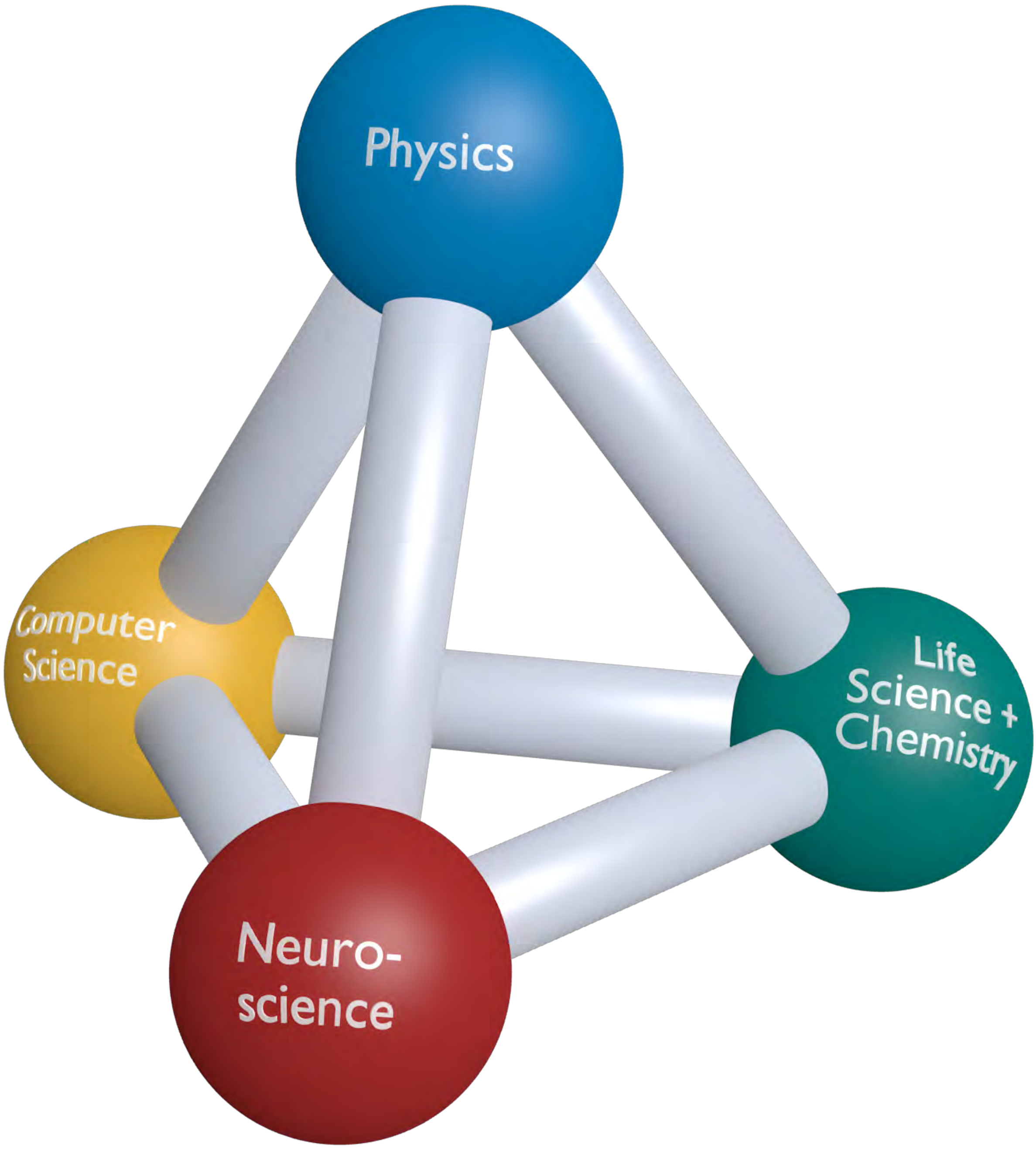
FIAS Frankfurt Institute for Advanced Studies



FIAS Scientific Report 2011

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Preface

The year 2011 has been a year of continuous development for the Frankfurt Institute for Advanced Studies. Scientists at FIAS have successfully continued to pursue their research in various branches of the natural sciences. There have been changes in personnel and in the funding situation, as outlined below, but no dramatic breakpoints. This Annual Report documents the scientific progress achieved in the past year through a collection of brief reports on individual research projects. In addition, important developments at cooperating institutions will be summarized, as well as colloquium schedules, conferences organized by FIAS, and the teaching activities in the framework of the Frankfurt International Graduate School for Science (FIGSS). The bibliography of publications by authors with FIAS affiliation, which complements the report, this time has been split into two parts, distinguishing between journal publications and conference reports/preprints.

Quite a number of leading scientists have either left or joined FIAS in 2011. In the field of physics, Fellow Paul Romatschke has left for a professorship at the University of Colorado, Boulder, CO and Junior Fellow Zhe Xu has become professor at one of the leading Chinese research universities, Tsinghua University in Beijing. A new arrival from Duke University, Durham, NC is Dr. Hannah Petersen who has won a grant to set up a Helmholtz Young Investigator Group. In the field of neuroscience a new Fellow has been appointed, Matthias Kaschube, who joined FIAS from Princeton University and also holds a new W2 professorship for Computational Neuroscience. A new Adjunct Fellow of FIAS is Prof. Visvanathan Ramesh who has accepted a W3 professorship for Software Engineering at the Department of Computer Science of Goethe University and has taken over as head of the Bernstein Focus Neurotechnology. Junior Fellow Gordon Pipa has been appointed to a professorship at the Institute of Cognitive Science at Osnabrück University.

The funding of FIAS to a large degree rests on external sources; therefore external reviews play an important role. In 2011 four major projects and collaborating institutions have undergone midterm evaluations. In the field of physics, the Helmholtz International Center for FAIR (HIC for FAIR) and the Extreme Matter Institute (EMMI) have been reviewed successfully and will receive substantial funding up to the year 2014 and 2013, resp. Also the program NanoBIC received a favorable evaluation and guarantees for continued funding from its backer, the Beilstein Institute. The Bernstein Focus Neurotechnology (BFNT) has received a mixed evaluation report. Presently BFNT is being restructured under the leadership of Prof. Ramesh, answering demands from the funding agency for a better integration of the various subprojects.

Several new research and collaboration projects have been started in 2011. FIAS is a member of the newly founded Nuclear Astrophysics Virtual Institute (NAVI) financed by the Helmholtz Association. Furthermore, FIAS will be at the center of a large international collaboration “Evaporation of microscopic black holes” (Principal Investigator: Dr. P. Nicolini) funded by a research grant from the German Research Foundation (DFG). The Meso-Bio-Nano Science team at FIAS (Prov. A.V. Solov’yov) coordinates the EU funded international COST Action Nano-IBCT (Nanoscale insights into ion beam cancer therapy). In the field of High Performance Computing, a Research and Development a contract with KACST (Saudi Arabia) has been signed with the intent to build a scalable HPC system prototype.

One long-standing problem of FIAS could not yet be resolved, i.e., the structural imbalance in favor of the branches of physics and neuroscience. In 2011 intense efforts were made to strengthen the branches of chemistry and/or life science, using the funds made available by the former president of the Board of Trustees, Dr. Helmut Maucher, and other sponsors. Twice a joint professorship was offered, in collaboration with Goethe University, to a high-profile scientist, first to a theoretical quantum chemist, then to a computational biologist. Unfortunately, in both cases competing offers from renowned institutions were given preference. FIAS will continue in its efforts to maintain and widen its broad interdisciplinary basis.

Research highlights 2011

Physics

To study *nonequilibrium phase transitions in relativistic heavy-ion collisions* the chiral fluid-dynamical approach was generalized to include dissipation and noise (Mishustin, Bleicher). The fluctuations of the order-parameter field were investigated in the dynamical environment. It is demonstrated that under such conditions the critical fluctuations associated with a second-order phase transitions are suppressed, while strong fluctuations associated with supercooling in the first-order phase transition survive.

In the group of I. Mishustin and W. Greiner a Geant4-based Monte Carlo model was developed to simulate spallation reactions in thick targets for Accelerator-Driven Systems (ADS). Using this model an efficient method of *destroying radioactive waste* was proposed and tested. With high-flux neutron pulses generated in such targets one can not only destroy actinide nuclei in (n,fission) reactions but also synthesize new elements in (n,gamma) reactions. This technology may open a new way to the hypothetical *"Island of Stability" of superheavy elements*.

A new mechanism for the *production of multi-hypernuclei* in relativistic heavy-ion collisions was investigated within several models (I. Mishustin, M. Bleicher). It assumes that, first, hyperons from the participant zone are absorbed in the nuclear spectators and second, these moderately-excited spectators break up into cold non-strange and hyper-fragments. Formation of multi-strange nuclei containing up to three hyperons is predicted on a measurable level.

In the group of E. Bratkovskaya a conceptually novel approach for the dynamical description of the *strongly interacting Quark-Gluon-Plasma (sQGP)* including a dynamical hadronization scheme has been developed – the Parton-Hadron-String Dynamics (PHSD) model – and successfully applied for the description of heavy-ion collisions from lower FAIR to LHC energies. The PHSD model reproduces a large variety of observables (as quark-number scaling of elliptic flow, transverse-mass and rapidity spectra of charged hadrons, dilepton spectra, collective flow coefficients, etc.), providing a solid tool to study the new stage of matter from a microscopic point of view.

In the area of astrophysics significant progress has been made in the development of a two-dimensional code to simulate *neutron star cooling* (S. Schramm). This code will allow for the correlated study of the spinning-down or accreting neutron star and the impact of rotation on the measurable cooling curves.

In a novel theoretical approach a *chirally symmetric hadron-quark model* for three flavors has been developed that is based on the parity-doublet model (S. Schramm). Within this model an equation of state for all values of temperature, chemical potential, and strangeness have been computed. The results will be used in simulations of heavy-ion collisions as well as in the study of compact stars.

Neuroscience

Infants in control: A fundamental learning problem for the developing infant (and other organisms or even robots) is to figure out which sensory events are caused by its own actions. This problem has been notoriously hard to study due to the limited motor repertoire of infants. J. Triesch's group, in collaboration with Prof. M. Knopf's developmental psychology group from Goethe University, has developed a new paradigm using automatic eye tracking technology to put infants in control of their environment. Specifically, the 6 and 8-month-old infants can trigger audio-visual events by looking at certain objects on a computer screen, thus putting young infants who are still learning to reach and grasp objects properly in control of their environment through their eye movements. A first study recently published has demonstrated that infants readily learn to utilize this new form of agency and that they anticipate the consequences of their actions in as few as three trials. This methodology has the potential to revolutionize infancy research, allowing to study virtually all aspects of infant cognition in a novel interactive fashion. The research may also have implications for cognitive training paradigms and may ultimately lead to new treatment methods for infants at risk of developing autism or other diseases.

The research group of Danko Nikolić has discovered that *spike timing of neurons in visual cortex* can change with high precision. A small change in stimulus properties can determine whether neuron A fires a few milliseconds before neuron B, or the other way around, B firing before A. Nikolić and collaborators propose that these relationships in spike timing have strong influence on the flow of information throughout the cortex.

Life Science and Chemistry

The Meso-Bio-Nano group at FIAS (A. Solov'yov) studies the structure and properties of a variety of objects on the nanoscale, e.g., atomic and molecular clusters, nanoparticles, nanowires, micro-droplets, and biomolecules.

Recently significant progress has been achieved in the quantitative molecular level understanding of the cascade of processes and mechanisms responsible for *damaging of biological targets by heavy-ion irradiation*. These studies extend significantly our knowledge about the physical mechanisms and molecular processes involved in ion-beam cancer therapy, and radiation damage in general. The MBN Science team at FIAS coordinates the EU funded COST Action Nano-IBCT (Nanoscale insights into ion beam cancer therapy) in which teams from 20 EU countries, Australia, Canada, USA, and Japan are involved.

A new patent for the invention of a scheme for the construction of a novel *source of coherent monochromatic radiation* operating in the range of high-frequency gamma rays (i.e. a *gamma laser*) has been granted (W. Greiner, A.V. Korol, A. Kostyuk, A.V. Solov'yov). The key element of the suggested gamma laser device is a periodically bent crystal through which energetic, ultrarelativistic and modulated charged particles (electrons or positrons) propagate in the channelling regime. The suggested scheme has similarities with the scheme of the so-called Free Electron Laser (FEL). Such lasers have been recently constructed in several countries including Germany and operate in X-ray frequency range. In the suggested gamma laser scheme the heavy and large magnets used in FEL are substituted with compact periodically bent crystals. This allows to reduce drastically the wavelength of electron/positron periodic motion and thus increase significantly the energy of the emitted photons.

Computer Science

The *ALICE high level trigger* was operated at CERN the entire year. It was used to analyze the entire event data stream of more than 20 GB/s in real time. In this process the on-line data was compressed by more than a factor 4. The ALICE HLT is the only system at CERN, which operates graphic cards as hardware accelerators. The entire tracking of the experiment is performed on less than 50 computers with 50 GPUs.

