluster of Excellence "Macromolecular Complexes" at Goethe University (DFG project EXC 115).

Related publication in 2012:

1) M.Th. Figge, A.S. Reichert, M. Meyer-Hermann, H. D. Osiewacz, *Deceleration of Fusion-Fission Cycles Improves Mitochondrial Quality Control during Aging*, PLoS Comput Biol 8(6): e1002576 (2012)

Quantitative approaches to tissue morphogenesis

Collaborators: Eric Wieschaus[1], Greg Beitel[2], Adam Martin[3], Matthias Kaschube[4]

[1]Department of Molecular Biology, Princeton University, Princeton NJ, USA; [2]Department of Molecular Biosciences, Northwestern University, Evanston IL, USA; Department of Biology, MIT, Cambridge MA, USA; [4]FIAS and Goethe University, Frankfurt, Germany

All body cells have an elaborate molecular machinery for generating forces and motions, and in multicellular organisms these molecules organize themselves to produce complex patterns of motion across whole tissues; a striking example is provided by gastrulation in embryonic development, where a single closed sheet of cells changes its topology, establishing the inside and outside of the organism (Fig. 1A). In recent work together with the experimental laboratory of Eric Wieschaus (Princeton) we have studied the dynamics of cell shape changes facilitating epithelial folding and tissue invagination (Fig1B; Gelbart et al., 2012; Wang et al., 2012). We have elucidated the role of volume conservation principles for tissue morphogenesis (Fig. 1C). In a related project together with the experimental laboratory of Greg Beitel (Northwestern), we applied similar techniques to identify the mechanisms regulating the size and shape of tubes in the tracheal (respiratory) system of the fruit fly. These studies shed new light on the complex processes through which cells and tissues sculpt our internal organs and body structure.

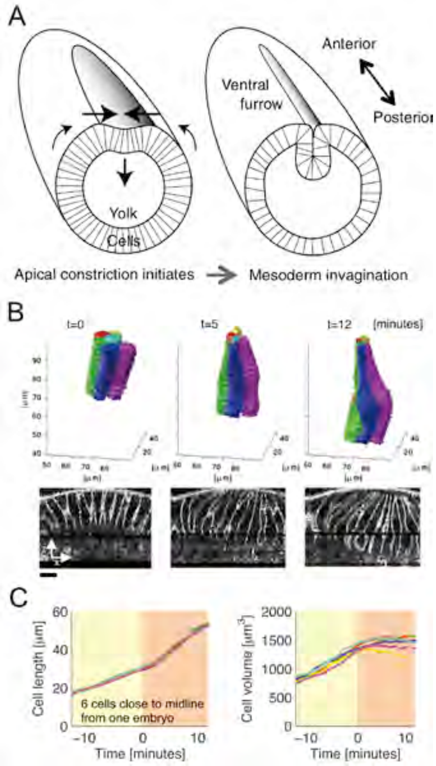


Figure1: (A) Schematic cross-sections through the *Drosophila* embryo at the beginning of gastrulation (Left) and a few minutes later (Right), illustrating tissue folding and invagination of mesodermal precursor cells. (B) Whole-cell reconstructions over time (Upper) from slices of the raw data (Lower). (Scale bar: 10 mm.). (C) Length (Left) and volume (Right) of the cells from B. Despite marked shape changes during gastrulation, cells largely preserve their volume (red region in C, Right). Modified from Gelbart et al, 2012.

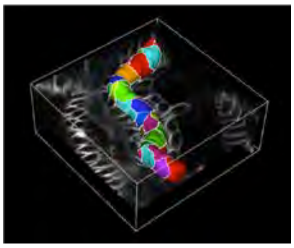


Figure 2: Quantitative analysis of an epithelial tube in the respiratory system of *Drosophila*. Different colors show the apical (tube facing) parts of Individual cells.

Related publications in 2012:

1. M.A. Gelbart, B. He, A.C. Martin, S.Y. Thiberge, E.F. Wieschaus, M. Kaschube, *Volume conservation principle involved in cell lengthening and d nucleus movement during tissue morphogenesis*, PNAS 109:19298–303 (2012)
2. K.S. Nelson, Z. Khan, I. Molnár, J. Mihály, M. Kaschube, G.J. Beitel, *Drosophila Src regulates anisotropic apical surface growth to control epithelial tube size*, Nat Cell Biol 14(5):518–25 (2012)
3. Y.C. Wang, Z. Khan, M. Kaschube, E.F. Wieschaus, *Differential positioning of adherens junctions is associated with initiation of epithelial folding*, Nature 484:390–393 (2012)

Photo-processes and Optical Properties

Collaborators: A.V. Verkhovtsev[1], A.V. Korol[1], A.V. Solov'yov[1], R.G. Polozkov[2], V.K. Ivanov[2], J.-P. Connerade[3], A. Müller[4]

[1] MBN@FIAS, [2] St. Petersburg State Polytechnic University, Russia, [3] Imperial College, UK, [4] Justig-Liebig-Universität Giessen, Germany).

Short description:
Investigation of photoexcitation processes in nanostructures. Special attention is paid to the accounting for the many-body correlation effects.

Main results:

A consistent many-body theory based on the jellium model has been applied recently for description of angular resolved photoelectron spectra of metal clusters anions Na_7^-, Na_{19}^- and Na_{57}^- [1]. Partial and total photoionization cross sections as well as angular anisotropy parameter were calculated within the single-particle Hartree-Fock (HF) approximation and with an account for many-electron correlations within the random phase approximation with exchange (RPAE) (see Fig. 1). Theoretical results were compared with experimental data of C. Bartels, C. Hock, J. Huwer, R. Kuhnen, J. Schwobel, B. von Issendorff (B. von Issendorff et al., Science **323**, 1323 (2009)). Good agreement between theory (RPAE) and experiment is demonstrated (see Fig. 2).

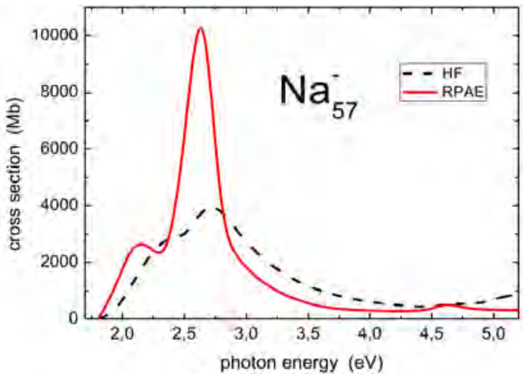


Fig. 1: The total photodetachment cross sections of Na_{57}^- anion within the HF and RPAE.

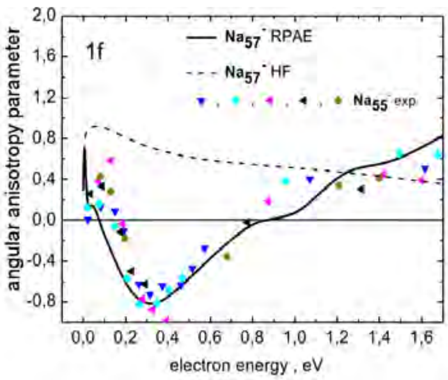


Fig. 2: The angular anisotropy parameter for the $1f$ shell of Na_{57}^- anion as a function of the photoelectron energy. Comparison between the HF, the RPAE results and the experimental from Bartels et. al (Science **323**, 1323 (2009)). Different experimental points correspond to the photoionization from the sublevels of the orbital split by the crystalline field of the cluster.

Related publications in 2012:

1. R.G. Polozkov, V.K. Ivanov, A.V. Korol, A.V. Solov'yov: *Photodetachment of metal cluster negative ions within many-body theory*, European Phys. J. D **66**, 287-(1-7) (2012)

2. A.V. Verkhovtsev, R.G. Polozkov, V.K. Ivanov, A.V. Korol, A.V. Solov'yov: *Photoionization of clusters and fullerenes*, The Second International Conference "Dynamics of Systems on the Nanoscale DySoN 2012" (30 September - 4 October, 2012, Saint Petersburg, Russia), Book of Abstracts, p. 47 (2012)

Free Atomic and Molecular Clusters, Nanoparticles

Collaborators: A.V. Verkhovtsev[1], A.V. Yakubovich[1], M. Hanauske[1], A.V. Solov'yov[1]

[1] MBN@FIAS

Short description:
Investigation of electronic structure and dynamical properties of atomic and molecular clusters.

Main results:

• We carried out the investigation of geometrical, electronic and magnetic properties of small transition metal clusters, namely pure and Ni-doped titanium clusters [1]. The optimized structures and geometrical properties of Ti_N and $Ti_{N-1}Ni$ clusters consisting of up to 15 atoms were studied using both the *ab initio* and classical approaches. It was shown that the geometrical properties, obtained within the classical simulations, are in good agreement with those obtained within the more sophisticated *ab initio* framework (see Fig. 1).

• We analyzed the influence of the Ni-doping on the stability and properties of the bimetallic Ni-Ti compounds (see Fig. 2). *Ab initio* analysis of electronic and magnetic properties of the clusters showed that the doping of titanium clusters by Ni atoms causes a significant charge transfer in a system and change of the magnetic properties.

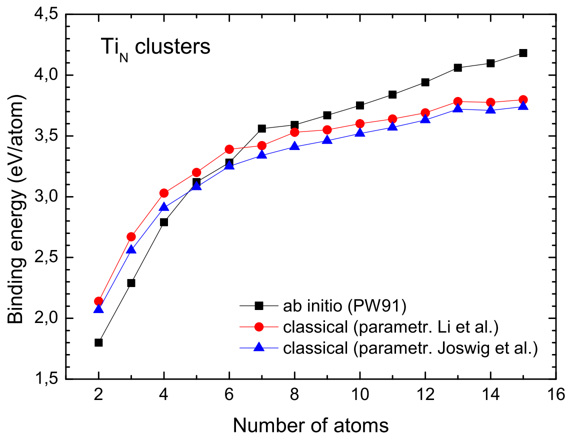


Fig. 1: Binding energies per atom for the most stable Ti clusters as a function of cluster size calculated within the *ab initio* (black line) and classical (red and blue lines) frameworks. Classical force fields were obtained using the Finnis-Sinclair potential. Two different parameterizations of the potential, proposed by Li et al. and Joswig et al., were used in the calculations.

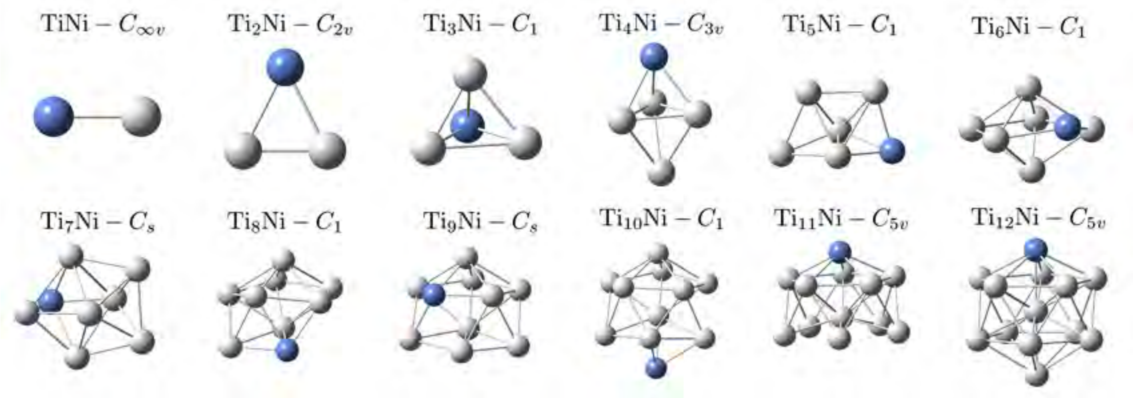


Fig. 2: Optimized geometries of Ni-doped titanium clusters $Ti_{N-1}Ni$ ($N \le 13$) calculated within the *ab initio* PW91PW91/DGDZVP2 method. Label above each cluster image indicates the point symmetry group of the cluster.

Related publication in 2012:

1. A.V. Verkhovtsev, M. Hanauske, A.V. Yakubovich, A.V. Solov'yov: *Characterization of small pure and Ni-doped titanium clusters: Ab initio versus classical approaches*, Comp. Mater. Sci. (2012) (submitted)

Nanocarbon Systems (Fullerenes, Nanotubes, Nanowires etc.)

Collaborators: A.V. Verkhovtsev[1], A.V. Korol[1], A.V. Solov'yov[1], R.G. Polozkov[2], V.K. Ivanov[2]

[1] MBN@FIAS, [2] St. Petersburg State Polytechnic University, Russia

Short description:

Investigation of electronic structure and dynamical properties of various nanocarbon systems, such as fullerenes, nanotubes etc.

Main results:

• We introduced a new type of correction for a more accurate description of fullerenes within the spherically symmetric jellium model [1]. As a case study we considered the C_{60} and C_{20} molecules. The correction represents a pseudopotential which originates from the comparison between the results of an accurate *ab initio* calculation and the jellium model calculations.

• Due to the alternating-sign shape of the pseudopotential (see Fig. 1), it affects the σ- and π-electrons of the system differently. Therefore, such a correction allows one to mimic partially the sp^2-hybridization, which occurs in formation of fullerenes, and, thus, to import the hybridization effects into the standard jellium model. The introduced pseudopotential may be considered as a more physically meaningful correction as compared with a structureless square-well pseudopotential which has been widely used earlier.

• It is demonstrated that the introduced correction improves significantly the electron density distribution as compared to the standard jellium model and the one with an additional square-well pseudopotential (see Fig. 2).

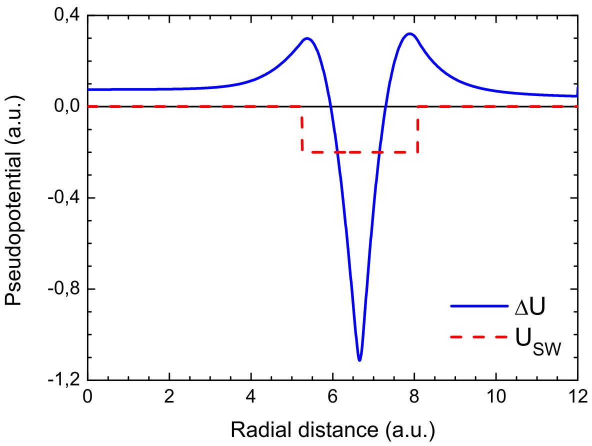


Fig. 1: The pseudopotential ΔU for the C_{60} fullerene (blue curve). The widely-used square-well pseudopotential U_{SW} is also shown for the comparison (dashed red curve).

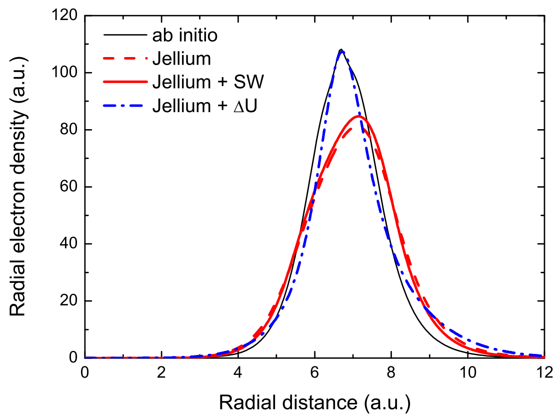


Fig. 2: Radial electron density of C_{60} obtained from the *ab initio* calculation (solid black curve) and calculated by means of the jellium model: the standard one (dashed red curve), with the additional square-well pseudopotential (solid red curve) and with the additional pseudopotential ΔU (dash-dotted blue curve).

Related publication in 2012:

1. A.V. Verkhovtsev, R.G. Polozkov, V.K. Ivanov, A.V. Korol and A.V. Solov'yov: *Hybridization-related correction to the jellium model for fullerenes*, J. Phys. B: At. Mol. Opt. Phys. **45**, 215101-(1-8) (2012)

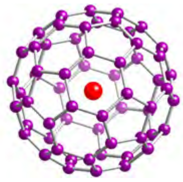
Endohedral Atoms and Molecules

Collaborators: A.V. Verkhovtsev[1], A.V. Korol[1], A.V. Solov'yov[1], R.G. Polozkov[2], V.K. Ivanov[2]

[1] MBN@FIAS, [2] St. Petersburg State Polytechnic University, Russia

Short description:

We investigate electronic structure and dynamical properties of endohedral complexes, consisting of an atom or a small molecule confined inside a fullerene cage. Special attention is paid to the noble gas endohedral fullerenes A@C_N, where A is a noble gas atom.



Main results:

A self-consistent Hartree-Fock calculation of electronic structure of noble gas endohedral fullerenes A@C_{60} (A = He, Ne, Ar) was carried out [1, 2]. All electrons of an encaged noble gas atom and 240 delocalized electrons of the C_{60} fullerene were considered simultaneously within a unified electronic configuration. It was shown [1, 2] that the account of the non-local exchange interaction within the Hartree-Fock approximation leads to the significant modification of the 3p and 4d electronic orbitals as opposed to the local exchange interaction within the local density approximation. As a result of the modification the redistribution of the electronic density of the 3p and 4d orbitals appears and causes the accumulation of the additional positive charge in the vicinity of the encaged atom and the additional negative charge on the fullerene core.

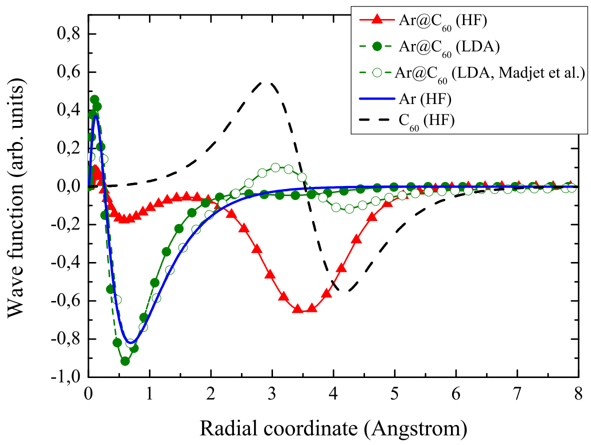


Fig. 1: The 3p wave function in free Ar atom (solid line), in pristine C_{60} (dashed line) and in Ar@C_{60} calculated within the HF approximation (line with triangles) and the LDA (filled-circled line). Results of the LDA calculation performed by Madjet et al. (2007) are also presented (open-circled line).

Related publications in 2012:

1. A.V. Verkhovtsev, R.G. Polozkov, V.K. Ivanov, A.V. Korol and A.V. Solov'yov: *Self-consistent Hartree-Fock approach to electronic structure of endohedral fullerene Ar@C_{60}*, Fullerenes, Nanotubes and Carbon Nanostructures **20**, 382-385 (2012)

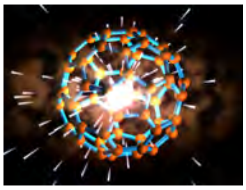
2. A.V. Verkhovtsev, R.G. Polozkov, V.K. Ivanov, A.V. Korol and A.V. Solov'yov: *Role of exchange interaction in self-consistent calculations of endohedral fullerenes*, Nucl. Instrum. Meth. B **279**, 202-204 (2012)

Collision Processes Involving Clusters and Biomolecules: Case of Clusters

Collaborators: A.V. Verkhovtsev[1], A.V. Korol[1], A.V. Solov'yov[1], A. Ruocco[2], P. Bolognesi[3], L. Avaldi[3]

[1] MBN@FIAS, [2] Università di Roma Tre, Rome, Italy, [3] CNR-IMIP, Monterotondo Scalo, Italy

Short description:
We study collision processes in nanostructures. Special attention is paid to the role of collective electron excitations (plasmons) and mechanisms of their relaxation.



Main results:

• We performed a joint experimental and theoretical investigation of inelastic scattering of fast electrons in collision with the C_{60} fullerene. To analyze the results of experimental measurements, we utilized a recently developed theoretical model [1] based on the classical description of collective electron excitations. The model describes the formation of the three collective electron excitations occurring in the system, namely two coupled modes of the surface plasmon as well as the volume plasmon.

• Theoretical results obtained within this model are in very good agreement with the experimental data (see Fig. 1). The results showed that collective excitations provide the main contribution to the inelastic scattering cross section of electrons over a broad energy range [2, 3] and, as opposed to the photoionization, both the two surface plasmon modes as well as the volume plasmon contribute to the cross section.

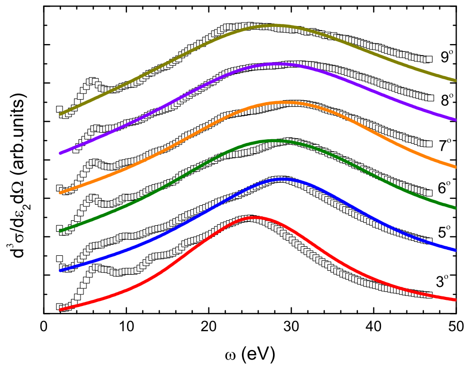


Fig. 1: Comparison of the experimental electron energy loss spectra with theoretical results obtained within the three-plasmon model [1] for the scattering angles $\theta = 3^\circ \ldots 9^\circ$. Black squares represent the experimental data, and solid lines represent results of calculations [3]. Both experimental and theoretical curves are normalized to 1. Horizontal bars at the left hand side of the figure show the zero cross section lines for each spectrum.

Related publications in 2012:

1. A.V. Verkhovtsev, A.V. Korol, A.V. Solov'yov: *Formalism of collective electron excitations in fullerenes*, European Phys. J. D **66**, 253-(1-11) (2012)

2. A.V. Verkhovtsev, A.V. Korol, A.V. Solov'yov, P. Bolognesi, A. Ruocco, L. Avaldi: *Interplay of the volume and surface plasmons in the electron energy loss spectra of* C_{60}, J. Phys. B: At. Mol. Opt. Phys. **45**, 141002-(1-6) (2012) (Fast Track Communication)

3. P. Bolognesi, L. Avaldi, A. Ruocco, A.V. Verkhovtsev, A.V. Korol, A.V. Solov'yov: *Collective excitations in the electron energy loss spectra of* C_{60}, European Phys. J. D **66**, 254-(1-9) (2012)

Collision Processes Involving Clusters and Biomolecules: Case of Biomolecules

Collaborators: A.V. Solov'yov[1], P. de Vera[2], R. Garcia-Molina[2], I. Abril[2]

[1] MBN@FIAS, [2] Universitat d'Alacant, Spain

Short description:
Impact ionization of complex biological media is studied by means of a newly suggested model.

Main results:

A semiempirical model has been developed for calculating the electron emission from any organic compound after ion impact. With the only input of the density and composition of the target we can evaluate its ionization cross sections using plausible approximations. The model is based on the dielectric formalism and some physically motivated approximations [1-3]. Results for protons impacting in the most representative biological targets (such as water or DNA components) show a very good comparison with experimental data (see Figs. 1 and 2). Due to its simplicity and great predictive effectiveness, the method can be immediately extended to any combination of biological target and charged particle of interest in ion beam cancer therapy.

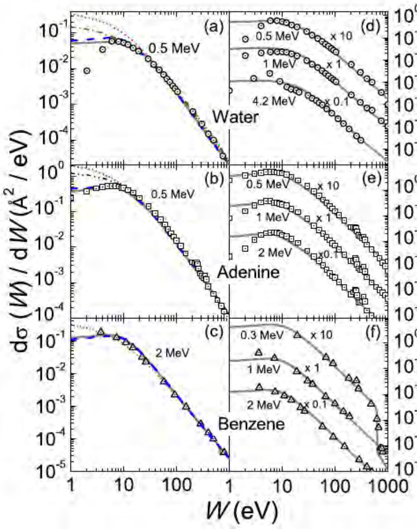


Fig. 1: Single differential cross sections for ionization of water (a), (d), adenine (b),(e) and benzene (c), (f) by protons of the indicated energies. Symbols represent experimental data. Solid lines – the current model. Dashed-and-dotted line - the *ab initio* calculations.

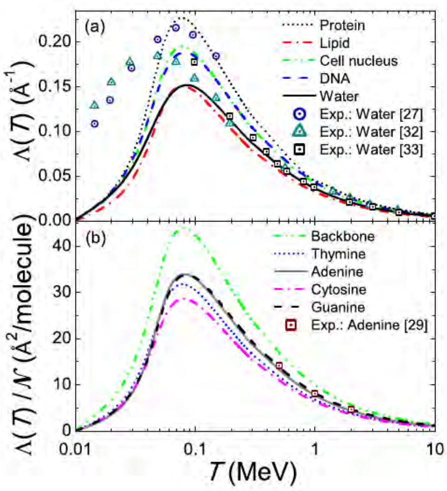


Fig. 2: Calculated macroscopic total ionization cross sections (TICS) (a) for proton impact in liquid water, DNA, protein, lipid, and cell nucleus, and (b) for proton impact in the indicated DNA components. Symbols represent experimental data.

Related publications in 2012:

1. P. de Vera, R. Garcia-Molina, I. Abril, A.V. Solov'yov: *A semiempirical model for the ion impact ionization of complex biological media*, Phys. Rev. Lett. (2012) (submitted)

2. P. de Vera, A.V. Solov'yov, I. Abril and R. Garcia-Molina: *Ionization of biomolecular targets by ion-impact: input data for radiaobiological applications*, The 2nd International Conference "Dynamics of Systems on the Nanoscale DySoN 2012" (September 30 - October 4, 2012, St. Petersburg, Russia), Book of Abstracts, p. 29 (2012)

3. P. de Vera, A.V. Solov'yov, I. Abril, R. Garcia-Molina: *Calculation of the energy spectra of secondary electrons emitted from ion tracks in biological targets.* NANO-IBCT Workshop on "Quantum Scattering Codes and Monte Carlo Simulations to Model Dynamical Processes in Biosystems" (QSMC 2012) (7-9 November, 2012, Madrid, Spain), Book of Abstracts, p. 40 (2012)

Collective Electron Excitations

Collaborators: A.V. Verkhovtsev[1], A.V. Korol[1], A.V. Solov'yov[1], A. Ruocco[2], P. Bolognesi[3], L. Avaldi[3]

[1] MBN@FIAS, [2] Università di Roma Tre, Rome, Italy, [3] CNR-IMIP, Monterotondo Scalo, Italy

Short description:
Investigation of collective electron excitations (plasmons) and mechanisms of their relaxation in photo- and collision processes in various nanostructures. Special attention is paid to the role plasmon excitations in fullerenes.

Main results:

• We studied the formation of collective electron excitations in the process of inelastic scattering of fast electrons on the C_{60} fullerene. Within a new theoretical model [1] we showed that the electron energy loss spectra of fullerenes are described by three collective excitations, namely two modes of the surface plasmon and the volume plasmon as well.

• It was shown [2, 3] that the three collective excitations provide a contribution to the inelastic scattering cross section over a broad energy range. The symmetric mode of the surface plasmon dominates at smaller scattering angles, while at larger angles the antisymmetric and the volume plasmons make the most prominent contribution (see Fig. 1).

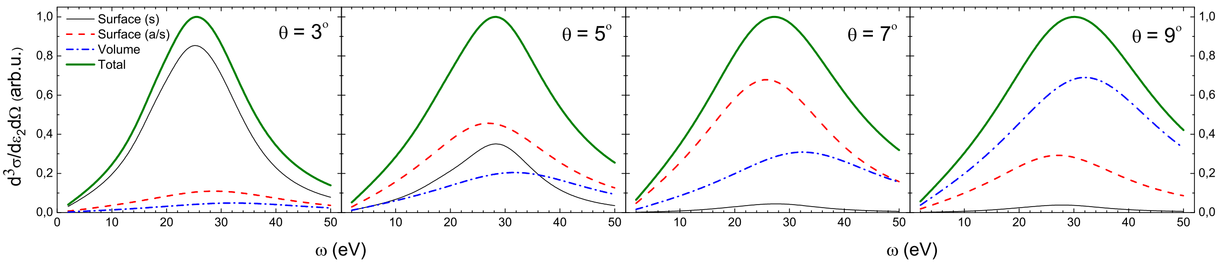


Fig. 1: Total cross section and the contributions of the volume and the two modes of the surface plasmon calculated for the scattering angles $\theta = 3°, 5°, 7°$, and $9°$. The symmetric and antisymmetric modes of the surface plasmon are shown by the thin solid black line and the dashed red line, respectively; the volume plasmon contribution is shown by the chained blue line. The total cross section is shown by the thick green line.

Related publications in 2012:

1. A.V. Verkhovtsev, A.V. Korol and A.V. Solov'yov: *Formalism of collective electron excitations in fullerenes*, European Phys. J. D **66**, 253-(1-11) (2012)

2. A.V. Verkhovtsev, A.V. Korol, A.V. Solov'yov, P. Bolognesi, A. Ruocco, L. Avaldi: *Interplay of the volume and surface plasmons in the electron energy loss spectra of* C_{60}, J. Phys. B: At. Mol. Opt. Phys. **45**, 141002-(1-6) (2012) (Fast Track Communication)

3. P. Bolognesi, L. Avaldi, A. Ruocco, A.V. Verkhovtsev, A.V. Korol, A.V. Solov'yov: *Collective excitations in the electron energy loss spectra of* C_{60}, European Phys. J. D **66**, 254-(1-9) (2012)

Dynamical Processes with Bio-Macromolecules: DNA Unzipping

Collaborators: A.V. Yakubovich[1], A.V. Solov'yov[2], S.N. Volkov[2], E.V. Paramonova[3]

[1] MBN@FIAS, [2] Bogolyubov Institute for Theoretical Physics, Ukraine, [3] Institute of Mathematical Problems of Biology RAS, Russia

Short description:
Computer simulations of the DNA double-helix unzipping, which is a compulsory stage of the biological processes of genetic information transfer. In this process the double-stranded (ds) DNA is separated into two single strands (ss), which allows us to read and to reproduce the genetic information recorded in the nucleic bases sequence. By means of classical molecular dynamics simulations we have investigated the process of unzipping of Drew-Dickerson dodecamer sequence and a hairpin (AAG) attached to the end of the double-helix chain.

Main results:

The performed simulations show that the dsDNA unzipping process involves both the degrees of freedom of the double-stranded helix and the degrees of freedom of the bases in the complementary pairs.
An important role in the unzipping process is played by the water environment. Shelves formed in the dependences of coordinates characterizing unzipping with time arise due to the involvement of water molecules in the unzipping process. The manifestation of metastable preopened states of the complementary base pairs is a result of the incorporation of water molecules in the space between the open bases in a pair.
The performed simulations confirm the assumption made in previous works on the existence of preopened states in the pathway of dsDNA unzipping. This essential feature may justify the bistability of the closed and preopened states of the complementary base pairs in the process of DNA unzipping.

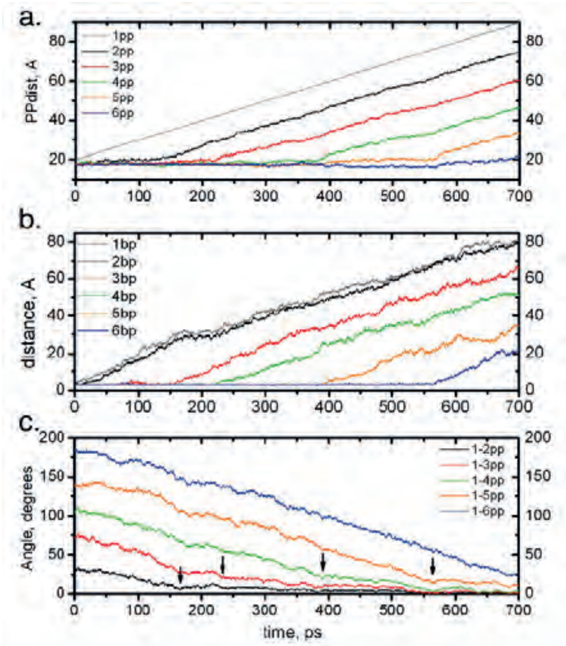


Fig. 1: (a) Growth of distances between phosphates, (b) distances between hydrogen atoms in the central H-bond of the base pairs, (c) the variation of the base pairs rotation angle with time during unzipping of the first 6-x base pairs in DD-h.

Related publication in 2012:

1. S.N. Volkov, E.V. Paramonova, A.V. Yakubovich, A.V. Solov'yov: *Micromechanics of base pair unzipping in the DNA duplex*, J. Phys.: Condens. Matter **24**, 035104-(1-6) (2012)

Dynamical Processes with Bio-Macromolecules: Statistical Mechanics of Protein Folding

Collaborators: A.V. Yakubovich[1], A.V. Solov'yov[1], Walter Greiner[2]

[1] MBN@FIAS, [2] FIAS

Short description:

We present a statistical mechanics formalism for the theoretical description of the process of protein folding↔unfolding transition in water environment. The formalism is based on the construction of the partition function of a protein obeying two-stage-like folding kinetics. Using the statistical mechanics model of solvation of hydrophobic hydrocarbons we obtain the partition function of infinitely diluted solution of proteins in water environment. The calculated dependencies of the protein heat capacities upon temperature are compared with the corresponding results of experimental measurements for staphylococcal nuclease.

Main results:

The constructed partition function of each state is a product of partition function of a protein in a given conformational state, partition function of water molecules in pure water and a partition function of H_2O molecules interacting with the protein. The introduced model includes a number of parameters responsible for certain physical properties of the system. The parameters were obtained from available experimental data and three of them were considered as being variable depending on a particular protein and pH of the solvent. We have compared the predictions of the developed model with the results of experimental measurements of the dependence of the heat capacity on temperature for staphylococcal nuclease. The experimental results were obtained at various pH of solvent. The suggested model is capable to reproduce well within a single framework a large number of peculiarities of the heat capacity profile, such as the temperatures of cold and heat denaturations, the corresponding maximum values of the heat capacities, the temperature range of the cold and heat denaturation transitions, the difference between heat capacities of the folded and unfolded states of the protein.

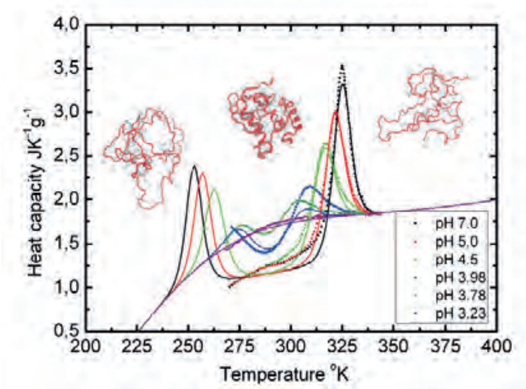


Fig. 1: Dependencies of the heat capacity on temperature for staphylococcal nuclease (PDB ID 1EYD) at different values of pH. Solid lines show results of the developed theoretical model. Symbols present experimental data. Structure of the protein in native and unfolded conformations are shown in temperature regions where the corresponding conformation exists.

Related publications in 2012:

1. A.V. Yakubovich, A.V. Solov'yov, W. Greiner: *Statistical mechanical theory of protein folding in water environment*, Proceedings of International Symposium on Exciting Physics: Quarks and Gluons, Atomic Nuclei, Biological Systems, Networks (13-20 November 2011, Makutsi Safari Farm, South Africa)

2. A.V. Yakubovich, A.V. Solov'yov, Walter Greiner: *Quantitative thermodynamic model for globular protein folding*, Phys. Rev. E (2012) (submitted)

Molecular Systems in Ubiquitous Environment and External Fields (Electric, Magnetic, Laser)

Collaborators: A.V. Yakubovich[1], A.V. Solov'yov[1], I.A. Solov'yov[2]

[1]MBN@FIAS, [2] UIUC, Urbana, USA

Short description:
Laser induced acoustic desorption (LIAD) is a procedure of gentle lifting of large neutral biomolecules into the gas phase. In LIAD experiments the biomolecules are deposited on a surface of a relatively thin ($\sim 10\mu m$) metallic foil. The back surface of the foil is irradiated by the laser pulse. The energy of the laser is adsorbed by the material of the foil which consequently causes the propagation of acoustic and thermal waves. The propagating waves induce vibration of the foil material which stimulates the emission of biomolecules from the foil surface to the gas phase.

Main results:

We have considered 13 lysine amino acid deposited on a (111)-nickel surface consisting of four monolayers. The size of the nickel surface in x an y directions was taken equal to 3 nm. The interactions between amino acids were described through the CHARMM22 force field and the interactions between nickel atoms were modeled using the many-body Sutton-Chen potential. Interaction between the atoms of nickel and atoms of lysines were described through the van der Waals potential.
Because of the acceleration of the foil, the loosely bound amino acids are desorbed from the foil surface in the course of the simulation. The desorption rate of the amino acids as a function of the surface acceleration has been analyzed. It was shown that the desorption rate has an exponential dependence on the value of the substrate acceleration. We have shown that in the coordinate frame moving with the speed of the substrate at the initial moment of time, the velocities of the molecules are inversely proportional to the substrate acceleration.

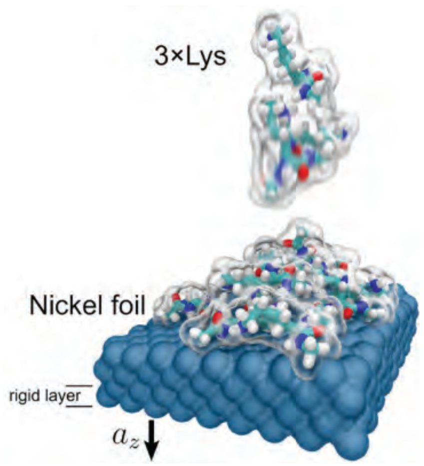


Fig. 1: Evaporation of a cluster of several lysine residues from the surface of a nickel foil. The evaporation is caused by the foil acceleration.

Nanoscale Phase Transitions (Folding, Melting, Solidification, Sublimation, Multifragmentation, etc.)

Collaborators: G.B. Sushko[1], A.V. Yakubovich[1], A.V. Solov'yov[1], S.Schramm[2]

[1] MBN@FIAS, [2] FIAS

Short description:

We have explored computationally the solidification process of large nickel clusters. This process has the characteristic features of the first order phase transition occurring in a finite system. The focus of our research is placed on the elucidation of correlated dynamics of a large ensemble of particles in the course of the nanoscale liquid-solid phase transition through the computation and analysis of the results of molecular dynamics (MD) simulations with the corresponding theoretical model. This problem is of significant interest and importance, because the controlled dynamics of systems on the nanoscale is one of the central topics in the development of modern nanotechnologies.

MD simulations in large molecular systems are rather computer power demanding. Therefore, in order to advance with MD simulations we have used modern computational methods based on the graphics processing units (GPU).

Main results:

We have conducted classical MD simulations of the Ni_{2047} cluster with the use of many-body Sutton-Chen potential on the time scales up to 65 ns. For the purposes of this work we have developed an efficient software code capable of performing large-scale MD simulations on GPUs. We have analysed the solidification kinetics of the clusters as a function of the over-cooling temperature and shown that the kinetics of the phase transition can be described within the framework of precursor formation theoretical model. Based on that theoretical model we had derived various characteristics of the systems such as solid-liquid surface tension coefficient, rate of the precursors formation, phase transition temperature for the clusters of arbitrary size.

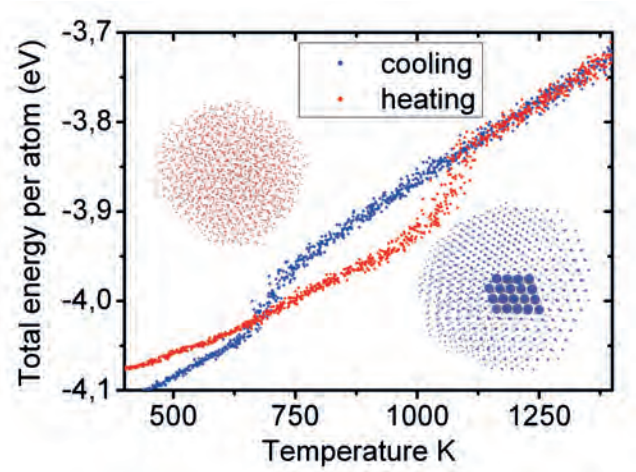


Fig. 1: Dependence of the total energy per atom in heating (red) and cooling (blue) simulations. The insets show the structures of Ni_{2047} in the molten (top-left) and solidified (bottom-right) states. The fragment of crystal structure is shown by blue spheres inside the crystallized structure.

Related publication in 2012:

1. Alexander V. Yakubovich, Gennady Sushko, Stefan Schramm, Andrey V. Solov'yov: *Kinetics of liquid-solid phase transition in large nickel clusters*, Phys. Rev. B (2012) (submitted) (http://xxx.lanl.gov/ arXiv:1210.3559v1 [physics.comp-ph])

Diffusion processes in MBN systems

Collaborators: A.V. Yakubovich[1], A.V. Verkhovtsev[1], G.B. Sushko[1], M. Hanauske[1], A.V. Solov'yov[1]

[1] MBN@FIAS

Short description:
We investigate the diffusion process occurring at the interface various MBN systems. A particular attention is paid to diffusion at the interface of transition metals, especially nickel and titanium crystals.

Main results:

• By means of classical molecular dynamics simulations we studied the diffusion process occurring at the interface of nickel and titanium surfaces. In particular, we studied surface diffusion at the interface of pure nickel and titanium crystals and derived the diffusion coefficient for Ni and Ti atoms in the temperature range 500-700 K (see Fig. 1). Assuming exponential dependence of the diffusion coefficient on temperature we predicted its value at room temperature.

• We studied also the diffusion of Ni_{55} cluster on the titanium surface in the presence of water environment (see Fig. 2). We analyzed the dynamics of nickel atoms in the cluster, described structural rearrangements occurring in the cluster due to the interaction with titanium surface and derived the diffusion coefficient for Ni atoms.

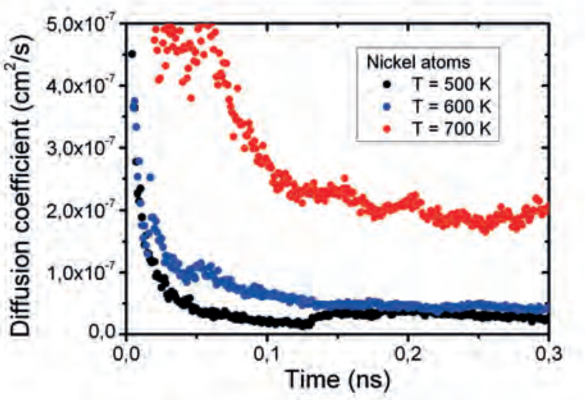


Fig. 1: One-dimensional diffusion coefficient of nickel atoms across the Ni-Ti interface at various temperatures.

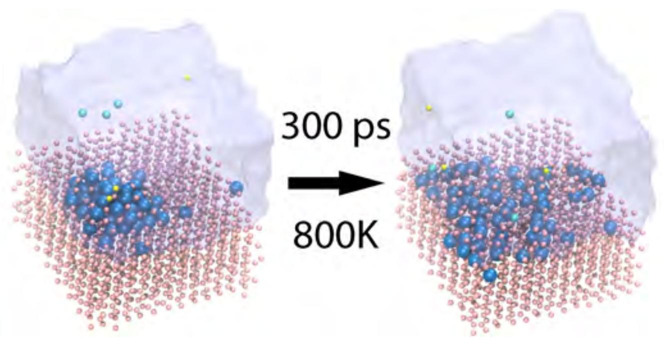


Fig. 2: Diffusion of the Ni_{55} cluster on the surface of titanium in the presence of water environment. After 300 ps at 800 K the cluster disintegrates and the nickel atoms intercalate under the first layer of titanium crystal. Titanium and nickel atoms are shown by red and blue colours, correspondingly Yellow and light-blue atoms represent sodium and chlorine ions in the solution. Transparent surface shows water atop the titanium surface.

Related publication in 2012:

1. A.V. Yakubovich, A.V. Verkhovtsev, M. Hanauske, A.V. Solov'yov: *Computer simulation of diffusion process at interfaces of nickel and titanium crystals*, Comp. Mater. Sci. (2012) (accepted for publication)

Nanostructured materials

Collaborators: A.V. Yakubovich[1], A.V. Verkhovtsev[1], G.B. Sushko[1], M. Hanauske[1], A.V. Solov'yov[1]

[1] MBN@FIAS

Short description: The aim of the study is to model nanoindentation and mechanisms of localized deformation of nanostructured biomaterials, nanocrystalline titanium and its alloys in particular. The study is focused on the investigation of the strength and mechanical properties of films and substrate/coating systems to be used in implants.

Main results:

• We performed molecular dynamics simulations of the nanoindentation process of the titanium crystal [1]. We considered the system consisting of approximately 120,000 atoms packed in the hexagonal close packed (hcp) lattice and studied its interaction with the diamond-like indenter. We considered the three different shapes of the indenter, namely the square, conical and spherical ones. In the performed simulations, the indenter moved with the velocity of 20 – 40 m/s and the maximum penetration depth into the crystal was approximately 4 nm.

• It was shown [1] that at the initial part of simulation the total energy of the system slightly decreases due to the Lennard-Jones interaction between the indenter and the surface of the titanium crystal. Further displacement of the indenter leads to the damage of the crystalline structure of the material and to the consequent increase of the total energy of the system (see Fig. 1 and 2).