A new algorithm was developed, allowing the highly efficient computation over Galois fields, which is required for redundant data coding. With the increasing data sizes in particular at CERN and at GSI such redundant coding is essential as no hardware can be reliable enough.

A new software package was developed, allowing *highly efficient vectorized programming*. Without such programming modern processors are used by less than 25% of their capabilities. This package is already in use at various sites and is planned to be incorporated into the ROOT package, which is used by physicists around the world.

A matrix multiplication and Linpack software package was developed, which outperforms all other existing solutions, in particular on ATI GPGPUS, which are used at the LOEWE-CSC. This software enabled the LOEWE-CSC to reach its high performance rating.

In cooperation with the physics groups a first version of a *Lattice QCD program* was developed to run on GPUs, which is highly efficient. In addition a new version of the Frankfurt UrQMD model was developed, which is also running on GPUs. The realized speed-up is a factor of 160.

1. Partner Research Centers

HIC for FAIR
Helmholtz International Center

An excellent year for HIC for FAIR

by Björn Bäuchle, Marcus Bleicher, Gabriela Meyer

After a successful evaluation in March 2011, the Helmholtz International Center for FAIR (HIC for FAIR) has been granted prolongation of the center for another three years. Thus, the ambitious research activities for FAIR conducted at the Universities of Frankfurt, Darmstadt and Gießen, the FIAS together with the partners GSI Helmholtz Zentrum für Schwerionenforschung (GSI), and the Helmholtz Association continue. Total support by the LOEWE program initiated by the state of Hesse amounts to 19.4 million Euro for the second funding period.

Ground-breaking research for FAIR

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, 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).

LOEWE professorships, Helmholtz Young Investigators and young scientists

The hiring of faculty members at the HIC for FAIR partner institutions is nearly completed: 13 W2/Fellow- and seven W3-positions out of 26 have been filled. HIC for FAIR is actively promoting young scientists. Out of nine W1/Junior Fellow positions, five have been filled. In addition, three Helmholtz Young Investigator (HYI) groups have succeeded in a competitive selection procedure of the Helmholtz Association and will join HIC for FAIR in 2012.

In 2011, the number of doctoral students working in HIC for FAIR has increased to nearly 200 young scientists coming from 30 different nations.

International visibility

More than 30 international conferences and workshops have been (co-)funded and organized by HIC for FAIR scientists. More than 150 visiting scientists from all over the world have contributed to the scientific program at HIC for FAIR.

Prof. Kester (on the right, HIC for FAIR, Univ. Frankfurt, head of the accelerator division at GSI) discussing with the reviewers sitting in the front row (left: Prof. Harris, Yale Univ.; right: Prof. Lippert, Jülich). MC in the left background: Prof. Bleicher.

Photo: © Uwe Dettmar, Frankfurt am Main.

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 international partner institutions; among 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 2011, more than 350 scientist 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 2011, EMMI members have published more than 250 papers in refereed journals, and more than 100 contributions to conference proceedings. EMMI runs an active workshop program. 8 EMMI workshops and one three-week EMMI program with strong international participation were organized in 2011. Among these workshops was the FIAS-EMMI Day that took place at FIAS. In December 2011, the first EMMI Rapid Reaction Task Force was organized and addressed the problem of thermalization in heavy ion collisions. The Rapid Reaction Task Forces are a new instrument which allows EMMI to gather a group of 15 to 20 world experts in order to address a particular scientific question in intense discussion. These meetings can be organized on a short timescale in order to react quickly to current and emerging questions. 11 renowned experts have visited EMMI partner institutions for extended periods in 2011 as EMMI Visiting Professor, and have made progress in their collaborations with EMMI members. These and further EMMI activities are listed at www.gsi.de/emmi.

In March 2011 EMMI has moved to the new office building at GSI. The building offers a lecture hall and four seminar rooms and provides a unique infrastructure for the activities of EMMI, in particular for workshops and programs.

In March 2011, as the first event organized in the new building, the Midterm Review of the ExtreMe Matter Institute and of the Helmholtz Alliance `Cosmic Matter in the Laboratory' took place. It was conducted by an international high-profile review committee in collaboration with the Helmholtz Association. More than 200 EMMI scientists from all participating institutions were present during the review. The review committee gave a very positive evaluation and strongly recommended to continue the activities of EMMI on a long-term basis.

For 17 days in August and September 2011, EMMI hosted the LHC exhibition `Weltmaschine' in the new building. The exhibition explained to the general public, with the help of genuine samples, how physicists investigate the fundamental questions about the Universe at the LHC. Pictures and displays showed the construction and functionality of the LHC. Physicists working at the LHC were present during the exhibition and answered the many questions raised by the visitors. Public lectures on the weekends informed the visitors about the current questions in elementary particle physics and cosmology. In total, the exhibition had more than 4500 visitors.

EMMI organized three masterclass events for high school students in 2011. In these masterclasses the students analyzed actual ALICE data. The total number of participants was about 70.

On November 23, 2011, EMMI participated in the nationwide `Tag der Weltmaschine', marking two years of particle collisions at the LHC. EMMI offered a public evening lecture and a video transmission of an interview with the CERN Director General, followed by ample opportunity to ask questions.

Bernstein Focus Neurotechnology Frankfurt

by Visvanathan Ramesh

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. A major goal of the initiative was to set up a collaborative research team in Frankfurt for sustainable long-term research in translating computational neuroscience advances to applications and several new professorships in the areas of machine learning, computational neuroscience and systems & software engineering were appointed by the end of 2011. Since the project start over the last two and a half years a number of scientific results have been produced in areas such as: developmental psychology, unsupervised machine learning, architectural models for vision, and high-performance computing. Progress was made in specific demonstrators illustrating learning of object representations for recognition via cue fusion and curiosity-driven learning, automated learning of mappings for relating camera views in video surveillance as well as exploitation of high-performance computing infrastructures for large scale offline learning.

It has to be noted, however, that the core system efforts have been hampered by delays in the hiring of the new professors and because of lack of agreement on technical integration aspects as well as execution process for integration among PI's. An interim project review was conducted in June 2011 and the feedback in the end of August emphasized the need for refocusing the efforts towards the core system construction goals, systems construction and the demonstrators. In response to the points of criticism raised by the reviewers, BFNT now is undergoing a restructuring which is led by its new coordinator, Prof. Ramesh, who succeeded Prof. von der Malsburg in this position. A restructuring plan that integrates all points of view and balances the needs of stakeholders (BMBF, FIAS, GU, PI's and Industry partners) was worked out. In order to account for the challenges faced in the first half of the project wherein the systems integration effort could not succeed, we proposed a management process and execution model that allows for modular execution of scientific projects while allowing seamless transfer to engineering of applications. This model reflects the strategic long-term need for establishment of an organizational structure and collaborative model that seamlessly translates scientific research to applications and allows for feedback of insights learned from systems science and engineering efforts into scientific components research.

The revised execution plan for BFNT will focus on specific research in scientific components involving autonomous learning, self-organization, cue-integration and fusion, and will phase out auxiliary research in neuroscience/psychology and neuroscience/neurophysiology that do not directly contribute to the systems effort. We will focus on two related but complementary application scenarios as case studies − icub robotics and video surveillance. The systems science and engineering research will:

- construct a large visual memory for general scene representation,
- develop virtual simulation tools for simulating large amounts of data for offline training,
- evaluate the ability to perform transfer learning on real data sets,
- develop novel autonomous learning methods for video representations,
- develop cue fusion and integration methods,
- develop modules for icub robotics and video surveillance to demonstrate autonomous learning in active vision context and event/activity analysis from video.

A modular execution model has been adopted wherein long-term science work-packages can be seamlessly integrated with systems science and engineering efforts planned. A committee based management model is adopted for various Phd students in order to achieve increased integration. Systematic processes and rigorous project management structure is setup in order to mitigate any future risks in the project.

2. Graduate Schools

HGS-HIRe for FAIR
Helmholtz Graduate School for Hadron and Ion Research

H-QM Helmholtz Research School Quark Matter Studies

Helmholtz Graduate School for Hadron and Ion Research

and

Helmholtz Research School for Quark Matter Studies

by Henner Büsching and Gerhard Burau

The Helmholtz Graduate School for Hadron and Ion Research (HGS-HIRe for FAIR) − a joint endeavor of the GSI Helmholtzzentrum and the universities at Darmstadt, Frankfurt, Giessen, Heidelberg and Mainz together with FIAS − looks back on a successful third year of operation. Established to provide a common platform for structured doctoral education in the scientific fields of hadron and ion research, HGS-HIRe is attracting an increasing number of participating students who perform their research projects in these fields at the partner institutions. More than 270 doctoral students are participating in the program of HGS-HIRe by the end of 2011. Nearly 30% of the participants have an international background, 19 participants of HGS-HIRe graduated in 2011.
The increasing number of participants in 2011 allowed for a consequent strengthening of the education program. In addition the Helmholtz Research School for Quark Matter Studies (H-QM) is more and more integrated in the structure of HGS-HIRe. H-QM is a joint project of the GSI Helmholtzzentrum, Goethe-Universität Frankfurt and FIAS to specially support a selected group of outstanding students performing research in the field of theoretical and experimental heavy-ion physics. Both, H-QM and HGS-HIRe are supported by the Initiative and Networking Fund of the Helmholtz Association.
Within the education program of HGS-HIRe and H-QM, numerous events on various topics, which addressed both, scientific and transferable skills, have been organized in 2011: five lecture weeks, three power weeks − one of them held at FIAS, and a total of ten seminars on transferable skills. With the latter HGS-HIRe is breaking new ground and has developed, together with experienced trainers from the UK, an integrated series of three courses focusing on various transferable skills, combining different aspects of professional and personal development. Additionally, the HGS-HIRe Perspectives events were introduced to facilitate the career planning of the students after finishing the PhD. Offered in 2011 on a regular basis, these events have been established as integral part of the program.
Last but not least three special events have been organized by HGS-HIRe in 2011:
The first joint Helmholtz-Rosatom School took place in Hirschegg (Austria) in February 2011. Participants of HGS-HIRe and fellows of the FAIR Russia Research Centre in Moscow came together to discuss and learn about various aspects of the new FAIR accelerator complex.
During the summer months of 2011 HGS-HIRe and GSI organized an international Summer Student Program which is offered to undergraduate students in physics or related natural science disciplines.
41 students from 14 countries, mostly from Europe but also from GSI/FAIR partner countries in Asia and South America took part in this year's program.
The second HGS-HIRe Graduate Days were held in Königstein/Taunus in October. Nearly 200 participants and members of HGS-HIRe joined this central event. Over the course of two days

participants reported on their projects, experienced researchers gave overview talks, and the HGS-HIRe Excellence Awards 2011 have been granted to Matthias Lochmann (Mainz) and Niels Strodthoff (Darmstadt).

Other pillars of the HGS-HIRe program were further strengthened. In the HGS-HIRe Abroad program participants can file a research proposal for a research stay abroad for a period of one to three months to facilitate their thesis project. A limited number of HGS-HIRe Abroad grants has been awarded in a competitive process several times per year.

In addition, HGS-HIRe and H-QM have been involved in a couple of public outreach activities:

- The 'International Masterclasses' which are organized in the framework of the European Particle Physics Outreach Group and the Initiative 'Netzwerk-Teilchenphysik' of the German BMBF
- An outreach program for elementary school kids with HGS-HIRe participants visiting elementary schools to talk about what it is like 'to be a scientist' (organized in cooperation with 'Polytechnische Gesellschaft' in Frankfurt)
- 'Tag der Weltmaschine' in November 2011 − an event including presentations and a small exhibition for the general public featuring the physics, the experiments and the technological challenges of the Large Hadron Collider LHC at CERN (organized in cooperation with the Physics Department of Goethe-Universität and FIAS)

Strongly supported by FIAS, HGS-HIRe provides and centrally organizes the very successful PhD scholarship programs of GSI, HIC for FAIR and EMMI.

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. Students are typically funded by research grants to their advisors, since FIGSS has no independent funding. The students are expected to obtain their PhD within three years.

In 2011 the number of FIGSS students has continued to rise. Enrollment went up from 56 in Decemeber 2010 to 66 in December 2011. Nine PhDs were awarded in 2011. The fraction of female students has been slightly decreasing from 20% to 15%, but the student population remains very international with 42% of our students being foreign nationals. The composition of FIGSS with respect to the different research disciplines has become somewhat more uniform last year. Neuroscience (35%) and Physics (33%) still make up the lion share (as has been the case from the founding days of FIAS), but Chemistry and Biology (15%) and Computer Science (17%) have been catching up a little.

We have updated and further developed our rules and procedures for FIGSS. Specifically, PhD committees are being introduced, which meet regularly and monitor the progress of the individual students. The cooperation with the ‘Goethe Graduate Academy’ (GRADE) is also being formalized.