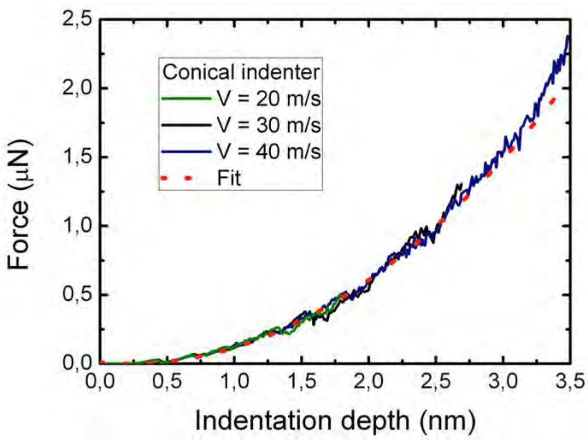


Fig. 1: Dependence of the force acting on the conical indenter on its pathway.

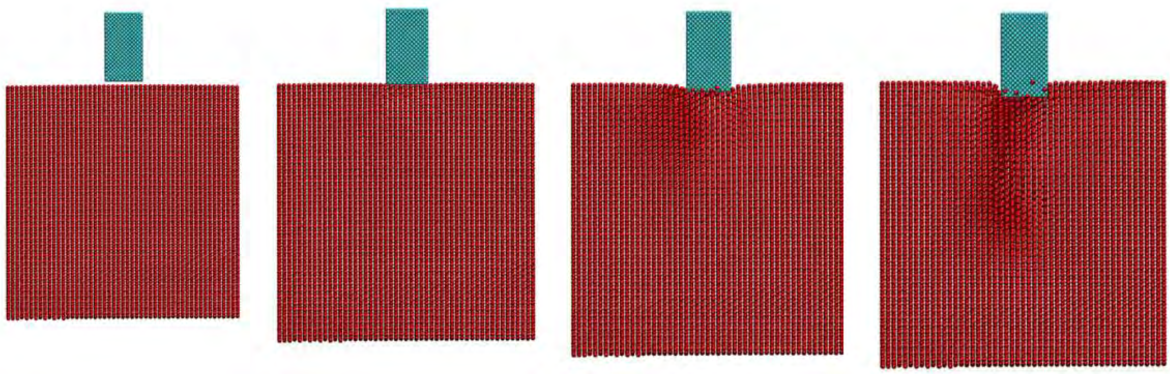


Fig. 2: Evolution of the crystalline structure of titanium during the nanoindentation process with a square indenter.

Related publication in 2012:

1. A.V. Verkhovtsev, A.V. Yakubovich, G.B. Sushko, M. Hanauske and A.V. Solov'yov: *Molecular dynamics simulations of nanoindentation process of titanium crystal*, Comp. Mater. Sci. (2012) (submitted)

Morphological Transitions

Collaborators: A.V. Solov'yov[1], C. Bréchignac[2], I.A. Solov'yov[3]

[1] MBN@FIAS, [2] CNRS, France, [3] UIUC, Urbana, USA

Main results:

In continuation of the last year investigation, we have now initiated the study of morphological transition of non-equilibrium fractal shapes by simulating diffusion of particles over a surface using the kinetic Monte Carlo (KMC) method implemented in the MBN Explorer computer package (I.A. Solov'yov et al., *J. Comp. Chem.* **33**, 2412 (2012)).

Experimentally, those nanofractals formed from deposition and diffusion of preformed silver clusters on cleaved graphite surfaces exhibit dendritic morphologies that are highly sensitive to any perturbation, particularly caused by temperature. We analyzed and characterized the morphological transition both in time and temperature using the recently developed Monte Carlo simulation approach for the description of nanofractal dynamics and compare the obtained results with the corresponding experimental data. The reported results revealed essential and general features of dynamical systems having dendritic shape.

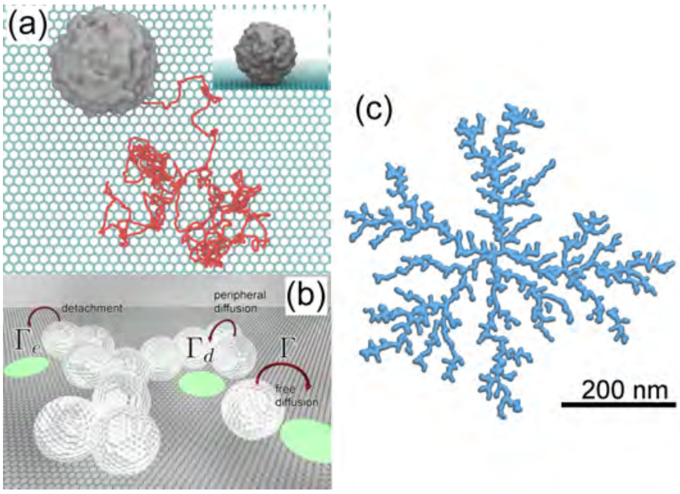


Fig. 1. A deposited silver cluster diffuses over a surface (a). The long time-scale motion of an ensamble of such clusters (b) is parameterized through kinetic rates Γ, Γ_d and Γ_e, corresponding to: the diffusion of a freely deposited cluster over a surface, the diffusion of a cluster along the periphery of an island on surface, and the detachment of a cluster from an island, respectively. Random deposition of new particles on the surface and accounting for the mentioned kinetic processes leads to formation of the fractal structure shown in (c).

Through studying the key elementary kinetic processes of nanocluster dynamics on a surface, shown in Fig. 1, we demonstrated that particle diffusion and detachment controls the shape of the emerging stable islands on a surface.

Related publication in 2012:

1. I.A. Solov'yov, A.V. Solov'yov: *Dynamics of nanofractal formation and fragmentation*, The Second International Conference "Dynamics of Systems on the Nanoscale DySoN 2012" (September 30 - October 4, 2012, Saint Petersburg, Russia), Book of Abstracts, pp. 42-43 (2012)

Computer Codes for the Description of Collective Electron Excitations in MBN Systems

Collaborators: A.V. Verkhovtsev[1], A.V. Korol[1], A.V. Solov'yov[1]

[1] MBN@FIAS

Main results:

• The package of Fortran codes was developed for the description of collective electron excitations (plasmons) which occur in a many-electron system interacting with an external electric field. The codes allow one to describe numerically plasmon excitations which are formed due to collisions with fast projectiles or electromagnetic irradiation. The codes are based on the recently introduced theoretical formalism [1] describing the formation of plasmon excitations in many-electron systems.

• The codes allow one to calculate:
(a) the photoionization and inelastic scattering cross sections using the so-called plasmon resonance approximation. The inelastic scattering cross sections can be calculated in a broad range of scattering angles;
(b) contributions of various types of plasmon excitations. One can evaluate the contribution of the surface plasmon, which occurs on a surface(s) of the system, as well as of the volume plasmon, which is formed due to local compression of the electric charge inside the system. For a fullerene there are two coupled modes of the surface plasmon, the so-called symmetric and antisymmetric ones, which are described, respectively, by the cophased and antiphase motion of the negative charge (see Fig. 1).

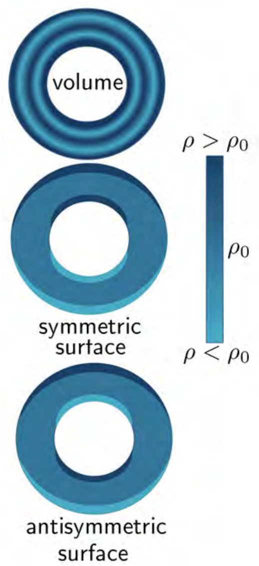


Fig. 1: Representation of the volume plasmon and the two modes of the surface plasmon for a spherically symmetric fullerene molecule.

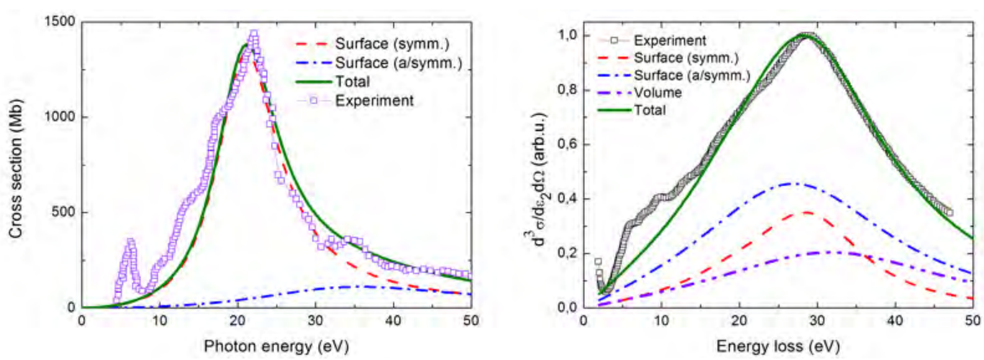


Fig. 2: Formation of plasmon excitations in photoionization (left) and electron impact ionization (right). The experimental electron energy loss spectrum corresponds to the scattering angle $\theta = 5^\circ$ (Bolognesi et al., *Eur. Phys. J. D* **66**, 254 (2012)).

Related publication in 2012:

1. A.V. Verkhovtsev, A.V. Korol and A.V. Solov'yov: *Formalism of collective electron excitations in fullerenes*, European Phys. J. D **66**, 253-(1-11) (2012)

Simulation of Ultra-Relativistic Electron and Positron Channeling and Radiation in Crystals

Collaborators: G.B. Sushko[1], V.G. Bezchastnov[1], A.V. Korol[1], A.V. Solov'yov[1], Walter Greiner[2], I.A. Solov'yov[3]

[1] MBN@FIAS, [2] FIAS, [3] UIUC, Urbana, USA

Main results: A new module, implemented as a part of the MBN Explorer package (I.A. Solov'yov et al., *J. Comp. Chem.* **33**, 2412 (2012)), was applied to simulate trajectories of an ultra-relativistic projectile in a crystalline medium. The motion of a projectile is treated classically by integrating the relativistic equations of motion with account for the interaction between the projectile and crystal atoms. The probabilistic element is introduced by a random choice of transverse coordinates and velocities of the projectile at the crystal entrance as well as by accounting for the random positions of the atoms due to thermal vibrations. The simulated trajectories (see Fig. 1) are used for numerical analysis of the emitted radiation (see Fig. 2). Calculations of the spectra were performed by means of the Fortran code built upon the revisited algorithm described in Korol et al. *J. Phys. G* **27**, 95 (2001). Initial approbation and verification of the code has been carried out by simulating the trajectories and calculating the radiation emitted by 6.7 GeV and 855 MeV electrons and positrons in oriented Si(110) crystal and in amorphous silicon.

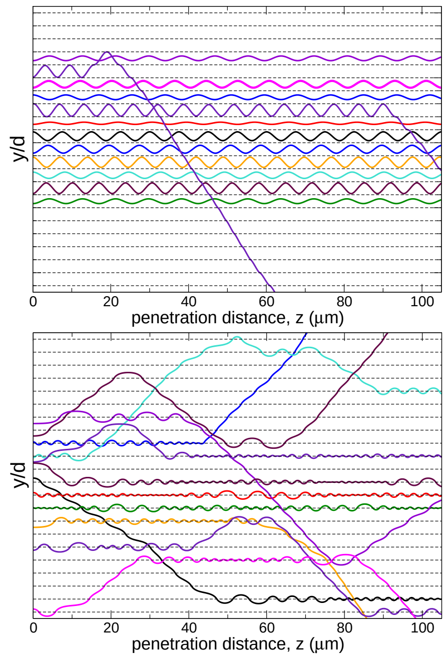


Fig. 1: Simulated trajectories of 6.7 GeV positrons (upper panel) and electrons (lower panel) in Si(110).

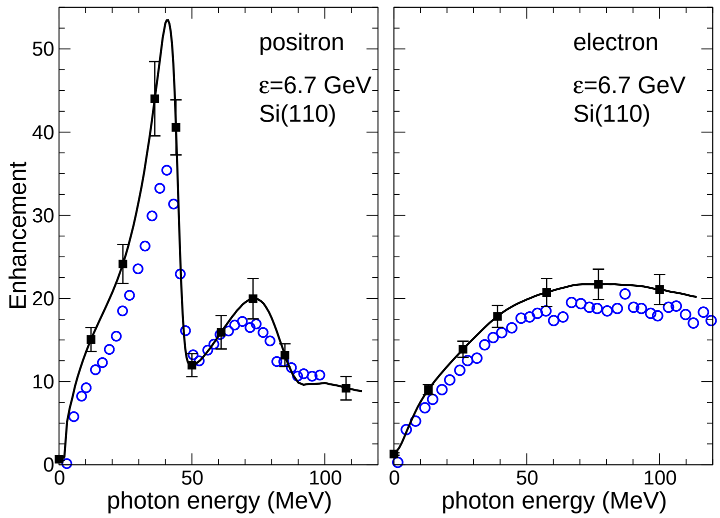


Fig. 2: Enhancement factor of the channeling radiation over the Bethe-Heitler spectrum. The left and right plots are for the positrons and electrons, respectively. Open circles stand for the experimental data from Bak et al. *Nucl. Phys.* B **242**, 1 (1984). The calculated data correspond to the incident angle lying within $\psi = [-\psi_L, \psi_L]$ with $\psi_L = 62\ \mu$rad being the Lindhard critical angle.

Related publications in 2012:

1. G.B. Sushko, V.G. Bezchastnov, I.A. Solov'yov, A.V. Korol, Walter Greiner, A.V. Solov'yov: *Simulation of ultra-relativistic electrons and positrons channeling in crystals with MBN Explorer*, J. Comp. Chem. (2012) (submitted)

2. A.V. Korol, A.V. Solov'yov, Walter Greiner: *Channeling and radiation in periodically bent crystals*, (Springer Berlin Heidelberg, 2012) 268 pp. (ISBN 978-3-642-31894-8)

Physics of Ion Beam Cancer Therapy: Investigation of a Possibility of Direct Thermomechanical Biodamage as a Result of Irradiation with Ions

Collaborators: A.V. Yakubovich[1], A.V. Solov'yov[1], E. Surdutovich[2]

[1] MBN@FIAS, [2] Oakland University, Michigan, USA

Short description:
When a heavy ion passes through tissue, a cylindrical shock wave is initiated due to a thermal spike near the ion's trajectory. In this project we investigate the possibility that this shock wave produces thermomechanical damage by a direct rupture of covalent bonds of DNA backbone. The Molecular Dynamics simulations were used to model the interaction of the shock wave and a DNA molecule.

Main results:

• We have performed full-atom molecular dynamics simulations of the shock wave in liquid water medium caused by a heavy ion for different values of the linear energy transfer (LET). The values of LET corresponded to those in the vicinity of the Bragg peak for carbon, neon, argon and iron ions. The wave interacts with a part of DNA molecule on the surface of nucleosome, as shown in Figure 1.

• The time dependence of energy in the covalent bonds of the DNA-fragment's backbone has been obtained and the evidence of a strand break has been inferred from these data (Fig. 2). The probability of direct strand breaking by a shock wave has been compared to that due to chemical mechanisms; the dependence of the radius of dominance of shock wave effects on LET has been predicted (Fig. 3).

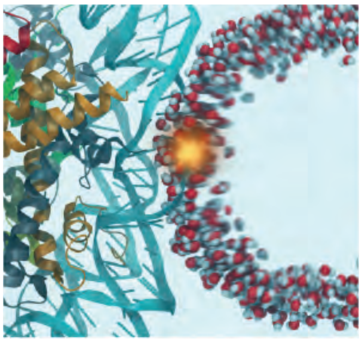


Fig. 1. The cylindrical shock wave front in water (on the right; ion's path is the cylinder axis perpendicular to the figure plane) interacts with a nucleosome (on the left) with a segment of a DNA molecule on the surface.

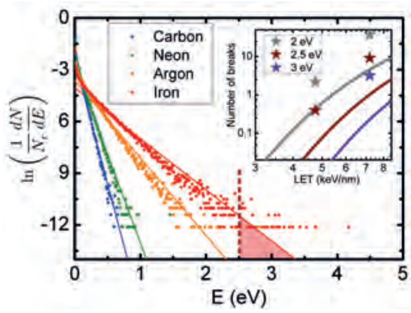


Fig. 2. Logarithm of the normalised number of the covalent bond energy records for a selected DNA fragment per 0.01 eV energy interval versus the bond energy for four values of LET: 0.9, 1.73, 4.745, and 7.195 keV/nm, corresponding to the Bragg peak values for several ions.

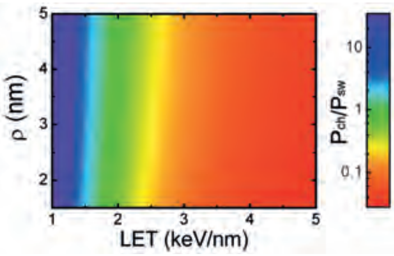


Fig. 3. The ratio of the probabilities, P_{ch}/P_{sw}, for producing at least one SSB in a 3-base-pair segment of DNA molecule. Yellow and red areas indicate the dominance of direct damage by shock waves.

Related publications in 2012:

1. A.V. Yakubovich, E. Surdutovich, A.V. Solov'yov: *Damage of DNA backbone by nanoscale shock waves*, J. Phys: Conf. Ser. **373**, 012014-(1-7) (2012)

2. A.V. Yakubovich, E. Surdutovich, A.V. Solov'yov: *Thermomechanical damage of nucleosome by the shock wave initiated by ion passing through liquid water*, Nucl. Instrum. Meth. B **279**, 135–139 (2012)

3. E. Surdutovich, A.V. Yakubovich, A.V. Solov'yov: *Biodamage via shock waves initiated by irradiation with ions*, Nature Scientific Reports (2012) (accepted for publication)

Physics of Ion Beam Cancer Therapy: Random Walk Approach for the Calculation of Radial Dose, Fluence of Secondary Electrons, and Other Problems

Collaborators: A.V. Yakubovich[1], A.V. Solov'yov[1], E. Surdutovich[2], A B. Rosenfeld[3], M.U. Bug[4], H. Rabus[4]

[1] MBN@FIAS, [2] Oakland University, Michigan, USA, [3] University of Wollongong, Australia, [4] Physikalisch-Technische Bundesanstalt, Germany

Main results:

In 2012 we successfully applied a random walk approach to describe the transport of secondary electrons produced by ions propagating through tissue. These works show that a relatively simple analytic tool can be quite powerful for applications in problems related to the analysis of radiation damage.

• The random walk approach was applied in order to consider the double-ionization events that may explain the mechanism of production of double strand breaks (DSBs) in DNA. The latter are considered to be due to action of two separate electrons. The double-ionization events taking place in the vicinity of DNA molecules increase the local density of electrons and thus increase the probability of DSBs [1].

• The random walk approach was used for the analytical calculation of the radial dose distribution around the ion's path. The results of the calculations were investigated at different distances (small and moderate) from the path and compared to the Monte Carlo simulations. The importance of the attenuation effects was analyzed [2].

• The random walk approach was used to calculate the fluence of secondary electrons and other physical quantities relevant for a target cylinder in the vicinity of the ion's path in liquid water. These calculations were compared with the Monte Carlo simulations of the same values done for the purposes of nano-dosimetry. The calculated and modelled fluences compared quite well, while the cluster distributions require further work [3].

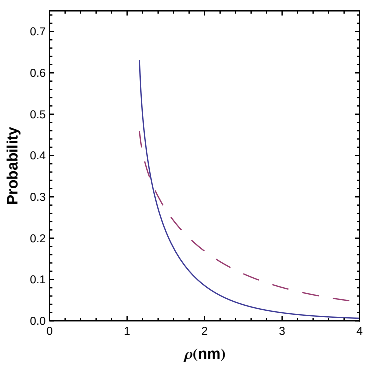


Fig. 1. The probability for two electrons to pass through a single convolution of DNA (solid line) compared to that of one electron (dashed line) [1].

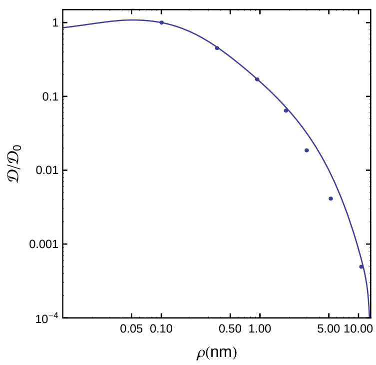


Fig. 2. The normalized radial dose determined from the random walk approximation (solid line) compared with Monte Carlo simulations (circles) for 1 MeV protons [2].

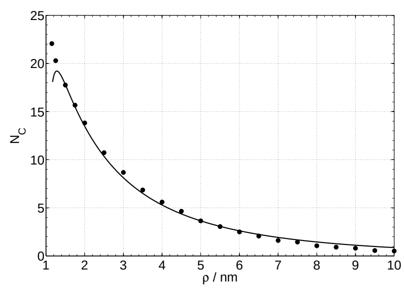


Fig. 3. Fluence of secondary electrons hitting the surface of the cylinder as function of the distance from the ion's path determined by the analytical approach (solid line) and PTra simulations (symbols) [3].

Related publications in 2012:

1. E. Surdutovich, A.V. Solov'yov: *Double strand breaks in DNA resulting from double-electron-emission events*, European Phys. J. D **66**, 206-(1-5) (2012)

2. E. Surdutovich, A.V. Solov'yov: *Random walk approximation for the radial dose dependence*, European Phys. J. D **66**, 245-(1-6) (2012)

3. M.U. Bug, E. Surdutovich, H. Rabus, A.B. Rosenfeld, A.V. Solov'yov: *Nanoscale characterization of ion tracks: MC simulations versus analytical approach*, European Phys. J. D **66**, 291-(1-6) (2012)

Theory of Crystalline Undulator (CU) Based Novel Light Sources

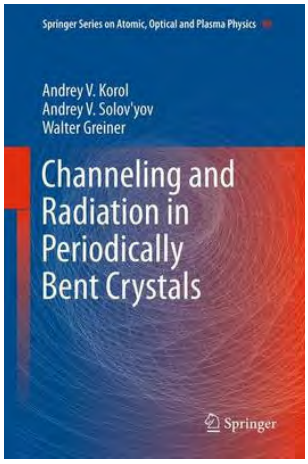
Collaborators: G.B. Sushko[1], V.G. Bezchastnov[1], A.V. Korol[1], A.V. Solov'yov[1], W. Greiner[2], H. Backe[3], W. Lauth[3], U. Uggerhøj[4], S. Connell[5], V. Guidi[4]

[1] MBN@FIAS, [2] FIAS, [3] Mainz Uni., Germany, [4] Aarhus University, Denmark, [5] Johannesburg University, South Africa;, [6] Ferrara University, Italy

Short description:
Investigation of the feasibility to construct a powerful source of high-energy ($\hbar\omega \sim 0.1 - 1$ MeV) monochromatic electromagnetic FEL-like radiation by a bunch of ultra-relativistic particles channelling through a periodically bent crystal (crystalline undulator, CU). Potential applications include plasma, nuclear and solid state physics, molecular biology, medicine and technology.

Main results:

- The feasibility of constructing a crystalline undulator and, on its basis, the light sources is a very recent concept. The book [1], published in 2012, represents the underlying fundamental physical ideas as well as the theoretical, experimental and technological advances made during the last one and a half decades in exploring the various features of crystalline undulators and the radiation formed in them. The book is addressed to a wide audience of researches and students since the phenomenon of crystalline undulator entangles the concepts from various research fields, such as material science, beam physics, physics of radiation, solid state physics, acoustics, etc, whereas its investigation implies the use and further elaboration of a variety of theoretical and computational methods, experimental techniques, technological and engineering approaches.