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 2011

T. Burwick	Visual System: Principles of Attention, 1h
E. Engel	Quantum many-particle theory, 2+1h
W. Greiner	Gauge Theory of Weak Interactions, 2h
C. Gros	Complex Systems and Neural Networks, 3+1h
J. Lücke	Recent Advances in Computational Neuroscience and Machine Learning, Seminar, 2h
I. Mishustin	Dynamical models for relativistic heavy-ion collisions, 2h
P. Romatschke	Thermal Quantum Field Theory, 2+2h
P. Romatschke	Hydrodynamics and Plasma Physics, Seminar, 2h
S. Schramm	Quantum theory on the lattice, 2+1h
D. Schuch	Nonlinearities and Dissipation in Classical and Quantum Physics, 2h
A. Solov'yov	Theoretical and computational methods in Meso-Bio-Nano Science, 2h
J. Triesch, C. Rothkopf	Systems Neuroscience, Seminar, 2h

Winter Semester 2011/12

T. Burwick	Brain Dynamics: From Neuron to Cortex, 1h
C. Gros	Complex Adaptive Dynamical Systems, 2+1h
W. Greiner	Gauge Theory of Weak Interactions, 2h
I. Mishustin	Physics of Strongly Interacting Matter, 2h
P. Nicolini	Gravity, matter and dualities, 2h
V. Ramesh	Systems Engineering for Computer Vision, 4h
S. Schramm	Nuclear and Neutrino Astrophysics, 2h
D. Schuch	Riccati and Ermakov Equations and the Quantum-Classical Connection, 2h
A. Solov'yov	Theoretical and computational methods in Meso-Bio-Nano Science, 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
Nuclear/Heavy ion group meeting	– Mishustin
Machine learning lunch seminar	– Lücke

Ph.D. degrees received by FIAS/FIGSS students in the year 2011

1	Martin Kober	26.01.2011	Über die Beziehung der begrifflichen Grundlagen der Quantentheorie und der Allgemeinen Relativitätstheorie
2	Urs Bergmann	04.04.2011	Pre- and postnatal development of topographic transformations in the brain
3	Jan Carsten Scholz	21.04.2011	Self-organizing structure and metrics of complex networks
4	Dominik Heide	21.04.2011	Statistical physics of power flows on networks with a high share of fluctuating renewable generation
5	Jan Steinheimer-Froschauer	06.06.2011	A model for heavy ion collisions with quark and hadronic degrees of freedom
6	Mirko Schäfer	13.07.2011	Dynamics of chaotic strings
7	Marlene Nahrgang	13.07.2011	Nonequilibrium phase transitions in chiral fluid dynamics including dissipation and fluctuation
8	Sophie Nahrwold	29.08.2011	Electroweak quantum chemistry: Parity violation in spectra of chiral molecules containing heavy atoms
9	Veronika V. Dick	12.10.2011	Mechanisms of nanofractal structure formation and post-growth evolution

3. FIAS Scientific Life

Seminars and Colloquia at FIAS in the year 2011

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.

Interdisciplinary FIAS Colloquium

20.01.2011 **Prof. Dr. Alfred Müller,** Institute for atomic and molecular physics, Justus Liebig University, Giessen
Soccer balls in the nano world

3.02.2011 **Dr. José Faraldo-Gómez,** Theoretical Molecular Biophysics Group, Max Planck Institute of Biophysics, Frankfurt
Mechanisms of selective ion binding and transport in F1Fo ATP synthases: Insights from quantitative computer simulations

10.02.2011 **Prof. Dr. Thierry Langer**, Prestwick Chemical Inc., France
Pharmacophore-based parallel in silico screening: An interesting concept for efficient activity profiling in drug discovery

14.04.2011 **Prof. Dr. Manfred Kappes**, Karlsruhe Institute or Technology (KIT), Physical Chemistry Institute and Nanotechnology Institute
Thermal and chemical properties of fractals generated by soft-landing of carbon clusters

28.04.2011 **Prof. Dr. Boris Sharkov,** FAIR GmbH, Darmstadt
FAIR and physics at FAIR

12.05.2011 **Prof. Dr. Valery Zagrebaev,** Flerov Laboratory of Nuclear Reactions, JINR, Dubna, Russia and FIAS
New prospects in the synthesis of superheavy nuclei

26.05.2011 **Dr. Gunnar Rätsch,** Friedrich Miescher Laboratory, Max Planck Society, Tübingen
Towards empirical models of the central dogma of molecular biology

9.06.2011 **Prof. Dr. Ulf Ziemann,** Division of Engineering, King's College, London
Homeostatic metaplasticity in human cortex: principles and applications

14.06.2011 **Prof. Dr. John Moffat,** Perimeter Institute for Theoretical Physics, Waterloo, Canada
Ultraviolet complete quantum field theory and its consequences for particle physics and quantum gravity

30.06.2011 **Prof. Dr. Joachim Denzler,** Friedrich Schiller University, Jena
Toward realistic real-world visual learning using Gaussian processes

7.07.2011 **Dr. Lucy Forrest,** Max Planck Institute for Biophysics, Frankfurt
A role for protein symmetry in moving ions across cell membranes

28.07.2011 **Prof. Dr. Victor Flambaum,** Niels Bohr Institute, Copenhagen
Lessons from phage biology

20.10.2011 **Prof. Dr. Christoph Düllmann,** GSI Darmstadt and Johannes Gutenberg University, Mainz
Superheavy Element Research - News from GSI and Mainz

27.10.2011 **Prof. Dr. Thomas Boller,** Max-Planck-Institute for Extraterrestrial Physics, Garching
Prospects in testing General Relativity theories in the strong field limit

10.11.2011 **Prof. Dr. Thomas Gasenzer,** Institut für Theoretische Physik, Universität Heidelberg
Superfluid Turbulence in an Ultracold Bose Gas

17.11.2011 **Dr. Ingo Ebersberger,** Center for Integrative Bioinformatics, Vienna, Austria
Biological data analysis in the post-genomic era:Looking for the needle in the hay

24.11.2011 **Dr. Jun Tani,** RIKEN Brain Science Institute, Saitama, Japan
Understanding Minds through Synthesis: A Neuro-Robotics Research Project

1.12.2011 **Prof. Dr. Irene Burghardt,** Institute for Physical and Theoretical Chemistry, Goethe-University Frankfurt
Quantum dynamics of photoprocesses in extended systems: coherence and correlations at the nanoscale

8.12.2011 **Prof. Dr. Debades Bandyopadhyay,** Saha Institute of Nuclear Physics, Kolkata
Supernova Explosions: Searching for Exotica

FIGSS Seminar

10.01.2011 **Quan Wang**
Studying motor sequence learning using a recurrent neural network

17.01.2011 **Dr. Lisa Scocchia**
Investigating the effects of visual working memory on perception: an empirical approach

24.01.2011 **Dr. Alexander Yakubovich**
Theory of phase transitions in polypeptides and proteins

31.01.2011 **Sophie Nahrwold**
Weak interaction effects in nuclear magnetic resonance spectra of chiral molecules

7.02.2011 **Jörg Bornschein**
Large scale machine learning using expectation maximization

14.02.2011 **Johan Bjerrum-Bohr**
Dynamics of a quark-gluon droplet

16.05.2011 **Jan Steinheimer**
Hypernuclei and strange clusters: Extending the nuclear chart

23.05.2011 **Torsten Schürhoff**
Neutron stars with small radii - the role of Delta resonances

30.05.2011 **Pengsheng Zheng**
Network self-organization explains the distribution of synaptic efficacies in neocortex

6.06.2011 **Dr. Andriy Kostyuk**
From crystalline undulator to gamma-laser

20.06.2011 **Prof. Dr. Yasuomi Sato**
Software and hardware developments for visual object recognition - Systems and practical applications

27.06.2011 **Dr. Harri Niemi**
Hydrodynamical description of ultrarelativistic heavy-ion collisions

4.07.2011 **Daniel Yueker**
Cosmic Phase Transitions within A Dynamical Background

11.07.2011 **Philip Rau**
Shock wave phenomena in nucleus-nucleus collisions

24.10.2011 **Dr. Hannu Holopainen**
Event-by-event hydrodynamics in modeling of ultrarelativistic heavy-ion collisions

31.10.2011 **Daniel Krieg**
A unifying functional view on synaptic plasticity

7.11.2011 **Dr. Rodrigo Picanço Negreiros**
Impact of rotation-driven particle repopulation on the thermal evolution of pulsars

21.11.2011 **Dr. Philip Sterne**
Neural Homeostatic Mechanisms from Information Theory

5.12.2011 **Alexey Verkhovtsev**
Investigation of carbon nanoscale hollow systems by means of many-body theory

19.12.2011 **Dr. Constantin Rothkopf**
Visuomotor behavior in naturalistic task: from receptive fields to value functions

Conferences and meetings (co)organized by FIAS in the year 2011

▷ **FIAS EMMI Day** Frankfurt, January 11, 2011

▷ **Ernst Strüngmann Forum,** ***"Cognitive Search - Evolution, Algorithms, and the Brain",*** Frankfurt, February 20 - 25, 2011

www.esforum.de/forums/esf09_cognitive_search.html

▷ **CUTE,** Kick-Off Meeting for the EU Supported Project (within FP7) **"Crystalline Undulator: Theory and Experiment",** Frankfurt May 6, 2011

▷ **Ernst Strüngmann Forum,** ***"Language, Music and the Brain - A Mysterious Relationship",*** Frankfurt, May 8 - 13, 2011

www.esforum.de/forums/esf10_language_music_brain.html

▷ ***"Ethics and Neuroscience: Empirical, Conceptual and Normative Issues",*** 14. Meeting of the Junior Research Group "Philosophy of Mind", Frankfurt, June 2-5, 2011

fias.uni-frankfurt.de/mindgroup/index.php/meeting-14.html

▷ **Ernst Strüngmann Forum,** ***"Evolving the Mechanisms of Decision Making - Toward a Darwinian Decision Theory",*** Frankfurt, June 19 - 24, 2011

www.esforum.de/forums/esf11_darwinian_decision_theory.html

▷ **ISACC 2011, Fifth International Symposium *"Atomic Cluster Collisions",*** Berlin, July 20 - 25, 2011

fias.uni-frankfurt.de/isacc2011

▷ **ICDL-EpiRob 2011, *"First Joint IEEE International Conference on Development and Learning and on Epigenetic Robotics",*** Frankfurt, August 24 - 27, 2011

www.icdl-epirob.org

▷ **NeD-2011, *"International Symposium on Non-equilibrium Dynamics",*** Heraclion, Crete, August 31 - September 3, 2011

▷ **Network Workshop "TORIC",** Heraclion, Crete, September 5 - 8, 2011

▷ **1st Nano-IBCT Conference *"Radiation Damage of Biomolecular Systems: Nano-scale Insights into Ion Beam Cancer Therapy",*** Caen, France, October 2 - 6, 2011

nano-ibct.sciencesconf.org

▷ **NUFRA2011, *"Third International Conference on Nuclear Fragmentation",*** Kemer, Turkey, October 2 - 9, 2011

fias.uni-frankfurt.de/nufra2011

▷ ***"Explanatory Models of Consciousness",*** 15. Meeting of the Junior Research Group "Philosophy of Mind", Frankfurt, October 20 - 23, 2011

fias.uni-frankfurt.de/mindgroup/index.php/meeting-15.html

Talks at the FIAS Forum in the year 2011

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.