- Simulation of 855 MeV of electron and positron channeling in straight Si (110) has been performed with a new computer code [2]. This case study is of interest in connection with the ongoing experiments with electron beams at Mainz Microtron as well as with the potentially feasible experiments at Frascati (Italy). By analyzing the simulated trajectories we estimated the electron dechanneling length. The emission spectra were calculated for both projectiles for the oriented crystal and for amorphous silicon as well (Fig. 1, left). The enhancement factor of the channeling radiation over the incoherent bremsstrahlung background was calculated (Fig. 1, right).

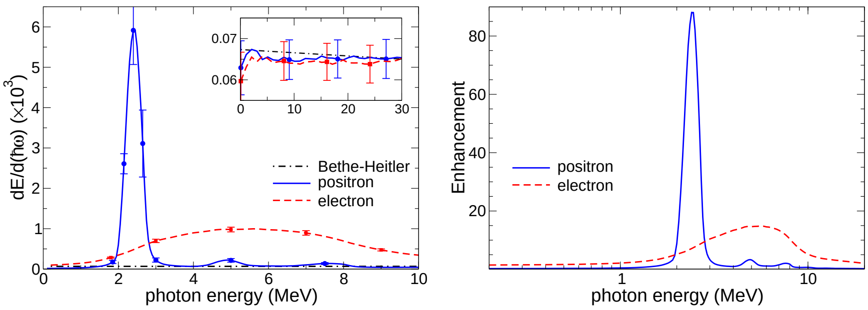


Fig. 1. *Left*: Spectra for 855 MeV positrons (solid line) and electrons (dashed line) passing through a 50 μm thick Si(110) crystal. The inset shows the spectra produced in amorphous Si and the Bethe-Heitler spectrum (dotted line). *Right*: Spectral enhancement of the channeling radiation with respect to the Bethe-Heitler values.

Related publications in 2012:

1. A.V. Korol, A.V. Solov'yov, Walter Greiner: *Channeling and radiation in periodically bent crystals*. (Springer Berlin Heidelberg, 2012) 268 pp. (ISBN 978-3-642-31894-8)

2. G.B. Sushko, V.G. Bezchastnov, I.A. Solov'yov, A.V. Korol, Walter Greiner, A.V. Solov'yov: *Simulation of ultra-relativistic electrons and positrons channeling in crystals with MBN Explorer*, J. Comp. Chem. (2012) (submitted)

Response of organotypic slice cultures to ionizing radiation

Collaborators: Mareike Müller[1,2,3,*], Marco Durante[2,3,4], Francesco Natale[2], Horst Stöcker[2,3], Horst-Werner Korf[1]

[1]Dr. Senckenbergisches Chronomedizinisches Institut, Fachbereich Medizin, Goethe-Universität Frankfurt/Main [2]GSI Helmholtzzentrum für Schwerionenforschung, Darmstadt [3]Frankfurt Institute for Advanced Studies, Frankfurt/Main [4]Institut für Festkörperphysik, Technische Universität Darmstadt, Darmstadt

* M. Müller is a PhD student at HGS-HIRe, funded by a Puschmann-scholarship

The aim of this work was to evaluate the response of liver and pancreas tissue to sparsely and densely ionizing radiation. For this, organotypic slice cultures (OSC) of liver (OLSC) and organotypic explant cultures (OEC) of pancreas (OPEC) were prepared from C3H wildtype (wt) mice and transgenic c-myc/TGF-α mice with an inducible liver tumor. OLSC from the transgenic c-myc/TGF-α mice were prepared from healthy (OHLSC) and neoplastic (ONLSC) parts of the liver. The pancreas from these animals was cultured as well (OTPEC). In order to evaluate a possible time dependence of the tissue response to ionizing radiation, OLSC and OPEC, OHLSC, ONLSC, and OTPEC were prepared at two different times of day: at the middle of the subjective day and at the middle of the subjective night.
Samples were cultured in a membrane-based culturing system with a liquid-air interface for several days. OLSC and OPEC from C3H wt-mice were irradiated with X-rays at doses of 2Gy, 5Gy, or 10Gy. OHLSC, ONLSC, OTPEC were irradiated with ^{12}C-ion extended Bragg peaks at the same doses. Mock-irradiated samples served as controls. All samples were fixed 1h and 24hrs post-irradiation, respectively, and immunohistochemically analyzed for markers of proliferation (Ki67), apoptosis (Caspase3), and DNA double-strand breaks (^{3} H2Ax).
While the pancreas samples, unfortunately, did not produce any meaningful results with regard to the evaluated parameters, healthy liver tissue showed distinct day-night differences with regard to all three analyzed parameters: the proliferation rate was significantly increased at the middle of the subjective day compared to the middle of the subjective night. Contrariwise, the apoptosis rate and rate of DNA double-strand breaks was significantly increased at the middle of the subjective night. These day-night differences were not detected in ONLSC. Regardless of the radiation type and dose, irradiation of healthy liver tissue did not influence the evaluated parameters. In ONLSC, however, the rate of DNA double-strand breaks increased dose-dependently.
The effects of ionizing radiation on the circadian clockwork were further examined in tissue samples of transgenic Per2^{luc}-mice. Per2^{luc}-mice express the enzyme luciferase under the control of the *Per2*-promoter, an important element of the circadian clockwork. Therefore, the analysis of these animals allowed to record the circadian rhythm of the molecular clockwork in liver and other tissues via real-time recordings of the luciferase-activity. As could be shown in OLSC and OEC from adrenal glands, ionizing radiation leads to a dose-dependent phase advance of the circadian clockwork.
The results of this project lead to the conclusion that ionizing radiation alter the circadian clockwork, but barely influence proliferation and apoptosis in healthy liver tissue.

Poster contribution
“Are ^{12}C radiation effects in murine liver tissue time-dependent?” at the Leopoldina Symposium “The circadian system: from chronobiology to chronomedicine”, 22.-23. March, 2012 at the Goethe Universität, Frankfurt am Main

Monte Carlo modeling of microdosimetry of therapeutic ion-beams and cosmic-rays

Collaborators: L. N. Burigo[1,2], I. A. Pshenichnov[1,3], I. N. Mishustin[1,4], M. Bleicher[1,2]

[1] Frankfurt Institute for Advanced Studies [2] Institut für Theoretische Physik, Johann Wolfgang Goethe University, Frankfurt am Main, Germany [3] Institute for Nuclear Research, Russian Academy of Sciences, Moscow, Russia [4] Kurchatov Institute, Russian Research Center, Moscow, Russia

The Monte Carlo simulation is a powerful method to account for the interactions of primary nuclei and all secondary particles with an extended medium. The Monte Carlo model for Heavy-Ion Therapy (MCHIT) based on the Geant4 toolkit was created in FIAS for simulation of complex radiation fields in ion-beam cancer therapy. The aim of the project is to study the stochastic impact of radiation at the level of individual cells.

Recent developments of MCHIT allowed the simulation of responses of Tissue-Equivalent-Proportional-Counters (TEPC) to neutron, proton and nuclear beams. The microdosimetric spectra measured by such devices are used to characterize the energy deposition to objects with effective size of few micrometers. The experimentally observed peak in the response function of the TEPC when an iron ion grazes the gas/wall interface of the detector is well reproduced by MCHIT simulations [1] as shown in Fig 1. The secondary particles produced in nuclear fragmentation of the ion beam can eventually contribute with the energy deposition in the TEPC. The model is suitable foridentifying the contributions from specific nuclear fragments. As an example, Fig 2 shows the contributions of individual fragments to microdosimetry spectra calculated with MCHIT [2]. As follows from our calculations, the energy deposition is provided by beam nuclei and nuclear fragments in regions near the beam, but by neutrona and protons far from it [3,4]. Further results include calculation of microdosimetric characteristics for a broad selection of ions and beam energies relevant for space research and cancer theapy.

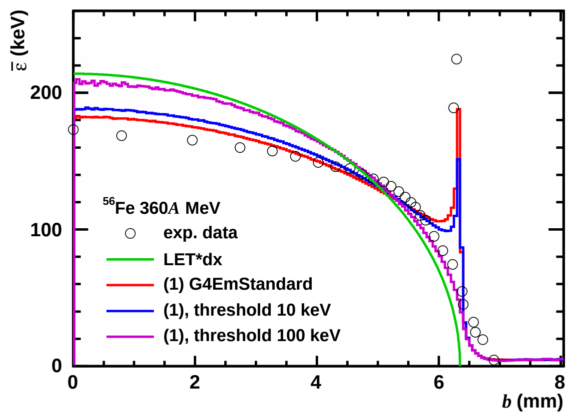


Figure 1: Energy imparted to TEPC by 360A MeV ^{56}Fe ions as a function of impact parameter. Experimental data from Gersey et al. 2002.

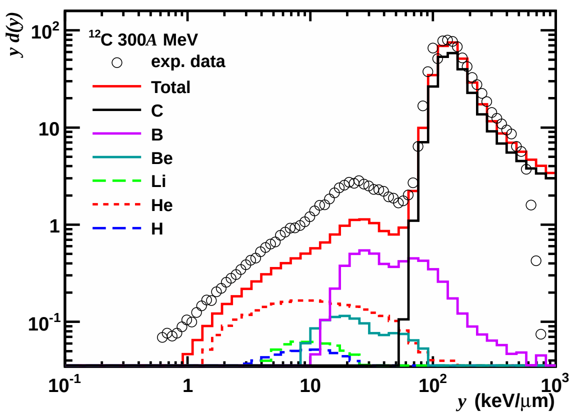


Figure 2: Microdosimetric spectra on the beam axis in the Bragg peak region for 300A MeV ^{12}C ions calculated with MCHIT. Data from Martino et al. 2010.

Related publications and talks in 2012:

1) L. Burigo, I. Pshenichnov, I. Mishustin, M. Bleicher, *Monte Carlo Simulations for Microdosimetry in Space Research at BIOMAT@FAIR*, FAIRNESS 2012, Hersonissos, Greece, September 3-8, 2012

2) M. Bleicher, L. Burigo, M. Durante, M. Herrlitz, M. Krämer, I. Mishustin, I. Müller, F. Natale, I. Pshenichnov, S. Schramm, G. Taucher-Scholz, C. Wälzlein, *Nanolesions induced by heavy ions in human tissues: Experimental and theoretical studies*, Beilstein J. Nanotechnol. 3, 556 (2012)

3) L. Burigo, I. Pshenichnov, I. Mishustin, M. Bleicher, *Microdosimetry of radiation fields from therapeutic C-12 beams in water: a study with Geant4 toolkit*. 2012. arXiv:1211.3648 [physics.med-ph]

4) I. Pshenichnov, L. Burigo, I. Mishustin, *Geant4 calculations of microdosimetric variables for neutrons and light nuclei in tissue-like materials*, 39th Annual Meeting of the European Radiation Research Society, Vietri sul Mare, Italy, October 15-19, 2012

Magnetic interactions and retardation in the electron emission from highly-charged ions

Collaborators: S. Fritzsche[1,2,3], A. Surzhykov[2,4], A. Gumberidze[1,2,5], T. Stöhlker[2,3,6]

[1] Frankfurt Institute for Advanced Studies, [2] GSI, Darmstadt, [3] Helmholtz Institute Jena, Germany, [4] Physikalisches Institut Heidelberg, Germany, [5] EMMI, Darmstadt, Germany, [6] University of Jena, Germany

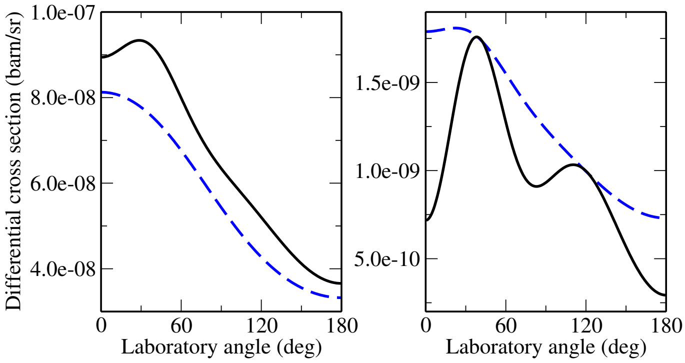
The x-ray spectroscopy of highly-charged, few-electron ions have shown that accurate energies and cross sections are obtained only if, apart from the static Coulomb repulsion among the electrons, the magnetic interactions and retardation as well as leading QED effects are taken into account into the thereotical description. In contrast to the spectrocopy of hard x-rays, however, little is known how the relativistic electron-electron (e-e) interactions affect their emission and, hence, the dynamics of electrons in strong fields. To obtain insight into this topic, we have re-analyzed the excitation and autoionization of highly charged ions with the goal to separate the magnetic and retardation contributions to the e-e interaction from the static Coulomb repulsion.

A remarkable change in the electron angular distribution due to the relativistic terms in the e-e interaction was found especially for the autoionization of (initially) beryllium-like projectiles, following a $1s \to 2p_{3/2}$ Coulomb excitation by some target nuclei. In this process, the angular distribution of the emitted electron is given by

$$W(\theta) \propto 1 + \sum_{k=2,4,\ldots} \mathscr{A}_k(\alpha_r J_r)\, f_k(\alpha_r J_r, \alpha_f J_f)\, P_k(\cos\theta),$$

where $\mathscr{A}_k(\alpha_r J_r)$ characterizes the alignment of the intermediate state after the excitation, θ is the polar angle with regard to the beam direction and where the $f_k(\alpha_r J_r, \alpha_f J_f)$ describe the dynamics of the autoionization. These functions merely depends on the e-e interaction, $V = V^{\rm Coulomb} + V^{\rm Breit}$, and provide access to both, the Coloumb repulsion and the (so-called) Breit interaction, i.e. the magnetic and retardation contributions.

For the excitation-autoionization process via the $1s2s^2 2p_{3/2}\ ^3P_2$ resonance, a diminished (electron) emission in forward direction as well as oscillations in the electron angular distribution due to the magnetic and retarded interactions are predicted especially for the electron emission into the $1s^2 2s\ ^2S_{1/2}$ ground and $1s^2 2p\ ^2P_{1/2}$ excited levels of the finally lithium-like ions; cf. Figure 1. This emission pattern is in strong contrast to a pure Coulomb repulsion between the bound and the outgoing electrons. Results in Figure 1 are shown in the laboratory frame and by incorporating only the Coulomb repulsion into the Auger amplitude (blue dashed lines) as well as for a full account of the e-e interaction (black solid lines). The lowering of the electron emission in forward direction ($\theta \approx 0^o$) is significant and enhanced in the laboratory frame due to the Lorentz transformation of the energetic electrons

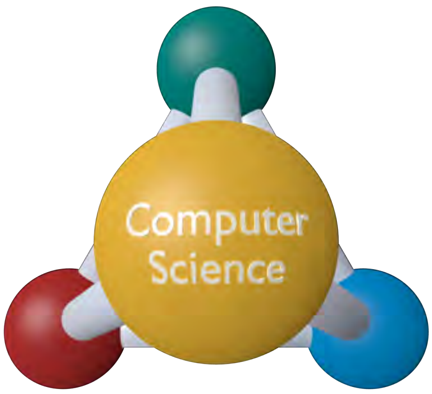


Angular distribution of electrons emitted in the $1s2s^2 2p_{3/2}\ ^3P_2 - 1s^2 2s\ ^2S_{1/2}$ (left panel) and $1s2s^2 2p_{3/2}\ ^3P_2 - 1s^2 2p\ ^2P_{1/2}$ (right panel) autoionization of U^{88+} projectiles with energy T_p = 5 MeV/u.

Related publications in 2012:

1) S. Fritzsche, A. Surzhykov, A. Gumberidze and T. Stöhlker, *Electron emission from highly charged ions: signatures of magnetic interactions and retardation in strong fields*, New J. Phys. 14, 083018 (2012)
2) L. Safari, P. Amaro, S. Fritzsche, J. P. Santos and F. Fratini, *Relativistic total cross section and angular distribution for Rayleigh scattering by hydrogen atom*, Phys. Rev. A 85, 043406 (2012)

4.4 Scientific Computing, Information Technology



The SANAM supercomputer

Collaborators: D. Rohr[1], S. Kalcher[1], V. Lindenstruth[1]
A. Alaqeeli[2], H. Alzaid[2]
S. Alkhereyf[2], A. Alharthi[2], A. Almubarak[2], I. Alqwaiz[2], R. Bin Suliman[2]

[1] Frankfurt Institute for Advanced Studies, [2] King Abdulaziz City for Science and Technology (KACST), Riyadh, Kingdom of Saudi Arabia

The SANAM supercomputer marks a milestone in power-efficient high-performance computing. Extending the success of the Goethe University's supercomputer LOEWE-CSC, the new computer achieves both, a significantly higher peak performance as well as an unprecedented power efficiency for compute clusters enhanced with commodity GPU accelerators. The relatively compact system (it is housed in less than 15 industry standard rack cabinets) is ranked number 52 on the Top500 list of the world's fastest supercomputers with a peak performance R_{max} of 421 TFlops [1]. In terms of power efficiency SANAM secured the second rank on the list of the most power-efficient supercomputers (Green500) delivering remarkable 2351 MFlops/W [2]. The development has been a joint effort between the King Abdulaziz City for Science and Technology (KACST), the Frankfurt Institute for Advanced Studies (FIAS), and the Helmholtz International Center for FAIR (HIC for FAIR). Figure 1 shows the integration of the system at the GSI Helmholtzzentrum in Darmstadt. Following the initial assembly and acceptance testing, the system will be transferred to KACST in Riyadh and is used for research activities related to petroleum, aerospace, bioinformatics, weather, and simulation of chemical reactions and particle movements.

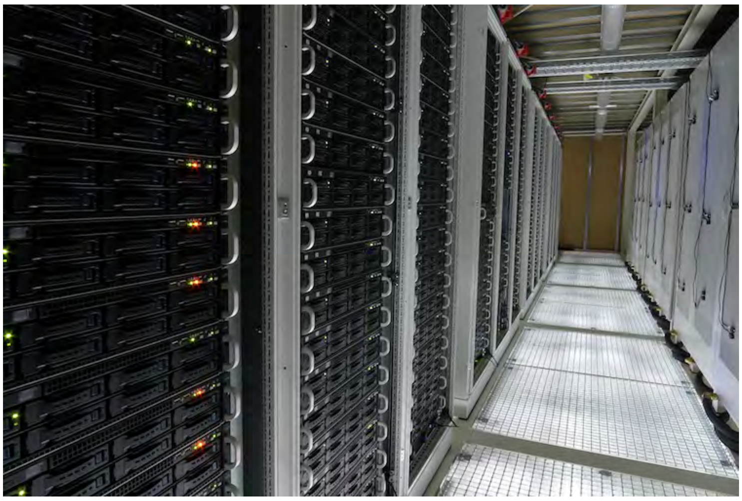


Figure 1: The SANAM supercomputer assembled at the GSI Helmholtzzentrum in Darmstadt.

SANAM is a cluster computer comprised of 210 (later extended to 300) commodity server nodes by ASUS (model ESC4000/FDR G2). Each node contains two Intel Xeon E5-2650 processors and 128 GB of RAM. The largest share of the compute performance is contributed by two AMD FirePro S10000 graphics cards per server. Each graphics card itself contains two graphics processing units (GPUs). In total the system is hence composed of 3360 CPU cores, 26880 GB of RAM, and 840 GPUs. The nodes are interconnected by an FDR InfiniBand high-performance fabric providing a throughput of 56 Gbit/s on a single link. The aggregate power consumption (measured during times of the highest computational workload) is only 179 kW and the theoretical peak performance R_{peak} is 1098 TFlops.

References:

[1] Top500 supercomputer sites, `http://www.top500.org/system/177996`
[2] The Green 500, `http://www.green500.org/lists/green201211`

Tracking, Triggering and Event Buffering with the ALICE TRD Global Tracking Unit

Collaborators: S. Kirsch[1], F. Rettig[1], V. Lindenstruth[1]

[1] Frankfurt Institute for Advanced Studies

The Global Tracking Unit (GTU) of the ALICE Transition Radiation Detector (TRD) is designed to provide triggers based on charged particle tracks reconstructed online within 6.5 µs after the interaction. Already on the detector, a total of 1.2 million analog channels are processed by ≈ 65500 multi-chip modules to find and parameterize segments of high-p_T tracks traversing the detector layers. Track segments and event raw data are transferred via 1080 optical links to the GTU, a systolic trigger processor and readout unit with 109 FPGAs arranged in a three-level (90-18-1) hierarchy. As central element of the detector readout chain, the GTU forms the resulting data stream and provides the TRD with multi-event buffer capability in order to reduce detector deadtime. Using the track segments, 90 units of the first stage perform a 3D event reconstruction of charged particle tracks in less than 2 µs. Reconstructed tracks are input to the 18 supermodule processing stages, where several trigger algorithms are applied. Results from the sectors are combined on the highest stage to form detector-wide trigger decisions, which are then transmitted to the central trigger processor of the experiment.

Online Tracking and Trigger Performance Online track reconstruction was provided throughout the data taking in 2012. Based on data recorded in 2012 and 2011, the online tracking performance was studied for pp and Pb-Pb collisions. A p_T resolution of better than 10-20% over the full trigger relevant range from 2 GeV/c to 8 GeV/c was achieved. A typical correlation of track-level transverse momenta from online tracking and offline reconstruction is shown in Figure 1. Mid 2012 a jet trigger was put into operation (see example event in Figure 2), later two single-electron triggers for heavy flavour and quarkonia studies followed. Sufficient data for the analysis of the physics performance of these triggers were recorded and the analysis is ongoing.

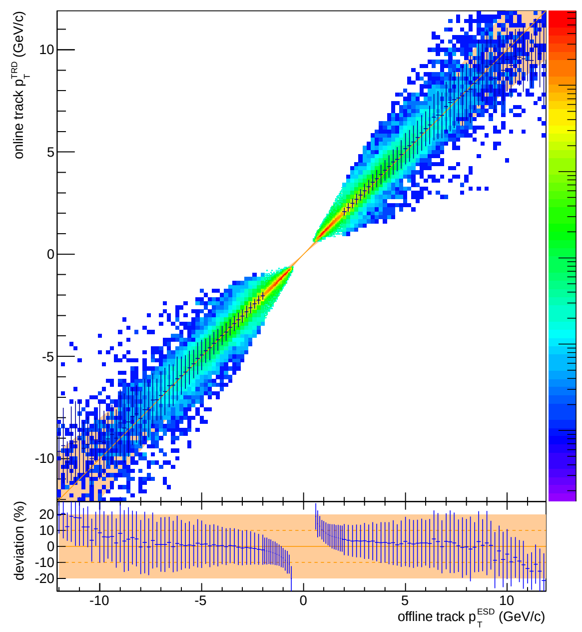


Figure 1: Correlation between offline and online estimate for transverse particle momentum

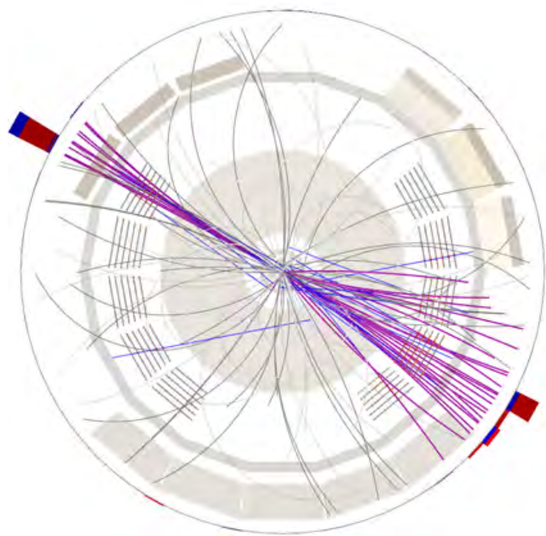


Figure 2: Di-Jet in pp event triggered with the TRD jet trigger

Reduction of Deadtime Throughout 2012 the GTU operated successfully with upgraded FPGA firmware designs providing multiple event buffers, thus decoupling detector front-end operation and event readout to the Data Acquisition. The required support for several interlaced trigger sequences required complex changes to the control logic and thorough verification with large statistics in pp and technical runs. In typical heavy-ion operation, a decrease in deadtime per event from ≈ 2000 µs to 150 µs was observed.

ALICE HLT TPC GPU Tracker

Collaborators: D. Rohr[1], S. Gorbunov[1], V. Lindenstruth[1]

[1] Frankfurt Institute for Advanced Studies,

The Large Hadron Collider (LHC) at the European Center for Particle Physics (CERN) is today's most powerful particle collider built to search for rare particles such as the Higgs boson and to study properties of dense hot medium. Alice is one of its four major detectors designed specifically for the second purpose. The ALICE High Level Trigger (HLT) is a compute farm of about 250 nodes and it is the first point where where all data from the various subdetectors are available together. The HLT is capable of a full online event reconstruction and uses data compression techniques in order to reduce the data rate stored to the tapes to a feasible rate.

Reconstruction of the trajectories (tracking) of particles measured in the Time Projection Chamber (TPC) is one critical part of event reconstruction and requires significant compute resources. The HLT implements a parallel tracking algorithm that can make use of GPUs. The tracker employs a pipeline which ensures continuous GPU utilization. Results of the GPU and the CPU version of the tracker match exactly except for artifacts caused by different rounding due to non-associate floating point arithmetic.

The HLT compute nodes are not exclusively used for tracking but also for other tasks like cluster transformation and vertexing. Hence, not all CPU cores are available for tracking. The below figure shows the speedup of both the GPU and the CPU implementation of the HLT tracker running on four CPU cores and, in the case of the GPU tracker, also on the GPU. The HLT tracker is 12 to 15 times faster than the offline version and the GPU tracker is faster by another order of magnitude.

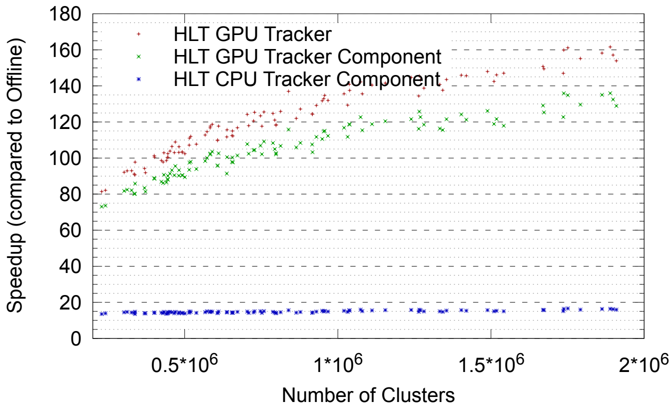


Figure: Speedup of HLT GPU tracker in comparison to CPU tracker and to offline tracker.

If the CPU tracker employs all available cores of one node, tracking takes about as long as tracking on the GPU. Hence, plugging a GPU in an existing node saves an entire node - and the required additional infrastructure. Overall, the GPU tracker enables TPC tracking with only about one tenth the investment which would be required otherwise.

Currently, the HLT is equipped with about 50 GTX480 GPUs achieving a maximum data rate of more than 200 Hz in central lead-lead collisions. The HLT was operated during the heavy ion phases at the end of 2010 and 2011 and is used for the proton-lead phase at the beginning of 2013.

Related publications:

1) S. Gorbunov, D. Rohr, et al., *ALICE HLT high speed tracking on GPU*, IEEE Transactions on Nuclear Science 58, 1845 (2011)
2) D. Rohr, S. Gorbunov, et al., *ALICE HLT TPC Tracking of Pb-Pb Events on GPUs*, Journal of Physics: Conf. Ser. 396, 12044 (2012)
3) D. Rohr *ALICE TPC Online Tracker on GPUs for Heavy-Ion Events*, Proc. of 13th Intl. Workshop on Cellular Nanoscale Networks and their Applications pp. 298-303 (2012)

Microdriver in High-Throughput and Real-Time Environments

Collaborators: D. Eschweiler[1], V. Lindenstruth[1]

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Compared to a system software engineer, the life of an application developer is rather easy. This is the case, because the **O**perating **S**ystem (OS) usually shields the really hard tasks from its users. Such tasks are for example direct hardware access, machine code programming, or memory management. The OS provides an **A**pplication **B**inary **I**nterface (ABI) to the user applications. It mainly maintains binary compatibility between a wide range of OS versions. The different parts of the OS itself are not binary compatible between versions, since there is no instance that provides an ABI to the OS. This usually means that, in case of an software update, all parts of the OS layer need to be replaced, even if only a single component needs updating. Another major difference is the aspect of fault tolerance. Buggy user applications usually crash, alter user data in an unwanted way, or are simply nonfunctional, but they should never compromise the integrity of the whole system. In contrast, when an OS component crashes it usually leaves hardware devices in an inconsistent or even deadlocked state and dynamically allocated memory regions are not freed automatically. Since there is no further instance below the OS, a crashed OS component usually also compromises the whole OS itself.

The software development paradigm of the Linux OS circumvents at least the compatibility issue by including all drivers and enhancements directly into the source package of the OS. This works in the most cases, but also forces vendors to provide their drivers as open source. Another common idea to improve the situation is, to execute the majority of OS components as a user application. Device drivers are a perfect target for such a relocation, since usually 80-90% of the OS code base is actually driver code. This microdriver / microkernel approach leads to much more compatible and robust systems, but is also seen as only suitable for low-performance and/or low-throughput applications. Drivers are also needed to operate certain custom devices, which are part physics experiments at CERN or GSI. The main demand to this particular range of software is, that it has to be fast as possible and efficient, to fulfill the throughput and real-time requirements of the used detector hardware. The related drivers must also be compatible with a wide range of OS versions, since the used version is usually determined by other proprietary drivers that need a dedicated version of the OS.

The aim of our PDA (**P**ortable **D**river **A**rchitecture) is to provide a simple to use **A**dvanced **P**rogramming **I**nterface, combined with a powerful library that already implements commonly needed functions such as interrupts, **P**rogrammed **I/O** (PIO), and **D**irect **M**emory **A**ccess (DMA). Furthermore, the PDA can control devices which are using the PCI bus to connected to the system. The PCI bus is one of the fastest internal interconnects that are currently available on the market. A library which can drive such a bus efficiently is likely to be able to drive other (slower) buses as well. The focus of the related research lays on how we can achieve to move as much code as possible into the userspace library and how we can enhance such a library for the needs of modern multiprocessor systems (memory pinning etc.). Such an approach leaves only the thin OS part that the related maintainer has to adjust for each new OS version. It also should remove the need to port the actual driver, since the ABI stays stable. The driver developer, which uses the PDA, therefore does not need to change anything in his code in case of an OS update. We intend to bring the final proof with the results of the PDA project, that the microdriver-concept can ultimately used for every kind of device drivers. A driver for readout hardware at the ALICE experiment at CERN will make use of the PDA to show the practical application of our microdriver system. Furthermore, the knowledge we will gain in ALICE will automatically apply to the CBM experiment at GSI. The gained synergies will shorten development times and improve the overall stability of the system software, which will work in CBM.

Reference:
1) D. Eschweiler, A. Brinkmann, *A Microdriver Architecture for Error Correcting Codes inside the Linux Kernel*, In Proc. of the ACM/IEEE Conference on Supercomputing (SC09), Portland. ACM, November 2009

Vc: Improvements to the C++ library for explicit, portable, and intuitive SIMD programming

Collaborators: M. Kretz[1,2], V. Lindenstruth[1]

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Current CPUs support vector (SIMD) instructions, which enable operations on Multiple Data with a Single Instruction. The trend shows that register sizes are increasing and thus the parallelism achieved with SIMD increases. The Vc library was developed to facilitate development of explicitly vectorized C++ code. The library aims to make SIMD development understandable to C++ beginners, be as fast as vector code developed directly for a given CPU, and enable portability of SIMD code. (See last year's report for details.)

At the beginning of 2012 Vc version 0.6 was released, being the first version to support AVX instructions. The Vc library was subsequently successfully integrated into a development branch of the ROOT libraries. It is planned that Vc 0.7 will additionally be released as part of ROOT in 2013. Furthermore, Vc has been integrated into the AliRoot framework, thus already reaching the wider ALICE community.

The development on Vc 0.7 focused on polishing the library for widespread use. To this end, a lot of work went into improved portability by additionally supporting the clang, MSVC, and ICC compilers as well as some older GCC versions. To a large extend, this work requires to debug and understand compiler bugs (miscompilations or deviations from the C++ standard), report these bugs to the compiler teams, if possible, and develop workarounds. It is important that every bug in a compiler is worked around in Vc. Otherwise, it would be very hard for any larger project to rely on Vc.

C++ supports automatic type conversion in many places. When two objects of different types are combined with an operator, often one of the types is converted before the operation is called. For the fundamental types the conversion rules are well-defined. Since the Vc types are simply small collections of fundamental types, they should follow the same conversion rules. Everything else would make the use of Vc more difficult. The issue is non-trivial and required thorough research. The implementation was finally done using SFINAE patterns.

A few issues in Vc had to be addressed to support compilation with C++11 compilers. Also, where it made sense, some patterns were improved with C++11 features.

The research on more intuitive and efficient memory access patterns and APIs continued. Many existing data structures cannot easily be modified for vector loads and stores. In those cases, scalar loads and stores are often used even though they quickly turn out to limit performance. A new API for interleaved memory access was researched and implemented. The API is similar to parallel assignment in Ruby or Python.

The trigonometric functions in Vc 0.6 were tuned for speed. For Vc 0.7 they have been reworked to achieve improved precision. As a result these functions are not inlined anymore, because the required code increased too much. Therefore, a pattern to support binaries with multiple implementations was developed. This is now used for the trigonometric functions in Vc's static library and available to users of Vc.

Project	Configure			Build			Test		
	Error	Warning	Pass	Error	Warning	Pass	Not Run	Fail	Pass
clang	0	0	6	0	2	4	0	0	3276
MSVC	0	0	8	0	4	4	0	92	3612
GCC	0	0	80	0	4	76	0	0	43582
ICC	0	0	2	0	0	2	0	0	2312
Open64	0	0	8	8	8	0			
mingw	0	0	1	0	0	1	0	456	122
experimental	0	0	14	0	2	12	0	86	7622

View of the dashboard on January, 25th 2013. It shows that the targeted compilers for Vc 0.7 (clang, MSVC, GCC, and ICC) are nearly at full support.

Optimized HPL for multi-GPU clusters

Collaborators: D. Rohr[1], S. Kalcher[1], V. Lindenstruth[1]

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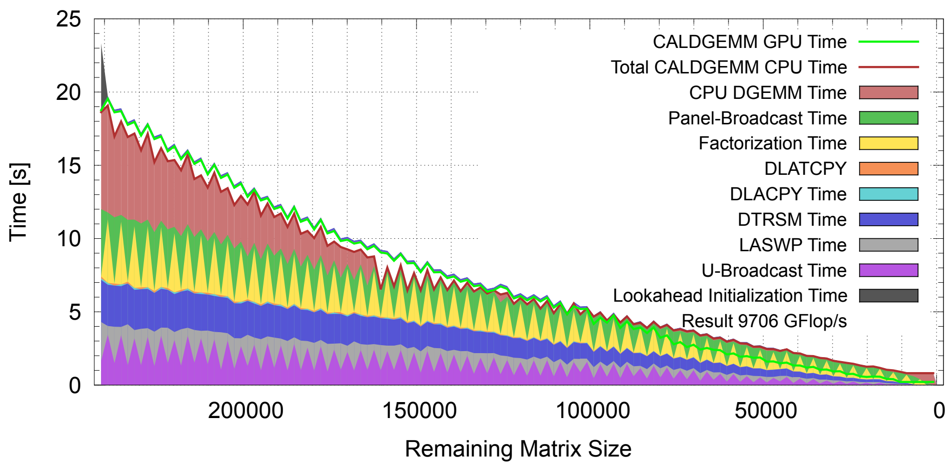
The High Performance Linpack implementation that was originally developed at the Frankfurt Institute for Advanced Studies for the LOEWE-CSC cluster of the Goethe-University, has been improved such that it can well utilize multiple GPUs of the current generation. It implements a recursive algorithm which solves a dense system of linear equations employing partial pivotization in order to guarantee numerical stability. With this implementation, the Sanam supercomputer achieved rank 52 in the November 2012 Top500 list and secured an excellent second rank in the Green500 list demonstrating 421 TFlop/s. In comparison to the LOEWE-CSC, Sanam offers four graphics cards per node, each of them faster than LOEWE's GPUs. For this reason, the GPUs are the contributors of most of the compute performance while the processors deliver only a minor portion. (The processors of the LOEWE-CSC provide about 30% of LOEWE's performance.)

The HPL implementation offloads the DGEMM tasks (generalized matrix multiplication) to the GPU and executes the rest of the algorithm on the processors. GPUs excel at simple tasks such as matrix multiplication where they can access a large fraction of their theoretical peak performance and hence also provide unbeatable power efficiency. Other tasks could benefit from GPU acceleration as well but it is very unlikely they can be sped up to the same extent as DGEMM. It is thus the best strategy to try to fully load the GPUs with DGEMM tasks all the time.

With the above approach it is essential to make the DGEMM on the GPU overlap with the CPU calculation. By design good performance cannot be achieved if the GPU idles during CPU calculation. A newly developed lookahead algorithm tackles this, which implements two optimizations. Each iteration the matrix update, which is based on DGEMM, processes the matrix columns in such an order that the factorization and the broadcast of the next iteration can run concurrently. In addition, the pivotization is pipelined with the update.

The following plot visualizes CPU execution time of all involved tasks in different colors. The green line is the GPU time of CALDGEMM, which is the optimized GPU DGEMM library. When the CPUs finish their tasks early, they can contribute to the DGEMM (red color). As long as the green line lies above the colored area, lookahead can completely hide all CPU calculations behind the DGEMM. Only at the end of the run, there is a period where GPU utilization drops. The measurement is based on a run with four nodes.



Certain parts of the algorithm can be implemented in two ways, one maximizing performance, the other optimizing power efficiency. To achieve an optimal ranking in both the Top500 and the Green500 list, two versions of the benchmark are maintained. The energy efficient version achieves around 2350 MFlop/J while the performance optimized version delivers about 2.4 TFlop/s per node - both showing only a negligible dependency on the number of participating nodes.

FLES: standalone First Level Event Selection package for CBM

Collaborators: V. Akishina[1,2,3], I. Kisel[2,3,4], I. Kulakov[2,3,4], M. Zyzak[2,3,4]

[1] Joint Institute for Nuclear Research, Dubna, Russia, [2] Goethe-Universität Frankfurt am Main, [3] GSI Helmholtzzentrum für Schwerionenforschung GmbH, Darmstadt, [4] Frankfurt Institute for Advanced Studies

The main focus of the CBM experiment (FAIR, Darmstadt, Germany) is the measurement of very rare probes, that requires interaction rates of up to 10 MHz. Together with the high multiplicity of charged particles (up to 1000) produced in heavy-ion collisions, this leads to huge data rates of up to 1 TB/s. Most trigger signatures are complex (short-lived particles, e.g. open charm decays) and require information from several detector subsystems.

The First Level Event Selection (FLES) package of the CBM experiment is intended to reconstruct the full event topology including tracks of charged long-lived particles and short-lived particles. The FLES package consists of several modules (see Figure 1): track finder, track fitter, particle finder and physics selection. As an input the FLES package receives the geometry of the tracking detectors and the hit measurements, which are created by the charged particles crossing the detectors. Tracks of the charged particles are reconstructed by the Cellular Automaton track finder and the Kalman filter based track fitter. The KF Particle Finder is used to find short-lived particles. In addition, a module for quality assurance is implemented, that allows to monitor the quality of the reconstruction at all stages.

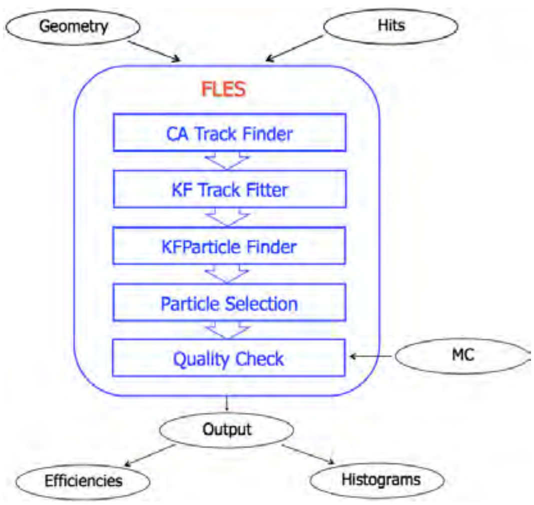


Figure 1: Block diagram of the KF Particle Finder algorithm.

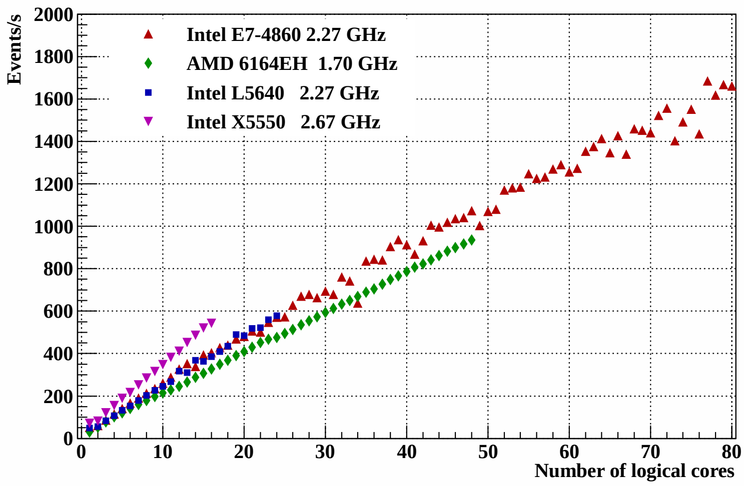


Figure 2: Scalability of the FLES package on many-core servers.

The package provides the high reconstruction efficiency and the high signal to background (S/B) ratio for the reconstructed decays. For instance, for 240 000 minimum bias Au+Au UrQMD events at 25 *A*GeV the reconstruction efficiency (normalized on 4π) for the K_s^0 meson is 15.3% with the S/B ratio 3.5 and for the Λ hyperon — 17.2% and 5.1 respectively.

The first version of the FLES package is optimized with respect to speed, intrinsically local and parallel. The implemenation is based on the SIMD instructions and have been parallelized between cores using the Intel Threading Building Blocks package, that provides scalable event-level parallelism with respect to the number of hardware threads and CPU cores. Four servers with Intel Xeon and AMD processors have been used for the scalability tests. The most powerful server has 4 processors with 10 physical cores each, that gives 80 logical cores in total. Figure 2 shows a strong scalability for all many-core systems. The achieved reconstruction speed is 1700 events per second on the 80-cores server.

The Cellular Automaton track finder at high track multiplicities for CBM

Collaborators: V. Akishina[1,2,3], I. Kisel[1,2,4], I. Kulakov[1,2,4], M. Zyzak[1,4]

[1] Goethe-Universität Frankfurt am Main, [2] GSI Helmholtzzentrum für Schwerionenforschung GmbH, Darmstadt, [3] Joint Institute for Nuclear Research, Dubna, Russia, [4] Frankfurt Institute for Advanced Studies

The CBM experiment at FAIR is being designed to study heavy-ion collisions at extremely high interaction rates (up to 10 MHz) and high track multiplicities (up to 1000). Since the beam in the CBM experiment will have no bunch structure, but continuous, the groups of events may be close or overlapped in time. Measurements in this case will be 4D (x, y, z, t). Thus, the reconstruction of time slices rather than events will be needed. In addition to such high input rate and complicated event topology, the full event reconstruction and selection will be done at the First Level Even Selection (FLES) stage. In this respect, both the speed of the reconstruction algorithms and their efficiency are crucial. The Cellular Automaton (CA) track finder is fast and robust and thereby is used both for the online and offline track reconstruction in the CBM experiment. The algorithm creates short track segments in each three neighbouring stations, then combines them into track-candidates and selects the best tracks according to the maximum length and minimum χ^2 criteria. The algorithm was further optimized for the case of high track multiplicity with respect to time: additional sorting of found hits according to 2-dimensional (y, z) grid was introduced in order to speed up the search for the next hit.

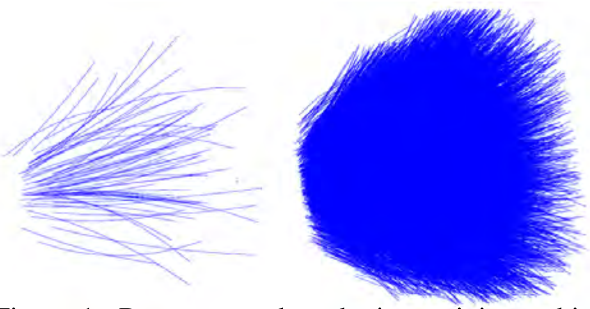


Figure 1: Reconstructed tracks in a minimum bias event (left) and a packed group of 100 minimum bias events (right), 109 and 10340 tracks on average respectively.

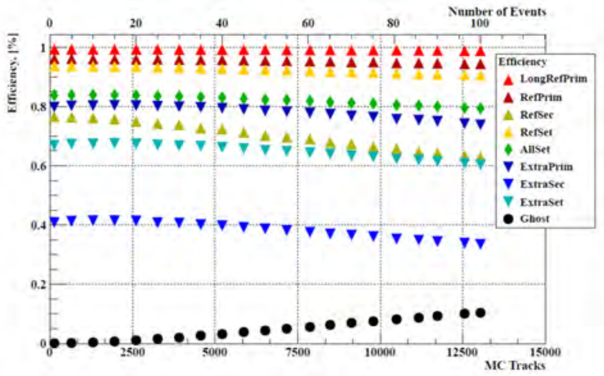


Figure 2: Track reconstruction efficiencies and ghost rate for different sets of tracks versus track multiplicity.