13.01.2011 **Prof. Dr. Michael Hausmann,** Kirchhoff-Institut für Physik, Universität Heidelberg
Medizinische Diagnostik der Zukunft – mit Computerchips Krankheiten diagnostizieren und Therapien entwickeln

17.02.2011 **Prof. Dr. Marcus Bleicher,** Institut für Theoretische Physik und Frankfurt Institute for Advanced Studies
Wie viele Dimensionen hat das Universum? Von drei zu sechsundzwanzig Dimensionen und zurück

31.03.2011 **Prof. Dr. Hermann Requardt,** Mitglied des Vorstands der Siemens AG, Chief Technology Officer, CEO Sektor Healthcare
Individualisierte Medizin - Zur Problematik moderner Gesundheitssysteme

19.05.2011 **Prof. Dr. Marc Thilo Figge,** Leibniz-Institut für Naturstoff-Forschung und Infektionsbiologie, Hans-Knöll-Institut, Friedrich-Schiller-Universität, Jena
Unser Körper kann nicht ohne Antikörper – über die lebenswichtige Bedeutung der Adaptiven Immunität

8.06.2011 **PD Dr. Peter Johannes Uhlhaas,** Max-Planck-Institut für Hirnforschung (MPI), Abteilung für Neurophysiologie, Frankfurt
Das Gehirn in der Pubertät – warum Jugendliche so sind, wie sie sind

6.07.2011 **Prof. Dr. med. Ingo Bechmann,** Institut für Anatomie der Universität Leipzig
Neues aus der Alzheimerforschung – das sterbende Immunsystem des Gehirns

9.11.2011 **Prof. Dr. Dieter Steinhilber und Prof. Dr. Theo Dingermann,** Goethe-Universität Frankfurt
Diabetes und das Metabolische Syndrom: Ursachen für das tragische Ende von Elvis Presley. Ein Vortrag mit Musik und medizinischen Fakten

4. Research Reports

4.1 Nuclear Physics, Particle Physics, Astrophysics

Nonequilibrium effects in hadronic fireball expansion

Collaborators: I.N. Mishustin, L.M. Satarov, and A.B. Larionov (FIAS & Kurchatov Institute, Moscow)

We consider a spherical volume of of hot and dense hadronic matter (fireball) expanding into a vacuum [1]. It is assumed that initially the fireball matter is in local thermal and chemical equilibrium with vanishing collective velocity. The initial radial profiles for energy (ε) and baryon (n) densities are parametrized by the Woods–Saxon distribution with some radius R and diffuseness a. We choose the initial values of ε and n at the fireball center, typical for hadronic matter created in heavy–ion collisions at $E_{\rm lab} \simeq 10$ AGeV. The time evolution of the fireball is studied in parallel within the GiBUU transport model (http://gibuu.physik.uni-giessen.de/GiBUU) and an ideal hydrodynamical model [2]. The equation of state of a a chemically equilibrated ideal hadronic gas is used in the hydrodynamic calculation. The same set of hadronic species is used in transport and fluid-dynamical simulations. Initial coordinates and momenta of hadrons in transport simulations have been randomly generated by using the Fermi and Bose distributions for (anti)baryons and mesons. The model results for radial profiles of densities and collective velocities of different hadronic species are compared at different times. We have found significant differences in space–time evolution of partial densities and collective velocities of hadrons predicted by these models. Also, the two models predict very different time evolution of hadron abundances which are especially pronounced for hyperonic species. In Fig. 1 one can see a qualitative difference between the results

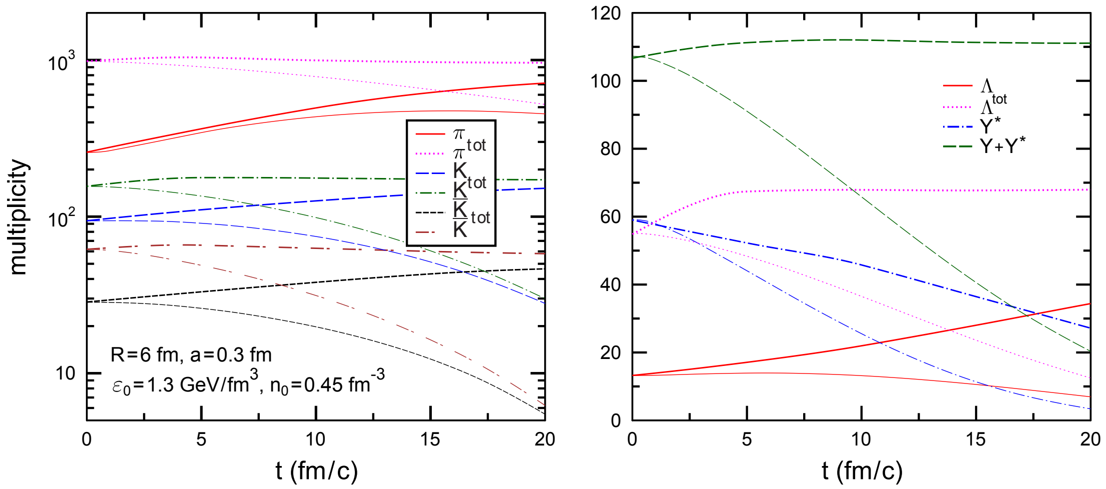


Figure 1: Multiplicities of mesons (left panel) and strange baryons (right panel) as functions of time in a hadronic fireball expanding into vacuum. Initial parameters of fireball are shown in the left panel. Thick lines represent the GiBUU results averaged over 5000 events. Thin lines are calculated within the hydrodynamical model. Symbols with the subscript 'tot' denote the total numbers of corresponding hadrons including those, hidden in hadronic resonances. $Y(Y^*)$ is the total multiplicity of stable (unstable) hyperons.

of two calculations. In particular, GiBUU predicts nearly constant total multiplicities of pions, (anti)kaons, and Λ hyperons (with inclusion of hadrons, hidden in resonances). However, these quantities decrease within the hydrodynamic model. We believe that strong deviations from chemical equilibrium predicted by transport calculations should be explicitly taken into account in future hydro–cascade simulations of relativistic nuclear collisions.

Related publications in 2011:

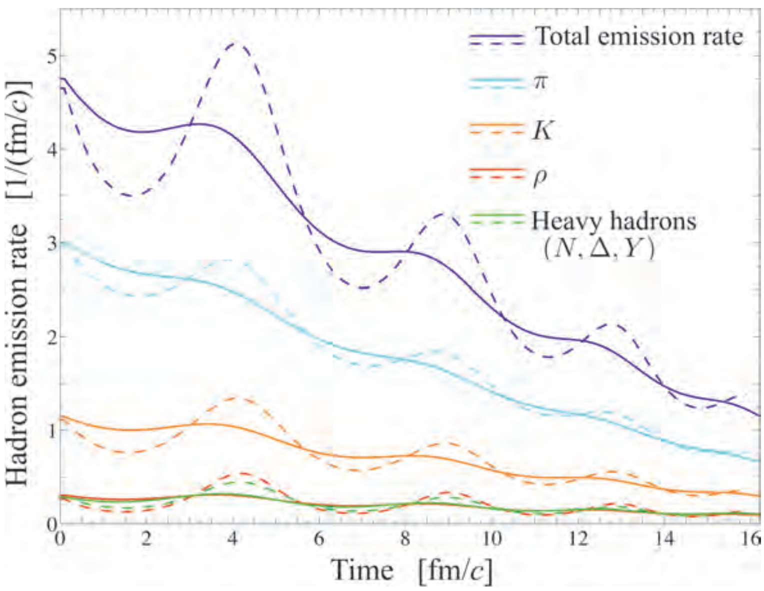
1) L.M. Satarov, A.B. Larionov, and I.N. Mishustin, Non-equilibrium effects in hadronic fireball expansion, submitted to Phys. Rev. C; ArXiv: 1201.552 [nucl-th].

2.) A.V. Merdeev, L.M. Satarov, and I.N. Mishustin, Hydrodynamic modeling of the deconfinement phase transition in heavy-ion collisions in the NICA-FAIR energy domain, Phys. Rev. C 84, 014907 (2011).

Hydrodynamics of a quark droplet

Collaborators: J. J. Bjerrum-Bohr, I. N. Mishustin, T. Døssing[1]
[1] Niels Bohr Institute, University of Copenhagen

We study the dynamics of small quark droplets, which might be created in heavy-ion collisions due to a strong collective expansion of the QGP. Our model takes into account thermal pressure of quarks, the vacuum pressure and surface tension effects. The model adopts the concept of the MIT bag model i.e. the droplet is described as spherical cavity with a bag constant, consisting of a plasma of massless quarks and antiquarks. The quark and antiquarks are described by hydrodynamics as a perfect fluid which is characterized by its rest frame energy density, isotropic pressure and a spherically-symmetric velocity field. The surface energy is associated with the gradients of the mean fields (condensates) in the transition region between inside and outside of the droplet. The hadronization is assumed to proceed via emission of hadrons from the droplet. We have applied Weisskopf's statistical model, where the double-differential emission rate is expressed through the ratio of the statistical weights before and after the particle emission to find equations for both total particle number and energy emission rates. As we can see from the figure, pions and kaons, are by far the most abundant emitted particles, since the emission of heavier species is suppressed by their mass. Nevertheless, the heavy particle spices contribute significantly to the energy loss as the emitted pions only carry away 50 % of the energy. We also see from the figure the damped oscillations of the droplet due to the initial expansion.



Emission rates of different hadron species (indicated on the figure) and the total emission rate as function of time. The dashed and solid lines represent calculation with and without an initial radial expansion of the droplet, respectively.

Related publications, posters and talks in 2011:

1) J.J. Bjerrum-Bohr, I. N. Mishustin, T. Døssing, Nucl. Phys A, (in press), arXiv:1112.2514v1 [nucl-th].

2) J.J. Bjerrum-Bohr in corporation with I. N. Mishustin and T. Døssing, *The dynamics of quark droplets*, poster presented at XXII International Conference on Ultrarelativistic Nucleus-Nucleus Collisions 2011,Quark Matter 2011.

Nonequilibrium chiral fluid dynamics

Collaborators: M. Nahrgang[1], C. Herold, M. Bleicher, I. N. Mishustin, S. Leupold[2]
[1] FIAS and SUBATECH, Nantes, [2] University of Uppsala

Investigating the QCD phase transition is one of the primary goals of heavy-ion collision xperiments. The crossover transition at low baryochemical potentials is well established by lattice QCD calculations. Model studies strongly indicate the first order phase transition at high baryochemical potentials. This implies the existence of a critical point at intermediate baryochemical potentials. In thermodynamic systems the correlation length and thus the fluctuations of the order parameter diverge at a critical point. In the same respect the relaxation time becomes infinite, which means that in a heavy-ion collision, where the expansion is fast, the system is necessarily driven out of equilibrium and any fluctuation signal of the critical point is diminished. On the other hand, at the first order phase transition such interesting phenomena as supercooling-reheating, nucleation and spinodal decomposition.

We have developed a consistent energy-conserving model describing a coupled dynamics of the order parameter for chiral symmetry, the sigma field, and an expanding fluid of quarks and antiquarks. This coupling gives rise to damping and noise. While the fluid expands the system cools and drives the sigma field through the phase transition. We investigate both scenarios: a critical point and a first order phase transition. In figure 1 we see the time evolution of the sigma field in x-direction in the center of the fireball. For the evolution through a critical point one observes a faster relaxation of the sigma field towards its equilibrium value (left plot) than for a first order phase transition (right plot). In the case of a first order phase transition, in the time interval 5-8 fm/c, the sigma field is still trapped in the chirally restored, high-temperature phase, leading to supercooling. It is due to the finite barrier that separates the unstable minimum from the stable minimum near the vacuum expectation value. The subsequent relaxation of the sigma field leads to a local reheating of the quark fluid. These effects at the first oder phase transition lead to an enhancement of coherently produced sigma excitations.

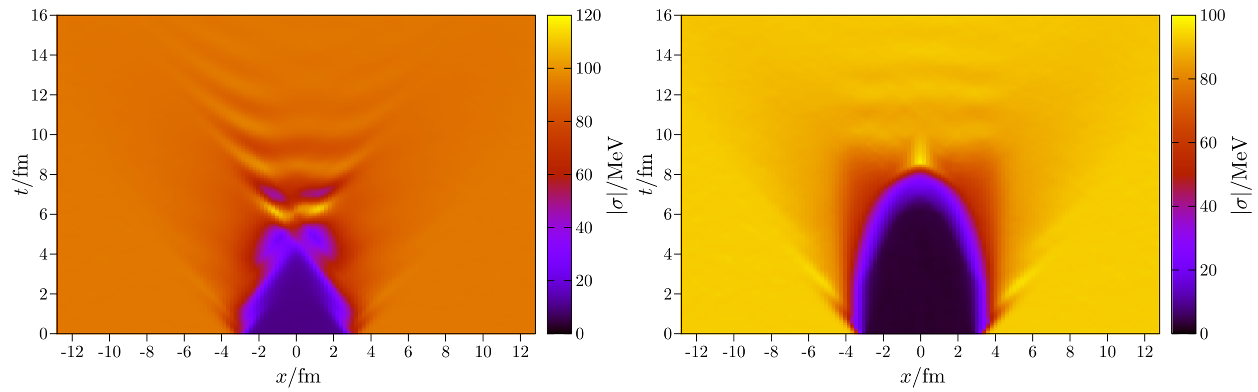


Figure 1: Time evolution of the sigma field along the x-direction in the plane $y = z = 0$ for a scenario with a critical point (left) and with a first order phase transition (right).

Related publications, posters and talks in 2011:

1) M. Nahrgang, S. Leupold, C. Herold, M. Bleicher, Phys. Rev. C84, 024912 (2011).
2) M. Nahrgang, S. Leupold, M. Bleicher, arXiv:1105.1396 [nucl-th].
3) M. Nahrgang, C. Herold, S. Leupold, I. N. Mishustin, M. Bleicher, arXiv:1105.1396 [nucl-th].
4) Igor Mishustin, *Hydrodynamic evolution of fluctuations in expanding quark matter*, invited talk at the Max Born Symposium "Three days on Quarkyonic Island" (Wroclaw, Poland, May 19-21, 2011).
5) M. Nahrgang, talk: *Dynamic fluctuation at the chiral phase transition* at 7th International Workshop on Critical Point and Onset of Deconfinement, November 2011.