The standalone FLES package was used to investigate the stability of the CA track reconstruction with respect to a track multiplicity per event. For the study 1000 of minimun bias Au+Au UrQMD events at 25 AGeV was simulated. As the first step towards 4D tracking a number of minimum bias events (up to 100) were packed into one group with no time measurement taken into account. The group was treated by the CA track finder as a single event and the regular reconstruction procedure was performed (Figure 1). The dependence of the track reconstruction efficiency on the track multiplicity is stable (Figure 2). In particular, the efficiency of the algorithm decreases only by 4% for 100 minimum bias events in one group, comparing to the case of a single minimum bias event. The efficiencies for the reference tracks ($p > 1$ GeV/c), which include tracks of particular physics interest, remains high for all range of track multiplicities. The efficiencies for extra (100 MeV/c$< p < 1$ GeV/c) and secondary tracks are also stable. The level of ghost tracks is less than 10%. The speed of the algorithm was studied as a function of track multiplicity. The time, which algorithm needs to proceed a grouped event, behaves as a second order polynomial with respect to a number events in the group. Due to this fact, the CA track finder needs less than 2 seconds in order to reconstruct a grouped event combined of 100 minimum bias events, that corresponds to about 10 000 reconstructed tracks.

Summarizing, the CA track finder reconstruction algorithm shows high speed performance and stability with respect to the track multiplicities, up to the extreme case of about 10 000 reconstructed tracks per event.

The KF Particle Finder package for short-lived particles reconstruction in CBM

Collaborators: M. Zyzak[1,2,3], I. Kisel[1,2,3], I. Kulakov[1,2,3], I. Vassiliev[1,3]

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Today the most interesting physics is hidden in the properties of short-lived particles which can not be registered directly by a detector system but only reconstructed from their decay products. A fast and efficient KF Particle Finder package for short-lived particles reconstruction and selection is developed for the CBM experiment. A search for about 50 decay channels has been currently implemented. At first, all tracks are divided into groups of secondary and primary tracks for further analysis. Primary tracks are those, which are produced directly in the collision of beam and target ions. Tracks from decays of resonances (strange, multi-strange and charmed resonances, light vector mesons, charmonium) are also considered as primaries since they are produced directly at the point of the primary vertex. Secondary tracks are produced by the short-lived particles, which decay not in the primary vertex point and can be well separated. These particles include strange particles (K_s^0 and Λ), multi-strange hyperons (Ξ and Ω) and charmed particles (D^0, $D^{\pm}$, $D_s^{\pm}$ and Λ_c). Then tracks are combined according to the block diagram in Figure 1 and particle-candidates are produced from these combinations. The particles are reconstructed with the KF Particle package, which is based on the Kalman filter (KF) method and finds parameters of the particle, such as decay vertex, momentum, energy, mass, etc., together with their errors. All particles of the event are reconstructed at once that makes the algorithm local with respect to the data and therefore very fast.

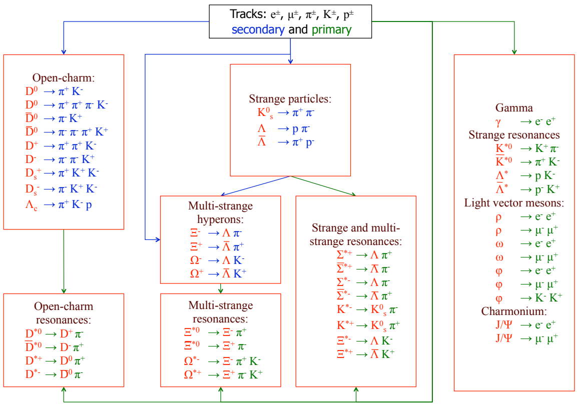

Figure 1: Block diagram of the KF Particle Finder algorithm.

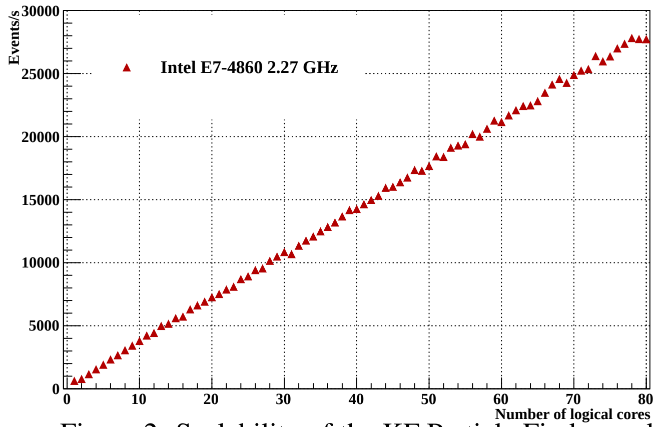

Figure 2: Scalability of the KF Particle Finder package with minimum bias Au+Au events at 25 AGeV on a many-core server lxir075 at GSI equipped with four Intel E7-4860 (2.27 GHz) CPUs.

KF Particle Finder achieves a high efficiency of the particle reconstruction. For example, efficiencies of K_s^0, Λ, Ξ^- and Ω^- reconstruction are 15.3%, 17.8%, 5.0% and 2.5% respectively for 240 000 of minimum bias Au+Au collisions at 25 AGeV. The corresponding signal to background ratios are 3.5, 5.1, 42.2 and 4.3.

In order to utilize all possible resources of modern CPUs and to achieve the highest possible speed KF Particle Finder is based on the SIMD instructions. Also, the algorithm has been parallelized between cores of the modern CPUs and demonstrates a strong linear scalability on many-core servers with respect to the number of cores (see Figure 2).

Summarizing, the KF Particle Finder package reconstructs about 50 of the most important decay channels for the CBM experiment with a high efficiency and a high signal to background ratio achieving speed of 1.5 ms per Au+Au minimum bias collisions at 25 AGeV on a single core.

Multi-strange baryons reconstruction in the CBM experiment

Collaborators: I. Vassiliev[1,2], I. Kisel[1,2,3], I. Kulakov[1,2,3], M. Zyzak[1,2,3]

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One of the predicted signatures of the phase transition from nuclear matter to deconfined quark gluon plasma is the enhanced production of multi-strange particles. Also the yield of particles carrying strange quarks is expected to be sensitive to the fireball evolution. The CBM detector will provide an unique opportunity to measure yields, direct and elliptic flows, excitation functions of multi-strange baryons at different energies and sizes of the colliding heavy ions. Ω^- baryon consists of 3 strange quarks, Ξ^- baryon contains 2 strange quarks and Λ — one strange quark. Multi-strange baryons will be measured in CBM by its decay into charged hadrons, which are detected in the Silicon Tracking System (STS) and in the Time-of-Flight detector (TOF).

To study the feasibility of multi-strange baryons reconstruction in the CBM experiment, a sets of 10^6 central Au+Au UrQMD events at 2, 4, 6, 8, 10, 15, 20, 25, 30 and 35 *A*GeV have been simulated. High statistic allows to calculate even $\Omega^\pm$ reconstruction efficiency directly, avoiding signal embedding into UrQMD events. Together with the wide range of beam energies, it allows to investigate systematic behavior of different physics observables, like direct and elliptic flows, excitation functions, antibaryon to baryon ratios and many others. In Fig. 1 the reconstructed multi-strange antibaryon to baryon production ratios versus beam energy is shown. Strange quarks number hierarchy is clearly visible. Black points correspond to Ω^+ to Ω^- ratios (S = 3), red points are Ξ^+ to Ξ^- ratios (S = 2) and blue points are $\bar{\Lambda}$ to Λ ratios (S = 1).

The Ω^- decays into ΛK^- with branching ratio 67.8% and $c\tau = 2.46$ cm, the Ξ^- decays to $\Lambda\pi^-$ with branching ratio 99.89% and $c\tau = 4.92$ cm, decays of Λ happen most often in the STS detector. The STS geometry with 8 double-sided segmented strip detectors, cables and support frames were used for event reconstruction. Particle identification with TOF was applied. The KF Particle Finder package was used to reconstruct about 50 particles and resonances including $\Omega^\pm$, $\Xi^\pm$, Λ and $\bar{\Lambda}$. Typical invariant mass spectrum is shown in Fig. 2. The Ω^- reconstruction efficiency is about 1.8% for central UrQMD events. The reconstructed mass value 1.672 ± 0.003 GeV/c^2 is in a good agreement with the simulated PDG's data. The invariant mass resolution is 2.3 MeV/c^2. The $\Omega^\pm$ and $\Xi^\pm$ particles are accepted, if they have good quality geometrical and topological detached vertices with $\chi^2_{geo} < 3\sigma$, $\chi^2_{topo} < 3\sigma$ and *z*-vertex farther than 3 cm downstream of the target plane.

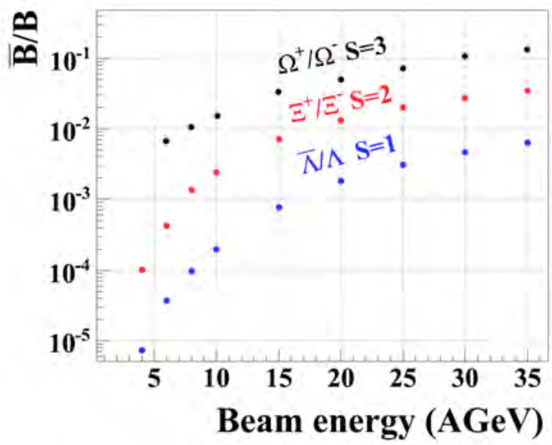


Figure 1: Recalculated ratios of anti-baryon to baryons yields versus beam energy.

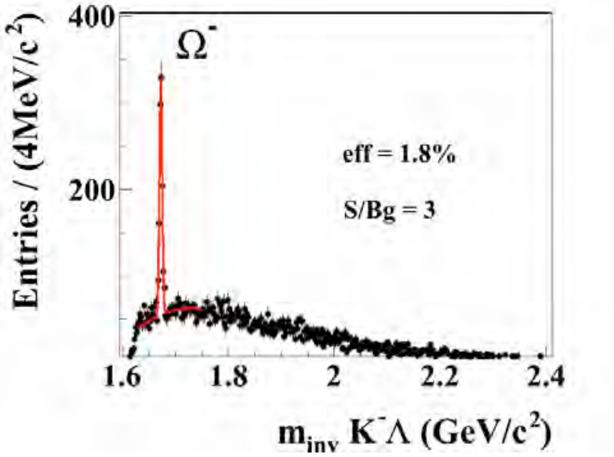


Figure 2: Reconstructed invariant mass distribution of ΛK^- pairs in central Au+Au collisions at 35 *A*GeV.

Lattice QCD on GPUs

Collaborators: M. Bach[1,2], V. Lindenstruth[1,2], O. Philipsen[3], C. Pinke[3]

[1] Frankfurt Institute for Advanced Studies, [2] Institut für Informatik, Goethe-Universität Frankfurt, [3] Institut für theoretische Physik, Goethe-Universität Frankfurt

Lattice Quantum Chromodynamics (LQCD) is the only a priori approach to describing the strong force. State-of-the-art lattice simulations require high-performance computing and constitute actually one of the most compute intensive problems overall. With processor clock speeds no longer improving and processors instead increasing their core count, Graphics Processing Units (GPUs) with their high peak performance and bandwidth have become an interesting platform for high-performance computing.

Originating in the high-end computer gaming market, GPUs nowadays offer highest computing capabilities at a very attractive price-per-flop ratio. Current high-end gaming GPUs by AMD and NVIDIA are priced at about 500 Euros. So far, however, most work on this field has been based on NVIDIA CUDA, locking the software to run on hardware by the single vendor NVIDIA.

We created the first application of OpenCL to Wilson fermions, enabling the code to be run on AMD and NVIDIA GPUs and also on classical CPUs. Last year we reported on a high performance $\not{D}$ implementation in OpenCL, which is the most compute intensive part of lattice calculation. In 2012 we have extended this work to a full hybrid Monte-Carlo application that shows major performance gains over a purely CPU based reference code. Additionally, the $\not{D}$ and the overall application has been tuned to a wider range of hardware, including the latest AMD GPUs.

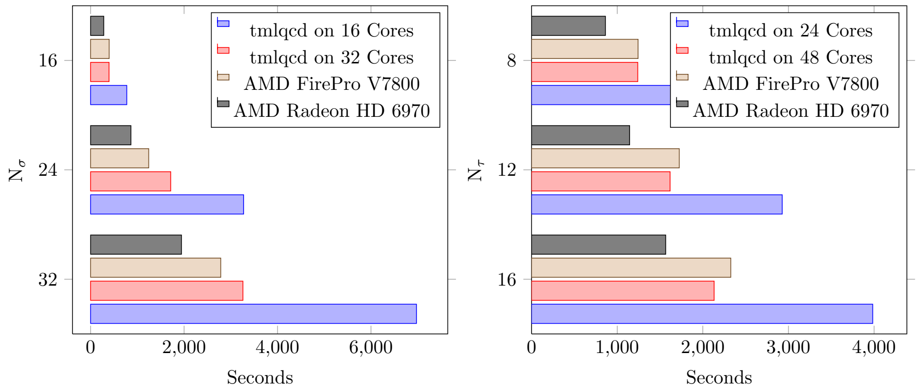


Figure: HMC runtimes in seconds using $\mu = 0.1$, $m_\pi = 520$, $\beta = 3.9$ and $\kappa = \kappa_c = 0.160856$ for fixed $N_\tau = 8$ and $N_\sigma = 24$, respectively.

For the Wilson $\not{D}$ kernel we were able to show excellent performance, utilizing more than 70 % of the available memory bandwidth for all lattice sizes on a variety of AMD GPUs, outperforming published performances of CUDA based codes. The code was also proven to work on NVIDIA GPUs, although with reduced performance, as no optimization has been performed for that hardware.

Extended to a full HMC for twisted-mass Wilson fermions we showed a speedup factor of four of our code running on an AMD Radeon HD 5870 compared to a reference code running on a single AMD Opteron 6172 socket. In addtion we could show the performance of the code to scale to newer generations of AMD GPUs.

First production usage of the code has been performed in December 2012. The data is currently being analyzed.

Related publications in 2012:

1) M. Bach, V. Lindenstruth, O. Philipsen, C. Pinke, *Lattice QCD based on OpenCL.* arXiv:1209.5942 [hep-lat].

Relativistic Hydrodynamics on Graphic Cards

Collaborators: J. Gerhard[1,2], V. Lindenstruth[1,2], M. Bleicher[1,3]

[1] Frankfurt Institute for Advanced Studies, [2] Institut für Informatik, Goethe-Universität, [3] Institut für Theoretische Physik, Goethe-Universität

Relativistic hydrodynamics is widely used in different areas of physics, ranging from the evolution of neutron stars over the collision of galaxies to the collision of heavy ions. All these simulations need to respect the relativistic nature of the dynamics, however the focus lies on different aspects. For the heavy ion collision case the algorithms have to be able to capture shock phenomena and cope with very sharp gradients.

Different models incorporate a hydrodynamic phase in order to explore different aspects of a collision. The possibility to incorporate hydrodynamic calculations into Monte Carlo models however, depends strongly on the execution time of the hydrodynamic computation.

The Frankfurt UrQMD model applies in its hybrid transport model, the *Sharp and Smooth Transport Algorithm* (SHASTA). Unfortunately the classic implementation is not capable of using the tremendous performance improvements of new hardware platforms. It is intrinsically serial and makes strong use of memory look-ups.

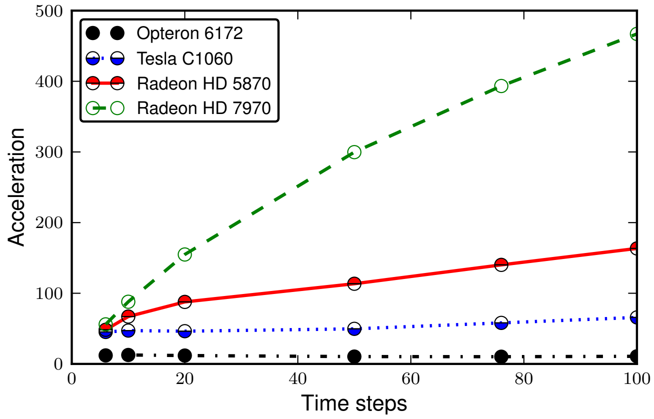


Figure: Acceleration of the compute velocity of a typical Au+Au collision event for $\sqrt{s} = 200\,A\,\text{GeV}$ with impact factor of $b = 7$. The identical optimized code is executed on different platforms.

The underlying serial *Sharp and Smooth Transport Algorithm* has been analysed and completely redesigned. A novel parallel form of the algorithm has been developed. The newly developed parallel SHASTA has been implemented in the *Open Compute Language* (OpenCL). The usage of OpenCL guarantees the vendor and architecture independence of the simulation code. Additionally to the tremendous speedups that can be achieved with accelerators such as GPUs, the implementation can still be executed on any commodity CPU present in the user community of UrQMD.

With this redesign, the hydrodynamic phase in the simulation model could be accelerated by almost a factor of 500 for a typical simulation scenario. This allows for better statistics, enhanced event-by-event analyses, and unprecedented stability studies of the simulation models. Specially under the light of the upcoming experiments at the FAIR facility a better statistical basis is of highest importance.

Related publication in 2012:

1) J. Gerhard, V. Lindenstruth, M. Bleicher, *Relativistic Hydrodynamics on Graphic Cards*, Comput. Phys. Commun., accepted for publication

Development of Computer Tools for Graphical Processors

Collaborators: A.V. Yakubovich[1], G.B. Sushko[1], A.V. Solov'yov[1], S. Schramm[2]

[1] MBN@FIAS, [2] FIAS

Short description: The aim of developing a code for GPU-based calculations is to exploit the advantages of a novel superiorly fast computational devices - special graphical cards available at novel supercomputer center LOEWE-CSC. The numerical solution of the MD equations becomes a challenging task if one studies systems with a large number of atoms. As the force calculation essentially implies the same type of calculation repeated many times over, this task is ideally suited to be implemented using a parallel-programming approach. If there are only few different types of forces involved, a single-instruction multiple-data (SIMD) hardware environment can be adopted in a natural way, since the same instructions are used for all pairs of particles. GPUs fulfil these requirements in an ideal way.

Main results:

We have developed a software code in order to get use of GPU facilities. The code includes a specific force fields for modeling the carbon-based materials, metal clusters and carbon-metal systems, treating composite alloys of transition metals. The code is written using OpenCL technology, which provides portability across different types of GPUs and other types of computing units.
During this year different properties of metallic clusters were studied using the code. The speed-up of a MD simulations of nickel clusters of different sizes comparing the CPU and GPU versions of the code can be up to two orders of magnitude (see Fig. 1). These results are consistent with theoretical estimation of performance of GPU and CPU in single precision.

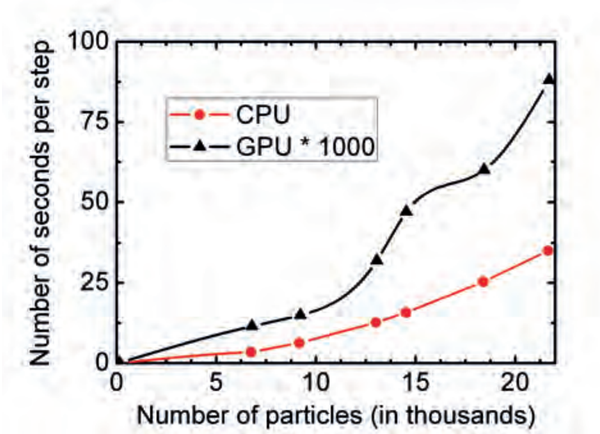


Fig. 1. Performance of the OpenCL version of the code as compared to the conventional CPU version. For systems consisting of more that 1 thousand of particles the computational advantage of the OpenCL version can be more than 100 times.

Related publication in 2012:

1. Alexander V. Yakubovich, Gennady Sushko, Stefan Schramm, Andrey V. Solov'yov: *Kinetics of liquid-solid phase transition in large nickel clusters*, Phys. Rev. B (2012) (submitted) (http://xxx.lanl.gov/arXiv:1210.3559v1 [physics.comp-ph])

Transmission needs in an increasingly renewable European power system

Collaborators: S. Becker[1], R. A. Rodriguez[2], G. B. Andresen[2], M. Greiner[2], and S. Schramm[1]

[1] Frankfurt Institute for Advanced Studies, [2] Department of Mathematics and Aarhus School of Engineering, Aarhus University, Denmark

We have investigated the effects of an increasing share of variable renewable energy sources (VRES), namely wind and solar photovoltaics, on the electric power transmission needs across Europe. The weather-caused fluctuation of VRES production can in part be mitigated by smoothing in out in space, i.e. power transmission. This requires an upgrade of the existing power grid, see the figure below.

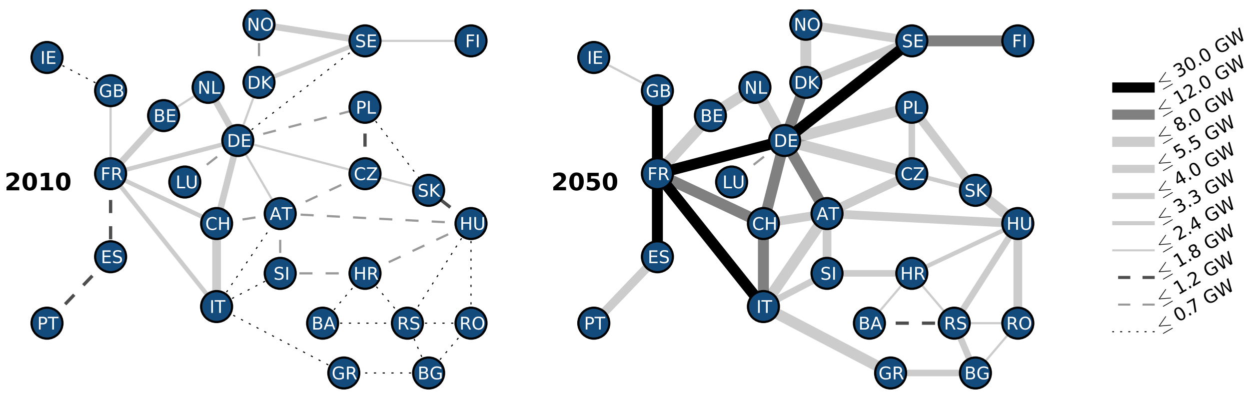
The mismatch Δ at each node, at time t in the network can be expressed as:

$$\Delta_n(t) = \gamma_n \left(\alpha_n^{\mathrm{W}} \frac{G_n^{\mathrm{W}}(t)}{\langle G_n^{\mathrm{W}} \rangle} + (1-\alpha_n^{\mathrm{W}}) \frac{G_n^{\mathrm{S}}(t)}{\langle G_n^{\mathrm{S}} \rangle} \right) \cdot \langle L_n \rangle - L_n(t)\,, \tag{1}$$

where G_n^{W} is the wind generation time series, G_n^{S} is the solar generation, and L_n the load. The generation time series were computed on the basis of real, high resolution weather data, and the load data are historical. These mismatches are reduced as far as possible by import and export, and if an uncovered load remains afterwards, it is assumed to be covered by a backup system.