Production of hyper-nuclei in reactions with relativistic ions

Collaborators: A.S. Botvina, K.K. Gudima[1], J. Steinheimer, I.N. Mishustin, M. Bleicher, H. Stöcker
[1] Institute of Applied Physics, Academy of Sciences of Moldova

We formulate a hybrid approach for describing formation of hyper-nuclei in peripheral collisions of relativistic light and heavy ions. The initial dynamical stage is simulated with transport models: the Dubna cascade model (DCM) and the ultra-relativistic quantum molecular dynamics (UrQMD) model. During this stage nucleons from the overlapping parts of the projectile and target (participant zone) interact intensively between themselves and with other hadrons produced in primary and secondary collisions. The hyperons ($Y = \Lambda, \Sigma, \Xi, \Omega$), produced in these interactions, can later on be captured by the projectile and target spectator residues (i.e., non-overlapping parts of colliding ions). In the Figure we demonstrate probabilities for producing spectator residues with different numbers of captured Λs together with their mean masses.

At the next stage these excited spectators will decay with production of normal and hyper-nuclei. For description of this process the statistical models of multifragmentation and Fermi-break-up were used. It was shown that a large variety of hypernuclei, including multi-strange and neutron-rich ones, can be formed in this way. We have performed analysis of preliminary experimental data on yields of light hypernuclei in projectile fragmentation reactions, reported recently by HypHI collaboration at GSI. We have found that the production of $^{3}_{\Lambda}$H, $^{4}_{\Lambda}$H, as well as exotic Λn ound state, which was never observed before, can be naturally explained within our approach.

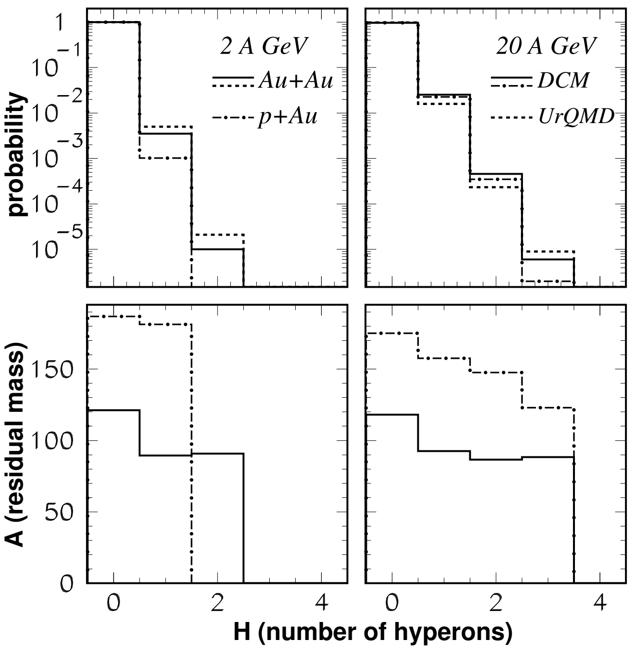


Figure: Probability for formation of conventional and strange spectator residuals (top panels), and their mean mass numbers (bottom panels) vs the number of captured Λ hyperons (H), calculated with DCM and UrQMD model for p + Au and Au + Au collisions with energy of 2 GeV per nucleon (left panels), and 20 GeV per nucleon (right panels).

Related publications and talks in 2011:

1) A.S. Botvina, K.K. Gudima, J. Steinheimer, I.N. Mishustin, J. Pochdzalla, A. Sances-Lorente, M. Bleicher, H. Stöcker, *Production of hyper-nuclei in peripheral collisions of relativistic ions*, mini-review to be published in Nucl. Phys. A.
2) A.S. Botvina et al., *Production of hyper-nuclei in reactions induced by relativistic light- and heavy-ions*, invited talk at the International Workshop "Strange Hadronic Matter" (ETC*, Trento, Italy, September 26-30, 2011).
3) A.S. Botvina et al., *Production of spectator hypermatter in relativistic light- and heavy-ion collisions*, talk at the Third International Conference on Nuclear Fragmentation - NUFRA2011 (Kemer, Antalya, Turkey, October 2-9, 2011).

Hypernuclei, dibaryon and antinuclei production in high energy heavy ion collisions

Collaborators: J. Steinheimer[1], K. Gudima[2], A. Botvina, I. Mishustin, M. Bleicher, H. Stöcker
[1] FIAS and Lawrence Berkeley National Laboratory, [2] Institute of Applied Physics, Academy of Sciences of Moldova

We obtained results on hyper-nuclei, anti-nuclei and di-baryon production in heavy-ion collisions over a wide beam energy range. To explore the theoretical uncertainties we applied two distinct approaches: firstly, the thermal production with the UrQMD-hydro hybrid model and secondly, the coalescence calculation within the Dubna hadron cascade model. Concerning most hyper-nuclei and di-baryons both approaches agree well in their predictions which gives us confidence in robustness and significance of the obtained results. We find that both the non-equilibrium and thermal models may be considered as appropriate approaches to describe strange cluster production. In agreement with previous studies we demonstrate that the most promising energy range to produce hyper-clusters will be provided by the FAIR and NICA facilities, $E_{lab} \approx 10$ - 20A GeV. Anti-matter clusters heavier than $\bar{t}$ are only feasible at RHIC and LHC energies. The most interesting result of our study is the apparent difference in the double ratio R_H when we compare our thermal results with the coalescence. This difference indicates that the information on correlations of baryon number and strangeness are visible in the microscopic coalescence approach, while they are washed out in the thermal picture. This could open the opportunity to directly measure the strangeness-baryon correlation, which may be sensitive to the onset of deconfinement. The present status of the experimental data does unfortunately not allow for a comprehensive comparison with our model calculations. We hope that this situation will improve in the upcoming RHIC energy scan and FAIR experiments.

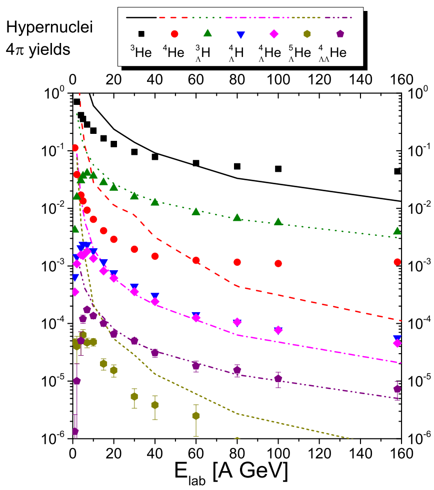


Figure 1: Full acceptance yields per event of different (hyper-)nuclei created in most central collisions of Pb+Pb/Au+Au. Shown are the results from the thermal production in the UrQMD hybrid model (lines) as compared to DCM based coalescence results (symbols).

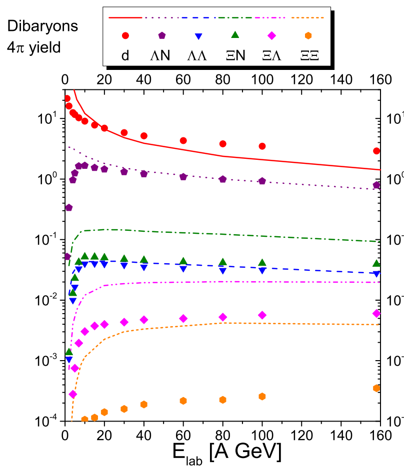


Figure 2: Full acceptance yields per event of different di-baryons created in most central collisions of Pb+Pb/Au+Au. Shown are the results from the thermal production in the UrQMD hybrid model (lines) as compared to DCM based coalescence results (symbols).

Related publications and talks in 2011:

1) J. Steinheimer, A. Botvina, K. Gudima, I. Mishustin, S. Schramm, M. Bleicher, H. Stöcker, *From FAIR to RHIC, hyper clusters and an effective strange EoS for QCD*, talk given at the international conference on Strangeness in Quark Matter 2011 in Krakow; arXiv:1112.5284 [hep-ph].

2) J. Steinheimer, A. Botvina, K. Gudima, I. Mishustin, S. Schramm, M. Bleicher, H. Stöcker, *Hypernuclei, dibaryons and antinuclei production in high-ebergy heavy-ion collisions: Thermal production vs. Coalescence*, to be submitted in Phys. Lett. B.

On production and properties of multi-lambda hypernuclei

Collaborators: C. Samanta[1], A.S. Botvina, I. Mishustin, W. Greiner
[1] Saha Institute of Nuclear Physics, Kolkata, India

Relativistic heavy-ion collisions offer the possibility of creating excited nuclear systems with hyperons. Hyperons are mostly produced in the midrapidity zone, where hadrons interact strongly whith each other. However, since Λ-particles have a broad rapidity distribution, some of them can be absorbed in the spectator residues of the projectile and target. Once produced and beeing excited, such spectator nuclear system begins to expand and finally breaks up into many composite fragments. Some fragments coming out of this disintegration may contain one or more hyperons. We use the statistical multifragmentation model, successfully used earlier, for the description of multifragmentation data, to predict relative yields of Λ-hypernuclei containing up to 4Λs. We have used two versions of the mass formula for calculation of observables to get a range of uncertainty associated with properties of unknown hyper-nuclei. Both mass formulae show increasing binding of Λ-hypernuclei with increasing Λ multiplicity, and, as a result, the large relative yield of multi Λ hypernuclei within some temperature range. The yields of hyper-fragments are found to be sensitive to the details of their mass formulae in the part related to the hyperon sector. Calculated mass distributions of the multi-lambda hypernuclei (Fig. 1) are found to be more probable for nuclei with higher Z values. All fragments have broad gaussian-like isotope distributions signaling that very exotic nuclei can be produced with noticeable probability.

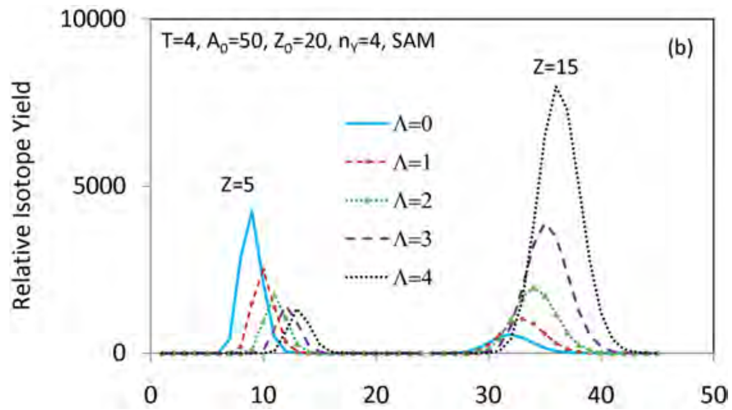


Figure 1: Mass distributions of hyperfragments with 0, 1, 2, 3 and 4Λs produced after multifragmentation of sources with $A_0 = 50$, $Z_0 = 20$ and $n_Y = 3$ (top) and $n_Y = 4$ (bottom) at temperature $T = 4$ MeV. Calculations are made with the the generalised mass formula of Samanta et al. Results are presented for total charge $Z = 5$ (left) and 15 (right) respectively.

Related publications and talks in 2011:

1) C. Samanta, *Strangeness: A new dimension in nuclear physics*, Symposium on Exciting Physics, Makutsi, South Africa, November 13-20, 2011.

2) C. Samanta, *Strange to superstrange nuclei, 5th DAE-BRNS workshop on Hadron Physics*, BARC, Mumbai, India, October 31-November 4, 2011.

3) C. Samanta, *Multi-strange nuclei in spectator fragmentation reactions*, International Conference on Nuclear Fragmentation 2011 (NUFRA2011), Kemer (Antalya), Turkey, October 2-9, 2011.

4) C. Samanta, A.S. Botvina, I. Mishustin, W. Greiner, *On production and properties of multi-lambda hypernuclei*, submitted for publication in J. Phys. G: Nucl. Part. Phys.

Isospin-dependent multifragmentation of relativistic projectiles

Collaborators: N. Buyukcizmeci[1], A.S. Botvina, I.N. Mishustin, W. Trautmann[2] et al.
[1] Selcuk University, Konya, Turkey [2] GSI, Darmstadt

Multifragmentation is an universal phenomenon occurring when a large amount of energy is deposited in a nucleus. It is challenging to describe the production of fragments in multifragmentation simultaneously with evaporation and fission which have been already studied extensively. It is also important that the physical conditions in some stellar processes (e.g., during collapses of massive stars associated with supernova explosions) is essentially determined by the state of hot nuclear matter at subnuclear density which can be investigated in multifragmentation reactions. There is a considerable interest to how the nuclear processes are modified with the neutron richness of matter. For this reason the ALADIN collaboration at GSI has performed experimental studies of fragmentation of relativistic projectiles with different mass and isospin content (^{107}Sn, ^{124}Sn, and ^{124}La), at beam energy of 600 MeV per nucleon.

In this work we have applied a well known statistical multifragmentation model (SMM) for simulation of the projectile break-up, and extraction of new information on properties of nuclear matter at various isospin asymmetries. We were able to reproduce simultaneously the charge yields of fragments, their mass (isotope) distributions, and correlations of these observables with excitation energy. For example, in Fig. 1 we show the quality of description of fragment charge distributions at different excitation energies (controlled by the charge bound in fragments) produced at disintegration of the ^{124}Sn projectile. We have demonstrated that in-medium reduction of the nuclear symmetry energy is necessary for successful description of the whole set of the data. Besides improving nuclear reaction models, this conclusion has consequences for many astrophysical processes, since the symmetry energy influences nuclear composition and weak reactions in stellar matter.

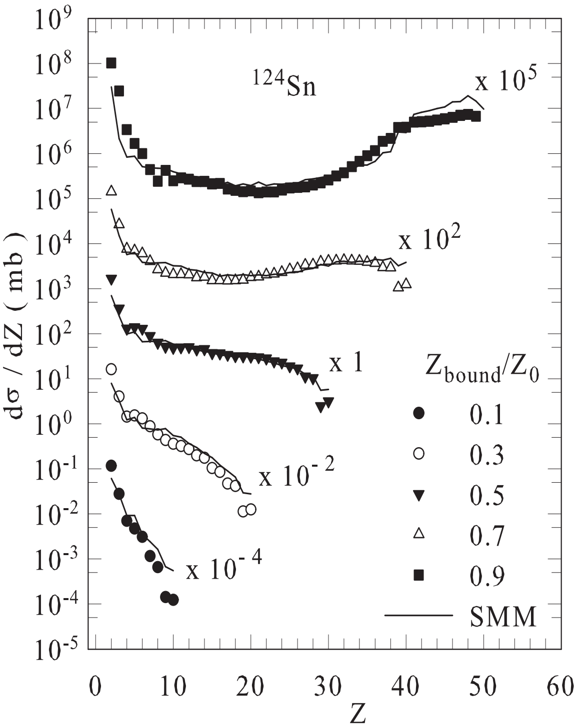


Figure 1: Experimental cross sections $d\sigma/dZ$ for the fragment production following collisions of ^{124}Sn projectiles sorted into five intervals of Z_{bound}/Z_0 with centers as indicated and width 0.2 (symbols) in comparison with normalized SMM calculations (lines). Different scale factors were used for displaying the cross sections as indicated.

Related publication in 2011:

1) R. Ogul, A.S. Botvina, U. Atav, N. Buyukcizmeci, I.N. Mishustin, W. Trautmann et al., *Isospin dependent multifragmentation of relativistic projectiles*, Phys. Rev. C83, 024608 (2011).

Monte Carlo modeling microdosimetry distributions from therapeutic beams

FIAS participants: L.N. Burigo, I.A. Pshenichnov, I.N. Mishustin, M. Bleicher

The Monte Carlo model for Heavy-Ion Therapy (MCHIT) created in FIAS was extended in order to simulate responces of Tissue-Equivalent-Proportional-Counters (TEPC) to neutron, proton and nuclear beams. The microdosimetric spectra measured by such devices characterize energy deposition to objects equivalent in size to living cells. The MCHIT model was used to predict microdosimetry distributions measured by a TEPC at 18 different positions inside a water phantom during an experiment at GSI (Martino et al., 2010). The simulation results reproduce the general trend of the lineal energy distributions as shown in Fig 1. However, the theory underestimates the data, far from the beam axis and in the tail area. This problem is related to an underestimation of yield of light fragments produced by primary nuclei in the phantom. The contributions from secondary neutrons, which propagate far from their production points, are also shown in Fig 1. This estimation will be useful for to evaluating biological effects of these neutrons far the target tumour volume. The MCHIT model was also applied to simulate microdosimetric experiments with quasimonoenergetic 40 and 65 MeV neutrons irradiating a PMMA phantom performed at JAERI (Nakane et al., 2001). The simulation results are in good agreement with the data, see Fig 2, and indicate that neutron-induced reactions are well described by MCHIT. All these results will appear in: L. Burigo, I. Pshenichnov, I. Mishustin, M. Bleicher. Microdosimetry of radiation fields from therapeutic ^{12}C beams in water: a study with Geant4 toolkit. (paper in preparation).

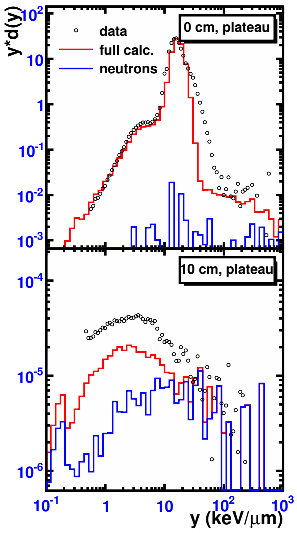


Figure 1: Microdosimetry spectra in water phantom irradiated by 300 A MeV ^{12}C nuclei. Upper (red) histograms are spectra calculated with MCHIT, lower (blue) - neutron contributions. Points - data by Martino et al., 2010.

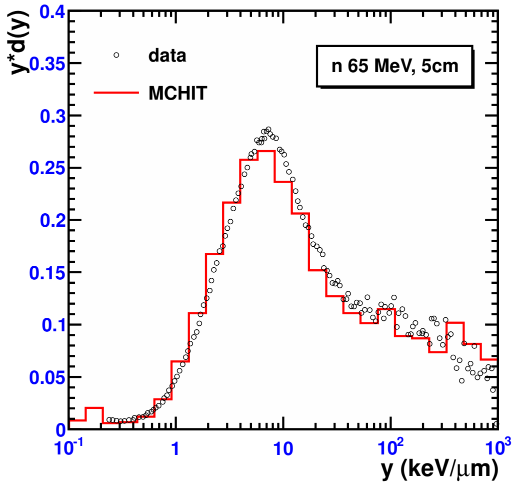


Figure 2: Microdosimetry spectra in PMMA phantom irradiated by ∼65 MeV neutrons. The histogram is a MCHIT simulation. Points – data by Nakane et al., 2001.

Related publications and talks in 2011:

1. Igor Mishustin, *MC simulations of ion-beam cancer therapy on macro and micro scales*, talk at NanoBIC Winter School (Arnoldshain, Germany, March 2, 2011).
2. L. Burigo, I. Pshenichnov, I. Mishustin, M. Bleicher, S. Schramm, *Monte Carlo simulations of ion-beam cancer therapy at macro- and microscopic scales*, talk at NanoBIC-Workshop on Structure Formation on the Nanometer Scale by Focused Energy Application, (Rauischholzhausen, Germany, October 9-11, 2011).
3. I.A. Pshenichnov, *Heavy-ion physics applied to cancer therapy: between basic science and medicine*, Bi-annual Russia-Spain conference on Particle Physics, Nuclear Physics and Astroparticle Physics (Barcelona, Spain, November 8-11, 2011).

Monte Carlo modeling of neutron production and transport in spallation targets

Collaborators: Yury Malyshkin, Igor Pshenichnov, Igor Mishustin, Walter Greiner

We study neutron production by energetic protons in extended targets made of non-fissile (e.g. tungsten) and fissile materials (e.g. uranium). Produced neutrons can be used to maintain nuclear fission reactions in a sub-critical assembly of an accelerator-driven system (ADS) designed for nuclear waste incineration. A dedicated software called MCADS (Monte Carlo for Accelerator-Driven Systems) was created in FIAS. MCADS is based on the Geant4 toolkit, which is widely employed in basic research to model propagation of particles and nuclei in extended media. The spatial distributions of neutron flux and energy deposition in the spallation target are calculated with MCADS. The even-by-event MC simulations are very useful to account for a large veriety of processes induced in the target. A history of a single 600 MeV beam proton and all secondary particles produced in a monolithic uranium target of a cylindrical shape is shown in Fig. 1 as an example.

The detailed spatial distribution of neutron flux is crucial for an ADS design process. In Fig. 2 the spatial distribution of neutron flux from 10 mA 600 MeV proton beam is shown for the uranium target . The average value of neutron flux over the whole target volume is $6.2 \cdot 10^{15}$ $n/(cm^2\ s)$, while the highest flux value of $2.5 \cdot 10^{16}$ $n/(cm^2\ s)$ is found on the beam axis at 5 cm depth.

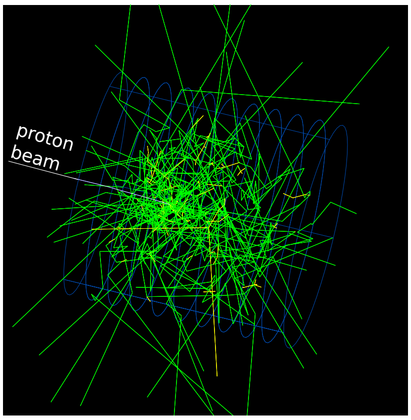


Figure 1: History of a single 600 MeV proton which hits a uranium target. Green – neutrons, yellow – gammas.

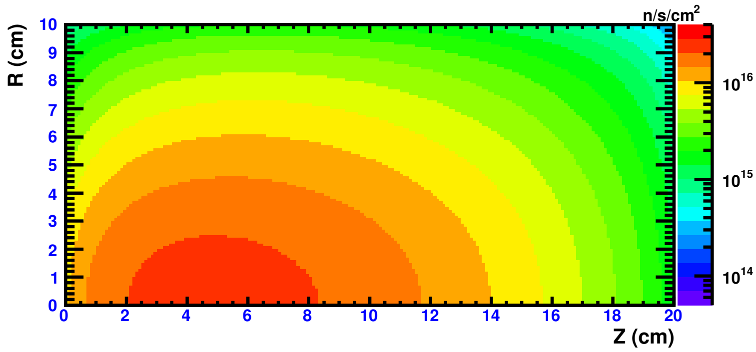


Figure 2: Spatial distribution of neutron flux inside the uranium target.

Our alculations show that by using uranium target one can obtain the same neutron yield with only 38% of the beam current needed for a non-fissile target made of tungsten. In this case the total heat deposition in fissile and non-fissile targets are similar too.

Related publications and talks in 2011:

1) Y. 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).
2) Yury Malyshkin, Igor Pshenichnov, Igor Mishustin, Timothy Hughes, Oliver Heid, Walter Greiner, *Monte Carlo modeling of neutron production and energy deposition in fissile spallation targets*, to be published in NIMB.

Monte Carlo simulation of the spallation target for the Advanced Gas-cooled Accelerator-driven Transmutation Experiment (AGATE)

Collaborators: I.A. Pshenichnov, I.N. Mishustin, W. Greiner

A concept study for a gas-cooled accelerator-driven transmutation facility AGATE [1,2] was performed in FIAS in cooperation with the Institute of Nuclear Fuel Cycle (INBK) of Aachen University, the Forschungszentrum Jülich and Siemens AG. Within the framework of the AGATE project the responsibility of the FIAS participants consisted in computer simulations of neutron production and heat deposition in several versions of a gas-cooled spallation target. Neutrons are produced in spallation reactions induced by intermediate-energy protons in collisions with heavy nuclei. Produced neutrons propagate to a subcritical reactor core placed around the spallation target. The facility is intended for transmutation of radioactive actinide nuclei which are present in spent fuel of nuclear reactors.

The considered spallation target has to be irradiated by a high-intensity proton beam to produce an intense flux of fast neutrons. A 10 mA beam of 600 MeV protons is suitable for this purpose, but such a beam creates a high thermal load on the target. Several target geometries were considered in our studies. A dedicated software application called Monte Carlo for Accelerator-Driven Systems (MCADS) was created in FIAS. MCADS is based on the Geant4 toolkit. Simulation results for various target geometries were compared to select an option with reduced total and specific heat deposition, but without essential reduction in the number of produced neutrons. Tungsten was selected as the material of the target due to its high melting point and resistance to corrosion.

Special efforts were undertaken to randomize as possible the neutron flux over the target depth in order to make it evenly distributed over the whole length (120 cm) of spent fuel elements loaded into the subcritical assembly. A segmented target consisted of 21 tungsten disks was proposed as a reliable design option, see Fig. 1. The thickness of each disk increases along the depth of penetration of the proton beam thus providing a flat distribution of the neutron flux along the beam axis, Fig. 2. The selected design option also provides better conditions for cooling with a flow of pressurised helium.