To model the growth of VRES installations, we obtained historical data as well as 2020 targets. For 2050, we assumed a gross share of VRES such that they cover the load, on average ($\gamma = 1$ in Eq. (1)). To these data, logistic growth curves were fitted.

In order to quantify the transmission needs, we set a target of a reduction in backup energy by 90 % of what is achievable by transmission. The flow on the network is calculated using the DC power flow paradigm. It has the advantage of minimizing dissipation, and yields lower bounds on the necessary flows. The line capacity upgrades are distributed across the links by setting each line capacity to a fixed quantile of the unconstrained flow. In this way, we arrive at the transmission line capacities shown below, which amount to roughly four times of today's total installed transmission capacities.



Topology of the European electricity network, as it is today (left), and as we predict it to be necessary in 2050 (right). Line thickness and linestyle indicate link capacity. Node size and positions are not to scale.

5. Talks and Publications

Conference and Seminar Talks by FIAS Members 2012

Jaan Aru

– Institute of Neurobiology, Free University Berlin, 22 Feb. 2012: *Scientific study of consciousness: where do we stand?*
– Technology, Entertainment, Design Conference (TEDx) Tallinn, 4. May 2012: *Why brain activity feels like something*
– Estonian Physics Society, Tallinn, 28. July 2012: *Brain science without a brain*
– Donders Discussions, Nijmegen, Netherlands, 25. Oct. 2012: *Distilling the neural correlates of conscious perception*
– Estonian Skeptics Society, Tallinn, 12 Dec. 2012: *The relationship between the brain and our subjective experience*

Maximilian Attems

– Xth Quark Confinement and the Hadron Spectrum, Munich, Germany, 8 Oct. 2012: *Longitudinal thermalization via the chromo-Weibel instability*
– High energy physics seminar, Bielefeld University, Gemany, 6 Nov. 2012: *Chromo-Weibel instabilities in Bjorken expansion*
– Second Norwegian Winter Workshop on QCD in Extreme Conditions, Trondheim, Norway, 14 Dec. 2012: *Longitudinal Thermalization via the Chromo-Weibel Instability*

Elena Bratkovskaya

– 50th International Winter Meeting on Nuclear Physics, Bormio, Italy, 22-27 January 2012: *In-medium effects on strangeness and dilepton production*
– Workshop on "Hadronic resonance production in elementary and heavy ion collisions", Austin, USA, 5-7 March 2012: *Resonances from PHSD*
– 28th Winter Workshop on Nuclear Dynamics, Dorado del Mar, Puerto Rico, USA, 7-14 April 2012: *Dilepton production from SIS to LHC energies*
– Bilateral FAIR–JINR-NICA Workshop "Matter at highest baryon densities in the laboratory and in space", Frankfurt, Germany, 2-4 April 2012: *Dynamics of the QGP in relativistic heavy-ion collisions*
– Workshop on Relaxation, Turbulence, and Non-Equilibrium Dynamics of Matter Fields (RETUNE 2012), Heidelberg, Germany, 21-24 June 2012: *Off-shell dynamical approach for relativistic heavy-ion collisions*
– Workshop "Study of the Baryonic Matter at Nuclotron" (BM@N) JINR, Dubna, Russia, 31 July - 1 August 2012: *Properties of dense and hot nuclear matter*
– 11th International Conference on Hypernuclear and Strange Particle Physics (HYP2012) Barcelona, Spain, 1-5 October 2012: *Antikaons in matter*
– 5th International Workshop on heavy quark production in heavy-ion collisions, Utrecht, The Netherlands, 14-17 November 2012: *'Open and hidden charm dynamics*
– International Workshop on Discovery Physics at the LHC (Kruger-2012), Kruger Gate, South Africa, 3-7 December 2012: *'The QGP dynamics in relativistic heavy-ion collisions'.*
– Workshop "Experimental data versus transport models", Munich, Germany, 17-18 December 2012: *Strangeness dynamics at SIS energies*

Zhenwen Dai

- 06/2012 Talk at the Conference of Computer Vision and Pattern Recognition (CVPR 2012), Providence, RI, USA, June 2012: *Autonomous Cleaning of Corrupted Scanned Documents - A Generative Modeling Approach*

Georgios Exarchakis

- 10th International Conference on Latent Variable Analysis and Source Separation (LVA/ICA 2012), 12 March 2012, Tel Aviv, Israel: *Ternary Sparse Coding*

Walter Greiner

- Advances in Astroparticle Physics and Cosmology 2012 (AAPCOS 2012), Darjeeling, India, 9 March 2012: *There are no black holes: Pseudocomplex general relativity*
- Third International Workshop “Crystalline Undulator and Related Phenomena”, St. Petersburg, Russia, 20-23 May 2012: *Strange matter and antimatter*
- Horizons of Innovative Theories, Experiments, and Supercomputing in Nuclear Physics (HITES2012), New Orleans, USA, 4 June 2012: *Extension of the Periodic System: Superheavy, Superneutronic, Superstrange Elements*
- International Summer School for Advanced Studies “Dynamics of open nuclear systems”, Predeal, Romania, 9 July 2012: *Nuclei: superheavy, superneutronic, -strange – and of antimatter*
- International Symposium on Exotic Nuclei (EXON 2012), Vladivostok, Russia, 2 October 2012: *How to create anti-nuclei and strange nuclei*
- Polytechnische Gesellschaft, Frankfurt, 30. October 2012: *Es gibt keine Schwarzen Löcher – Einsteins Relativitätstheorie neu formuliert*
- Fifth International Conference on Fission and Properties of Neutron-Rich Nuclei (ICFN5), Sanibel Island, Florida, USA, 9 November 2012: *There Are No Black Holes: Pseudo-Complex General Relativity – Review and Some Predictions*

Pasi Huovinen

- Helmholtz International Summer School “Dense Matter in Heavy-Ion Collisions and Astrophysics” (DM 2012), Dubna, Russia, 28 Aug. - 8 Sept. 2012: *Hydrodynamics of heavy-ion collisions*
- VIII Workshop on Particle Correlations and Femtoscopy (WPCF-2012), Frankfurt, 10-14 Sept. 2012: *Dynamical freeze-out in event-by-event hydrodynamics*
- Xth Quark Confinement and the Hadron Spectrum, Garching, 8-12 Oct. 2012: *Decade of hydrodynamics – what have we learnt?*

Yurii Karpenko

- VIII Workshop on Particle Correlations and Femtoscopy (WPCF-2012), Frankfurt, 10-14 Sept. 2012: *Recent results from hHKM model: radial, elliptic flows and interferometry at RHIC and LHC*
- Young scientists conference “Modern Problems of Theoretical Physics”, Bogolyubov Institute for Theoretical Physics, Kyiv, Ukraine, 23-26 Oct. 2012: *Hydrokinetic model for heavy ion collisions at RHIC and LHC energies*
- European Research Group (GDRE) meeting, Joint institute for nuclear research (JINR), Dubna, Russian Federation, 12-14 Dec. 2012: *Status of viscous hydrodynamic algorithm development*

Andrei Korol

- 2nd International Workshop “Crystalline Undulator and Related Phenomena”, Western Cape, South Africa, 4-8 March 2012: *Feasibility of the crystalline undulator for a heavy projectile*

- 3rd International Workshop “Crystalline Undulator and Related Phenomena”, St. Petersburg, Russia, 20-23 May 2012: *On the feasibility of electron-, positron- and proton-based undulators at high energies*
- 2nd International Conference “Dynamics of Systems on the Nanoscale” (DySoN2012), St. Petersburg, Russia, 30 Sept. - 4 Oct. 2012: *Crystalline undulator as a source of coherent radiation*
- 4th International Workshop “Crystalline Undulator and Related Phenomena”, St. Petersburg, Russia, 4-5 Oct. 2012: *Novel computer code for channeling simulation as a part of the MBN Explorer package*

Volker Lindenstruth

- IT2Green Jahrestagung 2012, Berlin, 23 May 2012, *Effiziente Rechenzentren*
- International Supercomputing Conference, Hamburg, 19 June 2012, *The FAIR Green-IT Cube data center*
- Night of Science Frankfurt, Campus Riedberg, 22 June 2012, *Das Frankfurt Institute for Advanced Studies – Forschung und Perspektiven , Hochleistungsrechnen auf dem LOEWE-CSC in Frankfurt*

  26.06.2012 Goethe Universität - Herausforderungen und Antworten, Frankfurt, Campus Westend, 22 June 2012, *Green-IT - Höchstleistungsrechner mit Kleinstverbrauch*
- Herbsttreffen des ZKI Arbeitskreises Supercomputing, Düsseldorf, 20 Sept. 2012, *MiniCube Rechenzentrum der GSI*
- International Workshop on Technology and Innovation (EPS-TIG), Erice, Italy, 24 Oct. 2012, *High Performance Computer*

Luca Lonini

- DGR-Tage 2012, Technical Univerisity Berlin, 6-7 September 2012: *Learning efficient representations of stereo-disparity perception and vergence movements using the iCub robot*

Jörg Lücke

- Dept. of Computer Science, University of Bonn, Germany, December 2012: *Unsupervised Learning for Computer Vision – Linear, Non-linear and Occlusive Components*
- Workshop on Image-based Systems Biology, German Conference on Bioinformatics 2012, Jena, Germany: *Representational Approaches for the Analysis of Microscopy Images*

Igor Mishustin

- NICA-FAIR Bilateral Workshop “Matter at highest baryon densities in the laboratory and in space”, Frankfurt, 2-4 April 2012: *Non-equilibrium phase transitions in expanding matter*
- 2nd International Symposium on Non-equilibrium Dynamics (NeD-2012) and 3rd Network Workshop on Theory of Ultra-Relativistic Heavy Ion Collisions (TURIC-2012), Hersonissos, Crete, Greece, 25-30 June 2012: *Non-equilibrium phase transitions in nuclear collisions*
- International Workshop “Strangeness in Nuclei”, ECT*, Trento, Italy, 15-19 Oct. 2012: *Hypernuclei production in relativistic nuclear collisions*
- International Workshop “Nuclear Equation of State for Supernovae and Compact Stars”, Frankfurt, 28-30 Nov. 2012: *Microscopic modeling of supernova matter*

Piero Nicolini

- Seminar talk at Max-Planck-Institut für Radioastronomie, Bonn, Germany, March 2012: *Beyond classical black hole spacetimes*
- Seminar talk at Universita degli Studi di Perugia, Perugia, Italy, March 2012: *Phenomenology of quantum black holes*

- COST Action MP0905 Black holes in a violent universe – 5th COST action meeting, Valletta, Malta, 24 April 2012: *Black holes meet quantum mechanics*, plenary talk
- Perspectives of Fundamental Cosmology - NORDITA, Stockholm, Sweden, 26. Nov. 2012: *Cosmological production of black hole pairs*, plenary talk
- 13th Marcel Grossmann Meeting, Stockholm, Sweden, 2012: *Production and evaporation of Planck scale black holes at the LHC*
- DPG-Frühjahrstagung, Fachverbände Gravitation und Relativitätstheorie, Göttingen, Germany, 2012: *Phenomenology of quantum gravity black holes*
- DPG-Frühjahrstagung, Fachverbände Gravitation und Relativitätstheorie, Göttingen, Germany, 2012: *Gravitational objects in the presence of a minimal length*

Vitalii Ozvenchuk

- 3rd Network Workshop of the European Network TURIC, Hersonissos, Crete, Greece, 25-30 June 2012: *Dynamical equilibration of strongly-interacting infinite parton matter*
- Conference of Young Scientists, Modern Problems of Theoretical Physics, Kyiv, Ukraine, 23-26 October 2012: *Dynamical equilibration of strongly-interacting 'infinite' parton matter*
- International Workshop on Hot and Dense Nuclear and Astrophysical Matter, Johannesburg, South Africa, 26-30 November 2012, *Dynamical equilibration and transport coefficients of strongly-interacting 'infinite' parton matter*

Daniela Pamplona

- 12th Annual Meeting of the Vision Sciences Society Meeting, Naples, USA, 12-16 May: *The statistics of looking: Deriving properties of retinal ganglion cells across the visual field*
- VISLAB, Institute for Systems and Robotics, Lisbon, Portugal, 24 July 2012: *The statistics of looking*, invited talk

Dorin Poenaru

- 4th International Conference on Current Problems in Nuclear Physics and Atomic Energy (NPAE-Kyiv2012), Kyiv, Ukraine, 3-7 Sept. 2012: *Cluster radioactivity and alpha decay of superheavy nuclei*
- 10th International Conference on Clustering Aspects of Nuclear Structure and Dynamics, Debrecen, Hungary, 24-28 Sept. 2012: *Heavy-particle radioactivity*
- Fifth International Conference on Fission and Properties of Neutron Rich Nuclei, Sanibel Island, Florida, USA, 4-10 Nov.2012: *Cluster decay of the heaviest superheavy nuclei*
- 2nd European Nuclear Physics Conference (EuNPC 2012), Bucharest, 17-21 Sept. 2012: *Alpha- and cluster decays of superheavy nuclei*

Viola Priesemann

- National Institute of Mental Health, Washington DC, USA, 23 Oct. 2012: *Neuronal avalanches change from wakefulness to deep sleep – A study of intracranial depth recordings in humans*
- University of Sussex, Brighton, UK, 27 Sept. 2012: *Organization principles of spontaneous neural activity from wakefulness to deep sleep – A study of intracranial depth recordings in humans*
- Conference "Systemic Risk: Economists Meet Neuroscientists", Frankfurt, Germany, 17 Sept. 2012: *Stability in self-organized networks*

Igor Pshenichnov

- XIII International Seminar on Electromagnetic Interactions of Nuclei, Moscow, Russia, 20-23 Sept. 2012: *Electromagnetic fragmentation of nuclei at heavy-ion colliders*

- 39th Annual Meeting of the European Radiation Research Society, Vietri sul Mare, Italy, 15-19 Oct. 2012: *Geant4 calculations of microdosimetric variables for neutrons and light nuclei in tissue-like materials*

Dirk Rischke

- Seminar talk at Helsinki University, Helsinki, Finland, 24 Feb. 2012: *Recent results from chiral effective models*
- Seminar talk at Yale University, New Haven, USA, 3 April 2012: *Recent results from chiral effective models*
- Seminar talk at Columbia University, New York, USA, 4 April 2012: *Recent results from chiral effective models*
- Seminar talk at Brookhaven National Laboratory, New York, USA, 6 April 2012: *Recent results from chiral effective models*
- 28th Winter Workshop on Nuclear Dynamics "WWND 2012", Dorado del Mar, Puerto Rico, 10 April 2012: *Recent results from chiral effective models*
- Conference "The physics and astrophysics of compact stars", Papeete, Tahiti, 4-8 June 2012: *Crystalline nuclear matter in a chiral effective model?*
- Quark Matter 2012, Washington, D.C., USA., 1-18 Aug. 2012: *Global Variables and Correlations*, invited talk, co-rapporteur (with B. Hippolyte)
- Final Colloquium GRK 881, Bielefeld, Germany, 12-14 Sept. 2012: *Fluid dynamics: theory and applications in heavy-ion physics*, invited talk
- Int. School of Nuclear Physics "Probing the Extremes of Matter with Heavy Ions", Erice, Sicily, 16-24 Sept. 2012: *Constructing and validating a chiral effective model for dilepton production in NN and AA collisions*
- Xth Conf. on "Quark Confinement and the Hadron Spectrum", Munich, Germany, 8-12 Oct. 2012: *The long-wavelength limit of the Boltzmann equation: recent insights in deriving dissipative relativistic fluid dynamics*
- Int. Workshop on "Discovery Physics at the LHC, Kruger 2012", Kruger Gate, South Africa, 3-7 Dec. 2012: *The long-wavelength limit of the Boltzmann equation: recent insights in deriving dissipative relativistic fluid dynamics*, invited talk

Constantin Rothkopf

- Center for Interdisciplinary Research, University of Bielefeld, Germany, 13 Nov. 2012: *Competition and priority control in mind and brain: new perspectives from task-driven vision*
- Department of Psychology at the University of Hong Kong, Hong Kong, 11 Oct. 2012, invited talk
- OCCAM conference, Osnabrück, Germany, 4-6 June 2012: *Visuomotor behavior in naturalistic tasks: from receptive fields to value functions*
- Computational and Biological Learning Lab, University of Cambridge, Cambridge, UK, 3 May 2012, invited talk
- Department of Cognitive Science, University of Osnabrück, Osnabrück, Germany, 1 Feb. 2012, invited talk

Chiriro Sasaki

- NICA/JINR-FAIR Bilateral Workshop "Matter at highest baryon densities in the laboratory and in space", Frankfurt, 2-4 April 2012: *Chiral Thermodynamics of Dense QCD – Baryons, Glueballs and Polyakov loops*.

- Third Year of APCTP-WCU Focus program "From dense matter to compact stars in QCD and in hQCD", APCTP Headquarter, Pohang, Korea, 9-18 April 2012; *Baryons at High Density and the Role of the Dilaton – Chiral Symmetry Breaking and Trace Anomaly* (invited talk)
- Hanyang University, Korea, 24 April 2012: *Hidden Local Symmetry in Medium with DLFP from Nuclei to Dense Matter* (seminar talk)
- Symposium for the 40th Anniversary of Devision of Nuclear Physics of the Korean Physics Society, Daejong, Korea, 26 April 2012: *Dense Hadronic Matter in Chiral Approaches* (invited talk).
- Yukawa Institute for Theoretical Physics, Kyoto, Japan, 15 May 2012: *Baryons at High Density and the Role of the Dilaton – Chiral Symmetry Breaking and Trace Anomaly* (seminar talk)
- Helmholtz-Institut für Strahlen- und Kernphysik, Universität Bonn, Bonn, Germany, 19 June 2012: *Baryons at High Density and the Role of the Dilaton – Chiral Symmetry Breaking and Trace Anomaly* (seminar talk)
- The 2nd International Symposium on Non-equilibrium Dynamics (NeD-2012) and the 3d Network Workshop on Theory of Ultrarelativistic Heavy Ion Collisions (TURIC-2012), Hersonissos, Crete, Greece, 25-30 June 2012: *Trace Anomaly, Chiral Symmetry Breaking and Baryons at High Density* (invited talk).
- Xth Quark Confinement and the Hadron Spectrum, TUM, Garching, German, 8-12 Oct. 2012: *Effective Gluon Potential and Yang-Mills Thermodynamics*

Stefan Schramm

- Advances in Astroparticle Physics and Cosmology (APCOS) in Darjeeling, India, 11 March 2012: *Properties of Compact Stars and Hot and Dense Matter in Quark-Hadron Models*
- HyperoNS 2012, Copernicus Astronomical Center, Warsaw, Poland, 22 Nov. 2012: *Modeling Hybrid Stars*
- Compact Stars in the QCD Phase Diagram III (CSQCD III), Guarujá, Sao Paulo, Brazil, 13 Dec. 2012: *Modeling Hybrid Stars in Quark-Hadron Approaches*

Wolf Singer

- IBRO International Workshop 2012, Szeged, Hungary, 19-21 Jan. 2012: *Janos Szentagothai Memorial Lecture: The dynamcial brain: In the footsteps of Janos Szentagothai*
- Studium Generale: "Grenzüberschreitungen – der Mensch im Spannungsfeld von Biologie, Kultur und Technik", Universität Tübingen, 2 February 2012: *Widersprüche zwischen Intuition und neurobiologischer Erkenntnis*
- Winter Conference on Neural Plasticity, 24th Annual Meeting, St. Kitts, Caribbean, 11-18 Feb. 2012: *The role of brain rhythms in cognition: Dynamic coordination of functional networks in the cortex*
- Veranstaltungsreihe "Neuronen – Lernen – Handeln", Stiftung Brandenburger Tor, Berlin, Germany, 18 April 2012: *Wie Wissen in den Kopf kommt – Was bieten die Neurowissenschaften der Pädagogik?*
- International Symposia for Contemplative Studies, Denver, Colorado, 26-29 April 2012: *The Nature of Consciousness: Contemplative, Neuroscientific, and Philosophical Perspectives* (Keynote Address)
- Transylvanian Experimental NeuroscienceSummer School (TENSS 2012), Pike Lake, Romania, 8 June 2012: *Coding Strategies (Rate versus Synchrony – temporal coding)*
- ZNZ Annual Symposium "Neural Plasticity and Repair, from basic Neuroscience to Therapy", Zurich, Switzerland, 14-15 June 2012: *Complexity and dynamics: the great challenges in neuroscience*
- Montreal Neurological Institute, Montreal, Canada, 3 July 2012: *Time Codes Space in Cortical Processing*
- ICS Summer School in Cognitive Sciences, Montreal, Canada, 5 July 2012: *Consciousness: Unity in Time Rather Than Space?*

- Gordon Research Conference “Neurobiology of Cognition”, Lucca, Italy, 8 July 2012: *Dynamic Coordination of Functional Networks in the Cerebral Cortex: Mechanisms, Development and Psychiatric Diseases* (Keynote Address)
- Symposium “Attention across Disciplines”, Mainz, 16 July 2012: *Perception, an Active Attention Dependent Process*
- 16th world congress of psychophysiology, Pisa, Italy, 13-17 Sept. 2012: *What binds it all together? Temporal coordination of neural responses in normal and pathological cognition*, (Keynote Address)
- 5th International Symposium on Schizophrenia, Göttingen, Germany, 21 Sept. 2012: *Disturbed Temporal Coordination of Distributed Cortical Processes as an Endophenotype of Schizophrenia*
- Symposium in Honor of Marc Jennerod, Lyon, France, 28-30 Oct. 2012: *Top-down causation – One of Marc’s legacies*
- The Pontifical Academy of Sciences: Plenary Session on Complexity and Analogy in Science, Vatican City, 5-10 Nov. 2012: *Gradual Increases in Complexity Lead to the Emergence of Novel Principles of Information Processing: The Cerebral Cortex as an Example*
- Katholische Akademie Bayern, München, Germany, 23-24 Nov. 2012: *Komplexität, Modularität und Synchronisation im menschlischen Gehirn und deren Bedeutung für das Menschenbild*
- Interdisziplinärer Workshop “Unser Bild vom Handeln: Aktuelle Kontroversen in Neurowissenschaft und Philosophie”, Münster, Germany, 3. Dec. 2012: *Neurobiologische Anmerkungen zur Bedingtheit von Entscheidungen*