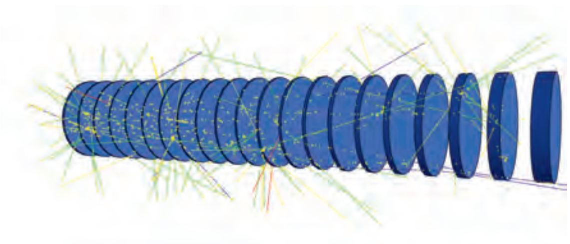


Figure 1: View of segmented target made of tungsten irradiated by 600 MeV protons from the left side

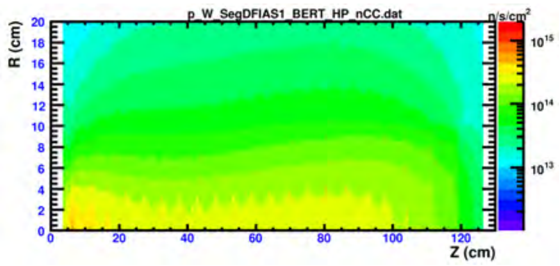


Figure 2: Spatial distribution of neutron flux from 10 mA proton beam

Related publications in 2011:

1) B. Thomauske, R. Nabbi, P. Bourauel et al., *Konzept einer gasgekühlten beschleunigergetriebenen Transmutationsanlage Advanced Gas-cooled Accelerator-driven Transmutation Experiment*, AGATE Synthese Report Aachen Nuclear Safety Reports (ANSR) Volume 1, Aachen, März 2011. http://www.inbk.rwth-aachen.de/index.php?cat=agate&lang=en

2) J. Kettler, K. Biss, K. Bongardt et al., *Advanced Gas-cooled Accelerator-driven Transmutation Experiment - AGATE*. Compact zur Jahrestagung Kerntechnik 2011, Berlin.

Production of hypermatter in relativistic heavy-ion collisions

Collaborators: Igor Mishustin, Jan Steinheimer, Konstantin Gudima, Alexander Botvina, Stefan Schramm, Horst Stöcker, Marcus Bleicher

We analyzed dilepton emission from hot and dense matter using a hybrid approach based on the Ultrarelativistic Quantum Molecular Dynamics (UrQMD) transport model with an intermediate hydrodynamic stage for the description of heavy-ion collisions at relativistic energies. During the hydrodynamic stage, the production of lepton pairs was described by radiation rates for a strongly interacting medium in thermal equilibrium. In the low mass region, hadronic thermal emission was evaluated assuming vector meson dominance including in-medium modifications of the rho meson spectral function through scattering from nucleons and pions in the heat bath. In the intermediate mass region, the hadronic rate was essentially determined by multi-pion annihilation processes. Emission from quark-antiquark annihilation in the quark gluon plasma was taken into account as well. When the system is sufficiently dilute, the hydrodynamic description breaks down and a transition to a final cascade stage was performed. In this stage dimuon emission was evaluated as commonly done in transport models. Focusing on the enhancement with respect to the contribution from long-lived hadron decays after freezout observed at the SPS in the low mass region of the dilepton spectra, the relative importance of the different thermal contributions and of the two dynamical stages is investigated. We found that three separated regions can be identified in the invariant mass spectra. Whereas the very low and the intermediate mass regions mostly receive contribution from the thermal dilepton emission, the region around the vector meson peak is dominated by the cascade emission.

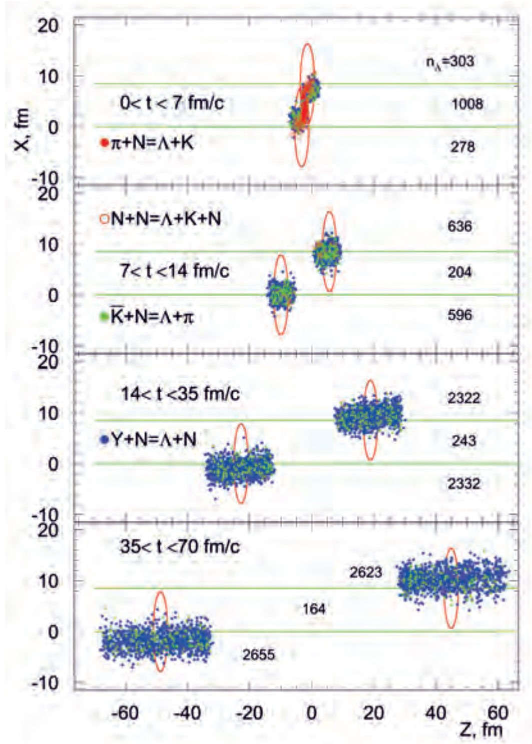


Figure: The symbols show the coordinates of absorption points in projectile and target spectators. Ellipses show the average positions of projectile and target nuclei during time intervals indicated.

Above the rho-peak region the spectrum is driven by QGP radiation. Analysis of the dimuon transverse mass spectra revealed that the thermal hadronic emission shows an evident mass ordering not present in the emission from the QGP.

This work has been supported by HIC for FAIR.

Related publications in 2011:

1) E. Santini, J. Steinheimer, M. Bleicher, S. Schramm, *Dimuon radiation at the CERN SPS within a (3+1)d hydrodynamic+cascade model*, Phys. Rev. C84, 014901 (2011). arXiv:1102.4574 [nucl-th].

2) E. Santini, B. Bäuchle, H. Petersen, J. Steinheimer, M. Nahrgang, M. Bleicher, *Hadronic and electromagnetic probes of hot and dense matter in a Boltzmann+Hydrodynamics model of relativistic nuclear collisions*, Nuovo Cim. C34N2, 119-126 (2011). arXiv:1102.1877 [hep-ph].

3) Elvira Santini, Marcus Bleicher, *Low mass dimuons within a hybrid approach*, J. Phys. Conf. Ser. 270, 012040 (2011). arXiv:1009.5266 [nucl-th].

Dimuon radiation within a (3+1)d hydrodynamic+cascade model

Collaborators: Elvira Santini, Jan Steinheimer, Hannah Petersen, Stefan Schramm, Marcus Bleicher

We analyzed dilepton emission from hot and dense matter using a hybrid approach based on the Ultrarelativistic Quantum Molecular Dynamics (UrQMD) transport model with an intermediate hydrodynamic stage for the description of heavy-ion collisions at relativistic energies. During the hydrodynamic stage, the production of lepton pairs was described by radiation rates for a strongly interacting medium in thermal equilibrium. In the low mass region, hadronic thermal emission was evaluated assuming vector meson dominance including in-medium modifications of the rho meson spectral function through scattering from nucleons and pions in the heat bath. In the intermediate mass region, the hadronic rate was essentially determined by multi-pion annihilation processes. Emission from quark-antiquark annihilation in the quark gluon plasma was taken into account as well. When the system is sufficiently dilute, the hydrodynamic description breaks down and a transition to a final cascade stage was performed. In this stage dimuon emission was evaluated as commonly done in transport models. Focusing on the enhancement with respect to the contribution from long-lived hadron decays after freezout observed at the SPS in the low mass region of the dilepton spectra, the relative importance of the different thermal contributions and of the two dynamical stages is investigated. We found that three separated regions can be identified in the invariant mass spectra. Whereas the very low and the intermediate mass regions mostly receive contribution from the thermal dilepton emission, the region around the vector meson peak is dominated by the cascade emission. Above the rho-peak region the spectrum is driven by QGP radiation. Analysis of the dimuon transverse mass spectra revealed that the thermal hadronic emission shows an evident mass ordering not present in the emission from the QGP.

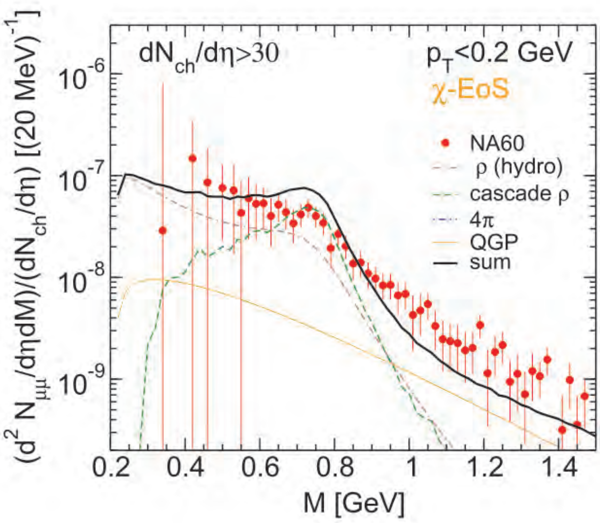


Figure: Acceptance-corrected invariant mass spectra of the excess dimuons in In-In collisions at 158A GeV.

This work has been supported by HIC for FAIR.

Related publications in 2011:

1) Marlene Nahrgang, Marcus Bleicher, Stefan Leupold, Igor Mishustin, *The impact of dissipation and noise on fluctuations in chiral fluid dynamics*, arXiv:1105.1962 [nucl-th].

2) Marlene Nahrgang, Stefan Leupold, Marcus Bleicher, *Equilibration and relaxation times at the chiral phase transition including reheating*, arXiv:1105.1396 [nucl-th].

3) Marlene Nahrgang, Stefan Leupold, Christoph Herold, Marcus Bleicher, *Nonequilibrium chiral fluid dynamics including dissipation and noise*, Phys. Rev. C84, 024912 (2011). arXiv:1105.0622 [nucl-th].

Effects of temperature dependent shear viscosity over the entropy density ratio on elliptic flow in ultrarelativistic heavy-ion collisions

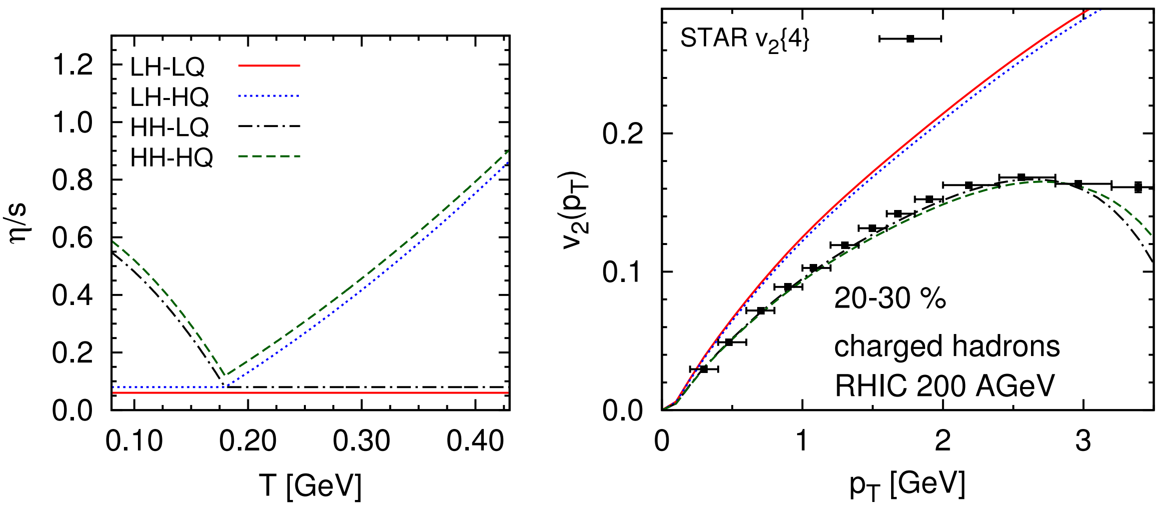
Collaborators: G.S. Denicol[1], P. Huovinen[1], E. Molnár[2,3], H. Niemi[2,4], D.H. Rischke[1,2]

[1]Institut für Theoretische Physik, Johann Wolfgang Goethe-Universität, [2]Frankfurt Institute for Advanced Studies, [3]MTA Wigner Research Centre for Physics, Budapest, Hungary, [4]Department of Physics, University of Jyväskylä, Finland

Presently, most hydrodynamical models of ultrarelativistic heavy-ion collisions assume a constant, temperature-independent shear viscosity to entropy ratio η/s. In several works it has been claimed that in order to describe elliptic flow data, this constant value cannot be significantly larger than the lower bound $\eta/s = 1/4\pi$ conjectured in the framework of the AdS/CFT correspondence. A constant η/s is, however, in contrast to the typical behavior observed in common fluids, where η/s has a strong temperature dependence and, typically, a minimum near phase transitions. A similar behavior of η/s is expected for finite-temperature matter described by quantum chromodynamics (QCD) near the transition from hadronic matter to the QGP (the QCD phase transition). We have investigated a question, whether the temperature dependence of η/s has an effect on the collective flow of hadrons in heavy-ion collisions.

In Au+Au collisions at RHIC, we find almost no difference in elliptic flow whether η/s is constant in the QGP phase or strongly increasing with temperature. In contrast, the elliptic flow is highly sensitive to the values of η/s in the low-temperature hadronic phase. On the other hand, we found that the sensitivity of the elliptic flow to the values of η/s in the high-temperature QGP increases with increasing collision energy, while the effect of the hadronic viscosity decreases. At the highest LHC energy, the above conclusion for RHIC energies is reversed: suppression of the elliptic flow is dominated by the viscosity of the QGP and insensitive to that of the hadronic phase.

The insensitivity of the elliptic flow to the high-temperature shear viscosity in Au+Au collisions at RHIC is illustrated in the Figure below, where our result from the hydrodynamical simulations are compared with the data from the STAR Collaboration.



Left: The parametrizations of η/s as a function of temperature *Right:* Elliptic flow of charged hadrons in 20-30 % centrality class in Au+Au collisions at RHIC. The data is 4-particle cumulant data from the STAR Collaboration

Related publications in 2011:

1) H. Niemi, G. S. Denicol, P. Huovinen, E. Molnar and D. H. Rischke, *Influence of the shear viscosity of the quark-gluon plasma on elliptic flow in ultrarelativistic heavy-ion collisions*, Phys. Rev. Lett. **106** (2011) 212302.