Andrey V. Solov’yov

- The General Kick-Off Meeting of the EU FP7 ViNaT Project, Technical University of Denmark, Roskilde, Denmark, January 2012
- Toulouse-Frankfurt Workshop on QCMD, Toulouse, France, February 2012
- Workshop on Nano-IBCT data base development (COST Action MP1002 Nanoscale insights into Ion Beam Cancer Therapy), Vienna, Austria, 24-26 February 2012: *COST action NANO-IBCT and data needs for multiscale modeling of radiation damage and nanodosimetry*
- 2nd International Workshop “Crystalline Undulator and Related Phenomena”, Western Cape, South Africa, 4-8 March 2012: *Crystalline undulator based Gamma-laser: Current status and perspectives*
- Department of Physical Sciences, The Open University, Milton Keynes, United Kingdom, April 2012
- Department of Applied Mathematics and Theoretical Physics, Queen’s University of Belfast, Belfast, United Kingdom, May 2012
- 3rd International Workshop “Crystalline Undulator and Related Phenomena”, St. Petersburg, Russia, 20-23 May 2012: *Crystalline undulator and crystalline undulator based Gamma-laser: Current status and perspectives*
- 12th International Workshop on Radiation Damage to DNA, Prague, Czech Republic, 2-6 June 2012: *Molecular level assessments of radiation biodamage: multiscale approach*
- 2nd General Meeting of EU FP7 ViNaT project, University of Science and Technology “MISIS”, Moscow, Russia, June 2012
- Second European Conference on Nanofilms (ECNF 2), Ancona, Italy, 17-22 June 2012
- The First International Workshop on NanoRadiation Chemistry (NaRaC-1), Belfast, United Kingdom, July 2012: *Multiscale modeling of radiation effects*
- French Academy of Sciences, Paris, France, July 2012
- 3rd International Conference Dubna-Nano 2012, Dubna, Russia, 9-14 July, 2012: *The multiscale physics of nanostructures self-assembling*

- International Conference on Many Particle Spectroscopy of Atoms, Molecules, Clusters and Surfaces (MPS 2012), Berlin, 28 August 2012: *Present status of the discussion on occurrence of plasmons in fullerenes*
- COST MPNS 6th annual progress conference (APC), Dublin, Ireland, September 2012
- 2nd International Conference "Dynamics of Systems on the Nanoscale" (DySoN2012), St. Petersburg, Russia, 30 Sept. - 4 Oct. 2012: *Dynamics of systems on the nanoscale: challenges for theory and experiment*
- 4th International Workshop "Crystalline Undulator and Related Phenomena", St. Petersburg, Russia, 4-5 Oct. 2012: *Current status of the crystalline undulator investigations*
- International Conference "Problems of Theoretical Physics", Kiev, Ukraine, 8 Oct. 2012: *Radiation damage in biomolecular systems: multiscale approach*
- Nano-IBCT workshop on quantum scattering calculations and Monte Carlo simulations of radiation damage Madrid, Spain, 7-9 Nov. 2012: *Multiscale physics of ion induced radiation damage*
- Australian Institute of Physics Congress, Syndey, Australia, Dec. 2012
- Micro-, Mini- and Nano- Dosimetry & International Prostate Cancer Treatment Workshop, Wollongong, Australia, 6 Dec. 2012: *Nanoscale Insights into Ion]Beam Cancer Therapy: Multiscale Approach*

Jochen Triesch

- Gaze Bias Learning – Linking neuroscience, computational modeling, and cognitive development, London, UK, 23-24 Jan. 2012: *Looking for Reward: From Gaze Following to Gaze Contingency*
- Kyutech-FIAS Joint Workshop on Brain System Technology: From Brain to Technology, Kyushu Institute of Technology, Japan, 8 Feb. 2012: *Let it learn!*
- Nonlinear Dynamics in Complex Neural Architectures, Lyon, France, 29-31 March 2012: *Self-Organization in recurrent neural networks*
- Max-Planck Institute for Mathematics in the Sciences, Leipzig, Germany, 15 March 2012: *Self-Organization and unsupervised learning in recurrent networks*
- Bernstein Conference on Computational Neuroscience, Munich, Germany, 12-14 Sept. 2012: *Self-Organization and unsupervised learning in recurrent networks*
- Hong Kong University of Science and Technology, Hong Kong, China, 5 Oct. 2012: *Self-Organization and unsupervised learning in recurrent networks*
- Int. Conf. on Development and Learning and Epigenetic Robotics, San Diego, USA, 7-9 Nov. 2012: *Infants in Control: Rapid Anticipation of Action Outcomes in a Gaze-Contingent Paradigm*
- Int. Conf. on Development and Learning and Epigenetic Robotics, San Diego, USA, 7-9 Nov. 2012: *Network Self-Organization*

Alexey Verkhovtsev

- 2nd International Conference "Dynamics of Systems on the Nanoscale" (DySoN2012), St. Petersburg, Russia, 30 Sept. - 4 Oct. 2012: *Study of collective electron excitations in fullerenes*
- VAMDC Regional workshop on atomic and molecular data, Belgrade, Serbia, 14-16 June 2012: *Development of the RADAM database*

Alexander Yakubovich

- Workshop on Nano-IBCT data base development (Nanoscale insights into Ion Beam Cancer Therapy), Vienna, Austria, 24-26 February 2012: *RADAM database development perspectives*
- VAMDC Regional Workshop on Atomic and Molecular Data, Belgrade, Serbia, 14-16 June 2012: *Development of the RADAM database*

- Second European Conference on Nanofilms (ECNF 2), Ancona, Italy, 17-22 June 2012: *Laser-induced acoustic desorption of lysine amino acids*
- 2nd General Meeting of EU FP7 Virtual Nanotitanium (ViNaT) Project, Moscow, Russia, 6-7 June 2012
- The First International Workshop on NanoRadiation Chemistry (NaRaC-1), Belfast, United Kingdom, 28-29 June 2012: *The RADAM database: future plans and data needs*
- 2nd International Conference “Dynamics of Systems on the Nanoscale” (DySoN2012), St. Petersburg, Russia, 30 Sept. - 4 Oct. 2012: *Diffusion and nanoindentation processes in titanium and nickel materials*
- Nano-IBCT Workshop on Quantum Scattering Codes and Monte-Carlo Simulations to Model Dynamical Processes in Biosystems (QSMC 2012), Madrid, Spain, 7-9 November 2012: *Thermomechanical mechanism of damage of biomolecules by the heavy ions*
- Nano-IBCT Workshop on Quantum Scattering Codes and Monte-Carlo Simulations to Model Dynamical Processes in Biosystems (QSMC 2012), Madrid, Spain, 7-9 November 2012: *Development of the RADAM database*
- Micro- Mini- and Nano- Dosimetry & International Prostate Cancer Treatment Workshop, Wollongong, Australia, 6 Dec. 2012: *DNA Damage by shockwaves produced by heavy ions*

FIAS conference abstracts and posters 2012

Symposium on New Developments in NMR and Conference of the National Magnetic Resonance Society

5-8 Feb. 2012, NMR Research Centre Indian Institute of Science, Bangalore

- P. Güntert, *Reliable and Flexible Automated Assignment with CYANA*

COSYNE - Computational and Systems Neuroscience

23-26 February 2012, Salt Lake City, Utah, USA

- C. A. Rothkopf, P. Schrater, *Optimally adapting heuristics: humans quickly abandon the constant bearing angle strategy*, abstract II-2
- Catalin V Rusu, Ulf Ziemann, Jochen Triesch, *A Model of I-Wave Generation during Transcranial Magnetic Stimulation (TMS)*, abstract II-99
- Juan Florez Weidinger, Wolfgang Keil, Dmitry Tsigankov, Michael Schnabel, Matthias Kaschube, Fred Wolf, *Active self-organization of disordered arrangements of orientation preference in cortical networks*, abstact III-25

Workshop on Nano-IBCT data base development (Nanoscale insights into Ion Beam Cancer Therapy)

24-26 February 2012, Vienna, Austria

- Matthias Hanauske, Alexander V. Yakubovich, Andrey V. Solov'yov, *Ion beam cancer therapy and scientific data infrastructure for simulation methods*
- Andrey V. Solov'yov, *COST action NANO-IBCT and data needs for multiscale modeling of radiation damage and nanodosimetry*
- A.V. Yakubovich1, E. Surdutovich, A.V. Solov'yov, *Multiscale approach: a theoretical tool for understanding radiation damage*

53rd Experimental Nuclear Magnetic Resonance Conference ENC2012

15-20 Apr. 2012, Miami, Florida

- Victor Jaravine, Suhas Tikole, Vladimir V. Rogov, Alexis Rozenknop, Frank Löhr, Volker Dötsch, Peter Güntert, *Fast Hyper-Dimensional NMR Spectroscopy of Short-Lived Biological Samples*, Abstract 197
- Suhas Tikole, Victor Zharavin, Peter Güntert, *Peak Identification Using Nonnegative Matrix Decomposition in Hyper Dimensional NMR Spectra*, Abstract 073

COST Action MP0905 Black holes in a violent universe – 5th COST action meeting

Valletta, Malta, 24-26 April 2012

- A. M. Frassino and P. Nicolini, *Remarks on the black string and alternative black objects*

Photonics Europe 2012, Conference 8432: Semiconductor Lasers and Laser Dynamics

16-19 April 2012, Brussels, Belgium

- O. D'Huys, L. Lean, R. Vicente, J. Danckaert, I. Fischer, *Dynamical properties of two delay-coupled lasers: on spectra, correlations, and synchronisation*, Proc. SPIE 8432, Semiconductor Lasers and Laser Dynamics V, 843215

12th Annual Meeting of the Vision Sciences Society Meeting

11 - 16 May 2012, Naples, FL, USA

- G. Diaz, J. Cooper, C. Rothkopf, M. Hayhoe, *Internal Models for Predictive Saccades In a Natural Interception Task*, Journal of Vision 12 (2012) 606
- D. Pamplona, J. Triesch, C.A. Rothkopf, *The statistics of looking: Deriving properties of retinal ganglion cells across the visual field*, Journal of Vision 12 (2012) 771
- B. Sullivan, L. Johnson, C. Rothkopf, D. Ballard, M. Hayhoe, *The effect of uncertainty and reward on fixation behavior in a driving task*, Journal of Vision 12 (2012) 1259

12th International Workshop on Radiation Damage to DNA

2-6 June 2012, Prague, Czech Republic

- A.V. Solov'yov: *Molecular level assessments of radiation biodamage: multiscale approach*, Book of abstracts L30

Second European Conference on Nanofilms (ECNF 2)

17-22 June 2012, Ancona, Italy

- A. Yakubovich, A.V. Solov'yov, *Solid-liquid phase transition in large metallic clusters*, Poster
- I. Solov'yov, V.V. Dick, A. Yakubovich, A.V. Solov'yov, *Nanoscale surface pattern formation*, Poster

1st Summer School on Thunderstorm Effects on the Atmosphere-Ionosphere System (TEA-IS)

17-22 June 2012, Torremolinos, Malaga, Spain

- A. Drozdov, A. Grigoriev, Yu. Malyshkin, *Neutron component of the radiation dose related to thunderstorm activity*, p. 146

16th annual meeting of the Association for the Scientific Study of Consciousness (ASSC16)

2-6 July 2012, Brighton, UK

- Jaan Aru, *Distilling the NCC: do local gamma band responses in visual cortex reflect conscious experience?*

8th FENS Forum of Neuroscience

14-18 July 2012, Barcelona, Spain

- N. G. Jaehner, C. A. Rothkopf, S. Voegler, J. Triesch, R.A.W. Galuske, *Topographic and functional organization of feedback axons from the middle suprasylvian sulcus to primary visual cortex in the cat*, Poster 39.38
- M. Kaschube, A. Sederberg, D. Tsigankov, *Generating a diverse repertoire of receptive fields in mouse visual cortex*, Poster 39.39

International Conference on Many Particle Spectroscopy of Atoms, Molecules, Clusters and Surfaces (MPS 2012)

28 Aug. - 1 Sept. 2012, Berlin,Germany

- A.V. Solov'yov, *Present status of the discussion on occurrence of plasmons in fullerenes*

Quark Matter 2012 International Conference,

13-18 August 2012, Washington DC, USA

- P. Huovinen, *Dynamical freeze-out in event-by-event hydrodynamics*, Poster
- H. Niemi, *Event-by-event distribution of azimuthal asymmetries in ultrarelativistic heavy-ion collisions*, Poster
- P. Rau, *Hadronic Resonance States in an Effective Chiral Model*
- D. Rischke, *A chiral effective theory for dilepton production in NN and AA collisions*

- G. Torrieri, *Scaling of high momentum harmonics: constraining energy loss models, and looking for opacity changes*
- G. Torrieri, *Theory and phenomenology of quarkyonic percolation of finite density QCD matter*
- H. van Hees, *Heavy-quark diffusion at the LHC within a UrQMD-hydrodynamical hybrid model*

Bernstein Conference 2012

12-14 September, Munich, Germany
- C. A. Rothkopf:, *Inferring human intrinsic rewards through inverse reinforcement learning*
- D. F. Pamplona, J. Triesch, C. A. Rothkopf, *Eyes are not cameras: Deriving properties of retinal ganglion cells from the natural input*
- Q. Wang, C. A. Rothkopf, J. Triesch, *Representations in a recurrent network model of motor sequence learning reveal unified view of procedural memory consolidation and structure learning*

16th World Congress of Psychophysiology

13-17 Sept. 2012, Pisa, Italy
- W. Singer *What binds it all together? Temporal coordination of neural responses in normal and pathological cognition*, Int. J. of Psychophysiology 85 (2012) 279

2nd International Conference "Dynamics of Systems on the Nanoscale" (DySoN2012)

30 Sept. - 4 Oct. 2012, St. Petersburg, Russia
- I.A. Solov'yov, A.V. Solov'yov, *Dynamics of nanofractal formation and fragmentation*, Book of abstracts p. 42-43
- P. de Vera, A.V. Solov'yov, I. Abril, R. Garcia-Molina, *Ionization of biomolecular targets by ion-impact: input data for radiobiological applications*, Book of abstracts p. 29
- A.V. Verkhovtsev, R.G. Polozkov, V.K. Ivanov, A.V. Solov'yov, *Photoionization of clusters and fullerenes*, Book of abstracts p. 47

11th Biannual Conference of the German Cognitive Society KogWis 2012

30 Sept. - 3 Oct. 2012, Bamberg
- Wanja Wiese and Thomas Metzinger, *Towards a Mereotopological Framework for the Unity of Consciousness*, Poster

International Conference "Problems of Theoretical Physics"

8 Oct. 2012, Kiev, Ukraine
- A.V. Solov'yov, *Radiation damage in biomolecular systems: multiscale approach*, Abstract O-15

39th Annual Meeting of the European Radiation Research Society

15-19 Oct. 2012, Vietri sul Mare, Italy
- N. Averbeck, O. Ringel, M. Herrlitz, B. Jakob, F. Tobias, M. Durante, G. Taucher-Scholz, *DNA end resection is required for the repair of complex lesions in human G1 cells*, Book of Abstracts, p. 150
- L. Burigo, I. Pshenichnov, I. Mishustin, *Influence of nuclear fragmentation on microdosimetry spectra from ^{4}He, ^{7}Li and ^{12}C beams in water*, Book of Abstracts, p.208
- I. Pshenichnov, L. Burigo, I. Mishustin, *GEANT4 calculations of microdosimetric variables for neutrons and light nuclei in tissue-like materials*, Book of Abstracts, p. 9

Fall Meeting of the APS Division of Nuclear Physics

24-27 Oct. 2012, Newport Beach, CA, USA
- R. Pokharel, S. Gavin, G. Moschelli, *Fluctuating Hydrodynamics Confronts the Rapidity Dependence of Transverse Momentum Fluctuations*, Bull. Am. Phys. Soc. 57 (2012) NB.00002

NANO-IBCT Workshop on "Quantum Scattering Codes and Monte Carlo Simulations to Model Dynamical Processes in Biosystems" (QSMC 2012)

7-9 Nov. 2012, Madrid, Spain
- P. de Vera, A.V. Solov'yov, I. Abril, R. Garcia-Molina, *Calculation of the energy spectra of secondary electrons emitted from ioin tracks in biological targets*, Book of abstracts p. 40

FIAS Publications 2012

In the following all publications from the year 2012 with at least one author quoting the FIAS affiliation are presented. The first listing collects the papers published in regular journals. In the second listing contributions to conference proceedings are displayed, as well as papers which have not (yet) been published in print, but are publicly available on a preprint server. Conference abstracts or posters are not included. A further section lists published books.

A. Journal publications

[1] K. Aamodt and others (ALICE collaboration), "Harmonic decomposition of two-particle angular correlations in Pb–Pb collisions at $\sqrt{s_{NN}} = 2.76$ TeV," *Phys. Lett.* **B708** (2012) 249–264, `arXiv:1109.2501 [nucl-ex]`.

[2] K. Aamodt and others (ALICE collaboration), "Particle-Yield Modification in Jetlike Azimuthal Dihadron Correlations in Pb-Pb Collisions at $\sqrt{s_{NN}} = 2.76$TeV," *Phys. Rev. Lett.* **108** (2012) 092301, `arXiv:1110.0121 [nucl-ex]`.

[3] B. Abelev and others (ALICE collaboration), "D_s meson production at central rapidity in proton–proton collisions at $\sqrt{s} = 7$ TeV," *Phys. Lett.* **B718** (2012) 279–294, `arXiv:1208.1948 [hep-ex]`.

[4] B. Abelev and others (ALICE collaboration), "Heavy flavour decay muon production at forward rapidity in proton–proton collisions at $\sqrt{s} = 7$ TeV," *Phys. Lett.* **B708** (2012) 265–275, `arXiv:1201.3791 [hep-ex]`.

[5] B. Abelev and others (ALICE collaboration), "Inclusive J/psi production in pp collisions at $\sqrt{s} = 2.76$ TeV," *Phys. Lett.* **B718** (2012) 295–306, `arXiv:1203.3641 [hep-ex]`.

[6] B. Abelev and others (ALICE collaboration), "J/psi polarization in pp collisions at $\sqrt{s} = 7$ TeV," *Phys. Rev. Lett.* **108** (2012) 082001, `arXiv:1111.1630 [hep-ex]`.

[7] B. Abelev and others (ALICE collaboration), "J/psi production as a function of charged particle multiplicity in pp collisions at $\sqrt{s} = 7$ TeV," *Phys. Lett.* **B712** (2012) 165–175, `arXiv:1202.2816 [hep-ex]`.

[8] B. Abelev and others (ALICE collaboration), "J/psi suppression at forward rapidity in Pb-Pb collisions at $\sqrt{s_{NN}} = 2.76$ TeV," *Phys. Rev. Lett.* **109** (2012) 072301, `arXiv:1202.1383 [hep-ex]`.

[9] B. Abelev and others (ALICE collaboration), "K^0_s-K^0_s correlations in pp collisions at $\sqrt{s} = 7$ TeV from the LHC ALICE experiment," *Phys. Lett.* **B717** (2012) 151–161, `arXiv:1206.2056 [nucl-ex]`.

[10] B. Abelev and others (ALICE collaboration), "Light vector meson production in pp collisions at $\sqrt{s} = 7$ TeV," *Phys. Lett. B* **710** (2012) 557–8, `arXiv:1112.2222 [nucl-ex]`.

[11] B. Abelev and others (ALICE collaboration), "Measurement of charm production at central rapidity in proton-proton collisions at $\sqrt{s} = 7$ TeV," *JHEP* **1201** (2012) 128, `arXiv:1111.1553 [hep-ex]`.

[12] B. Abelev and others (ALICE collaboration), "Measurement of charm production at central rapidity in proton-proton collisions at $\sqrt{s}$ =2.76 TeV," *JHEP* **1207** (2012) 191, `arXiv:1205.4007 [hep-ex]`.

[13] B. Abelev and others (ALICE collaboration), "Measurement of electrons from semileptonic heavy-flavour hadron decays in pp collisions at $\sqrt{s} = 7$ TeV," *Phys. Rev.* **D86** (2012) 112007, `arXiv:1205.5423 [hep-ex]`.

[14] B. Abelev and others (ALICE collaboration), "Measurement of event background fluctuations for charged particle jet reconstruction in Pb-Pb collisions at $\sqrt{s_{NN}} = 2.76$ TeV," *JHEP* **1203** (2012) 053.

[15] B. Abelev and others (ALICE collaboration), "Measurement of prompt J/ψ and beauty production cross sections at mid-rapidity in pp collisions at $\sqrt{s} = 7$ TeV," *JHEP* **11** (2012) 065, `arXiv:1205.5880 [hep-ex]`.

[16] B. Abelev and others (ALICE collaboration), "Measurement of the cross section for electromagnetic dissociation with neutron emission in Pb-Pb collisions at $\sqrt{s} = 2.76$ TeV," *Phys. Rev. Lett.* **109** (2012) 252302, `arXiv:1203.2436 [nucl-ex]`.

[17] B. Abelev and others (ALICE collaboration), "Multi-strange baryon production in pp collisions at $\sqrt{s} = 7$ TeV with ALICE," *Phys. Lett.* **B712** (2012) 309–318, `arXiv:1204.0282 [nucl-ex]`.

[18] B. Abelev and others (ALICE collaboration), "Neutral pion and η meson production in proton-proton collisions at $\sqrt{s} = 0.9$ TeV and $\sqrt{s} = 7$ TeV," *Phys. Lett.* **B717** (2012) 162–172, `arXiv:1205.5724 [hep-ex]`.

[19] B. Abelev and others (ALICE collaboration), "Pion, Kaon, and Proton Production in Central Pb–Pb Collisions at $\sqrt{s_{NN}} = 2.76$ TeV," *Phys. Rev. Lett.* **109** (2012) 252301, `arXiv:1208.1974 [hep-ex]`.

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[24] B. Abelev and others (ALICE collaboration), "Underlying event measurements in pp collisions at $\sqrt{s} = 0.9$ and 7 TeV with the ALICE experiment at the LHC," *JHEP* **1207** (2012) 116, `arXiv:1112.2082 [hep-ex]`.

[25] A. Alink, F. Euler, E. Galeano, A. Krugliak, W. Singer, and A. Kohler, "Auditory Motion Capturing Ambiguous Visual Motion," *Front. Psychology* **2** (2012) 391.

[26] A. Alink, F. Euler, N. Kriegeskorte, W. Singer, and A. Kohler, "Auditory Motion Direction Encoding in Auditory Cortex and High-Level Visual Cortex," *Human Brain Mapping* **33** (2012) 969–978.

[27] M. Alvioli, H. Holopainen, K. J. Eskola, and M. Strikman, "Initial state anisotropies and their uncertainties in ultrarelativistic heavy-ion collisions from the Monte Carlo Glauber model," *Phys. Rev.* (2012) 034902, `arXiv:1112.5306 [hep-ph]`.

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