Initial state anisotropies and their uncertainties in ultrarelativistic heavy-ion collisions from the Monte Carlo Glauber model

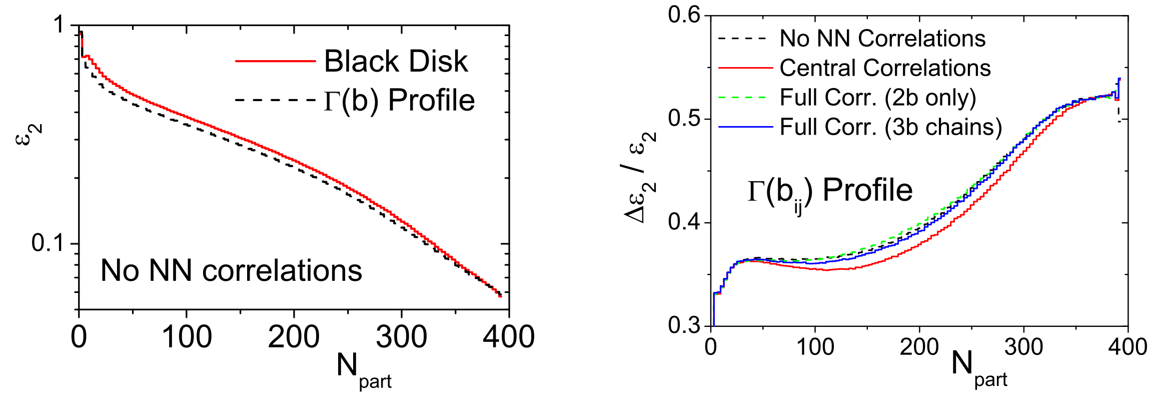
Collaborators: M. Alvioli[1], H. Holopainen[2,3,4], K.J. Eskola[3,4], M. Strikman[5]

[1] ECT*, European Centre for Theoretical Studies in Nuclear Physics and Related Areas, [2] Frankfurt Institute for Advanced Studies, [3] University of Jyväskylä, [4] Helsinki Institute of Physics, [5] The Pennsylvania State University

Significant azimuthal momentum distribution anisotropies measured in ultrarelativistic heavy-ion collisions can be explained with relativistic hydrodynamics: the initially produced QCD-matter contains spatial anisotropies and during the hydrodynamical evolution these anisotropies are transferred to the momentum distributions of final state particles. In this work we consider two sources of uncertainties related to the Monte Carlo Glauber (MCG) model which is often used to initialize the hydrodynamical simulations. All results are for Au+Au collisions at $\sqrt{s_{NN}} = 200$ GeV.

In the MCG modeling one needs to know the positions of the initial state nucleon configurations. In most cases the nucleon positions inside the colliding nuclei are sampled using the Woods-Saxon potential, neglecting nucleon-nucleon correlations. Here we studied the effects of realistically correlated configurations on initial anisotropies. In addition, we used two different nucleon-nucleon interaction models. In the *black disk* approach two nucleons collide always when their transverse separation b is small enough, while in the *profile function* ($\Gamma(b)$) approach we have a transverse separation dependent probability for the collision to happen.

First we considered the different interaction models, neglecting all nucleon-nucleon correlations for simplicity. We saw that for every ε_n with $n = 1,2,3$ the black disk interaction model leads to larger anisotropies. In central collisions the difference between different interaction models is small and it grows towards peripheral collisions. At largest the difference is order of 10%.



Left: Eccentricity as a function of number of participants (N_{part}) with two different nucleon-nucleon interaction models. *Right:* The relative fluctuations of eccentricity as a function of N_{part} with different nucleon-nucleon correlations.

Next we studied the effects of the nucleon-nucleon correlations. We studied four different cases here: no correlations, central correlations and two sets with different approximations of full correlations. We found that including only central correlations makes the anisotropies smaller (by at most 10-20%), while the full correlations return the results quite close back to the no correlations case. The effects of the correlations are largest in the most central collisions and the difference gets smaller in the more peripheral collisions. As far as the relative fluctuations of the anisotropies are concerned, we found that the full correlations reduce the effects produced by the central ones to a very small deviation from the uncorrelated case.

Related publication in 2011:

1) M. Alvioli, H. Holopainen, K.J. Eskola, M. Strikman, *Initial state anisotropies and their uncertainties in ultrarelativistic heavy-ion collisions from the Monte Carlo Glauber model*, arXiv:1112.5306 [hep-ph].

Aspects of transport coefficients in relativistic hydrodynamics

Collaborators: X. G. Huang[1,2], P. Huovinen[1,2], K. Kodama[3], T. Koide[1,3], D. H. Rischke[1,2], A. Sedrakian[2]

[1] Frankfurt Institute for Advanced Studies, [2] Institute for Theoretical Physics, Frankfurt, Germany [3] Instituto de Fisica, Universidade Federal do Rio de Janeiro, Rio de Janeiro, Brasil

Relativistic hydrodynamics is one of the most often used approaches in studying the collective phenomena in heavy-ion collisions, supernova explosions, and neutron stars. However, including viscosities in the relativistic hydrodynamics is not easy. A naive relativistic generalization of Navier-Stokes theory does not work, because it violates causality and is usually unstable, and hence does not permit numerical simulations. A solution to this problem has been known since works of Mueller, and Israel and Stewart more than 30 years ago, and the resulting theory is usually called second-order hydrodynamics. Different from Navier-Stokes theory where the viscous stress tensors Π and $\pi^{\mu\nu}$ are completely fixed by the distribution of velocity fields, in second-order hydrodynamics, Π and $\pi^{\mu\nu}$ are treated as independent dynamical variables which should be solved simultaneously with the velocity fields. As was proven, second-order hydrodynamics is causal and stable, but the cost is the appearance of new transport coefficients. The microscopic formulas for the shear viscosity η, the bulk viscosity ζ and corresponding relaxation times τ_π and τ_Π of causal dissipative relativistic fluid-dynamics are obtained at finite temperature and chemical potential by using the projection operator method. The non-triviality of the finite chemical potential calculation is attributed to the arbitrariness of the operator definition of the bulk viscous pressure. We show that, when the operator definition for the bulk viscous pressure Π is appropriately chosen, the leading order result of the ratio of ζ and τ_Π coincides with the same ratio obtained at vanishing chemical potential. In applying these formulae to the pionic fluid, we find that the renormalizable energy-momentum tensor should be employed to obtain consistent results.

Quarks produced in the early stage of non-central heavy-ion collisions could develop a global spin polarization along the opposite direction of the reaction plane due to the spin-orbital coupling via parton interaction in a medium that has finite longitudinal flow shear along the direction of the impact parameter. We study how such polarization evolves via multiple scattering in a viscous quark-gluon plasma with an initial laminar flow. The final polarization is found to be sensitive to the viscosity and the initial shear of local longitudinal flow.

Relativistic magnetohydrodynamics of strongly magnetized relativistic fluids is derived in the ideal and dissipative cases, taking into account the breaking of spatial symmetries by a quantizing magnetic field. A complete set of transport coefficients, consistent with the Curie and Onsager principles, is derived for thermal conduction, as well as shear and bulk viscosities. It is shown that in the most general case the dissipative function contains five shear viscosities, two bulk viscosities, and three thermal conductivity coefficients. We use Zubarev's non-equilibrium statistical operator method to relate these transport coefficients to correlation functions of equilibrium theory. The desired relations emerge at linear order in the expansion of the non-equilibrium statistical operator with respect to the gradients of relevant statistical parameters (temperature, chemical potential, and velocity.) The transport coefficients are cast in a form that can be conveniently computed using equilibrium (imaginary-time) infrared Green's functions defined with respect to the equilibrium statistical operator.

Related publications in 2011:

1) X. -G. Huang, P. Huovinen and X. -N. Wang, *Quark polarization in a viscous quark-gluon plasma*, Phys. Rev. C84, 054910 (2011)

2) X. -G. Huang, A. Sedrakian and D. H. Rischke, *Kubo formulas for relativistic fluids in strong magnetic fields*, Annals Phys. 326, 3075 (2011)

3) X. -G. Huang and T. Koide, *Shear viscosity, bulk viscosity and relaxation times of causal dissipative relativistic fluid-dynamics at finite temperature and chemical potential*, arXiv:1105.2483 [hep-th]

4) X. -G. Huang, T. Kodama, T. Koide and D. H. Rischke, *Bulk viscosity and relaxation time of causal dissipative relativistic fluid dynamics*, Phys. Rev. C83, 024906 (2011)

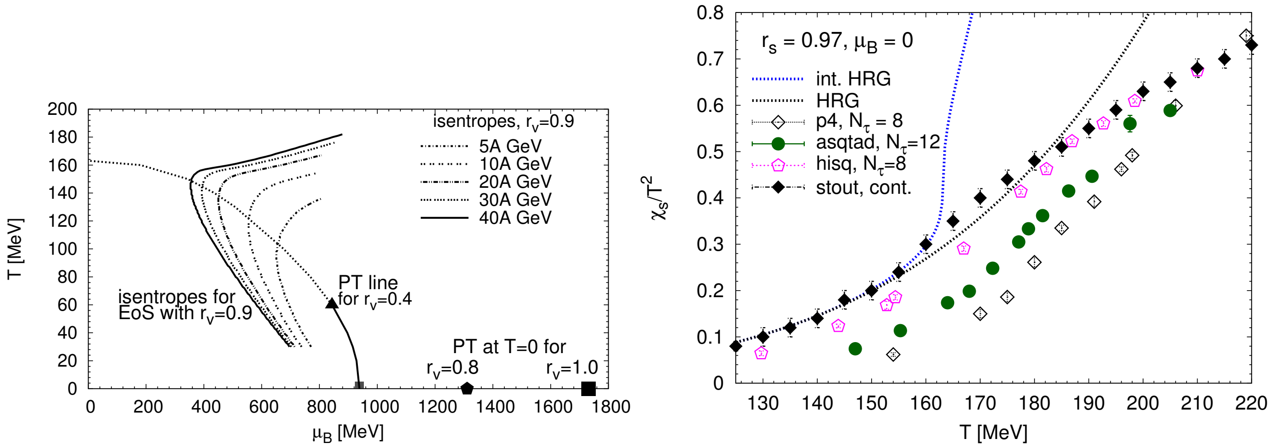
Chiral hadronic model including resonances

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

[1] FIAS, [2] Institut für Theoretische Physik, Goethe Universität Frankfurt, [3] GSI - Helmholtzzentrum für Schwerionenforschung, Darmstadt.

We extended the existing effective chiral flavour SU(3) model for the QCD equation of state which was developed in Frankfurt over the last years to include all hadronic resonances up to masses of $m \leq 2.6$ GeV. All particles are coupled to the scalar σ-field and the vector ω-field. We introduce a parameter r_v controlling the coupling strength to the repulsive vector fields and thus primarily affecting the particles' abundancies. Therefore, by varying r_v we are able to study the impact of heavier resonances on the phase diagram of strongly interacting matter with particular interest on the chiral phase transition.

By studying the thermodynamic properties of our model we observe a good agreement to latest continuum extrapolated lattice data if we chose a physically reasonable vector coupling close to one. This finding is supported by our results for the susceptibilities of conserved charges on the phase transition which are again comparable to lattice QCD for $r_v \sim 1$. However, in this case our model rules out a first order phase transition in favour of a smooth cross over transition not only at vanishing baryochemical potentials $\mu_B = 0$ but in the whole μ_B-regime ruling out the postulated existence of a critical end point.



a): QCD phase diagram from our model with isentropes for various beam energies for a vector coupling $r_v \sim 1$ where there is only a broad crossover phase transition. The shown phase transition line depicts the situation for the lowest reasonable coupling strength $r_v = 0.4$. **b):** Strange quark susceptibility from our model at $\mu_B = 0$ (blue dashed line) compared to lattice QCD results from various lattice actions. Good agreement is obtained with latest continuum extrapolated data up to the critical temperature T_c.

Related publications in 2011:

1) P. Rau, J. Steinheimer, S. Schramm and H. Stöcker, *Baryon resonances in a chiral hadronic model for the qcd equation of state*, arXiv:1109.3621 [hep-ph], accepted by Phys. Rev. C.

2) P. Rau, J. Steinheimer, S. Schramm and H. Stöcker, *Resonance states in an effective chiral hadronic model*, arXiv:1201.3834 [hep-ph].

The phase structure of a chiral model with dilatons in hot and dense matter

Collaborators: C. Sasaki[1], I. Mishustin[1,2]

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

In this work we have studied thermodynamics and the phase structure of a QCD-like model whose degrees of freedom are constituent quarks and gluons. Both chiral and scale symmetries are implemented in the model by introducing mean fields representing $\bar{q}q$ and $G_{\mu\nu}G^{\mu\nu}$. These symmetries are dynamically broken at low temperature and density. The model thus mimics the features of QCD in the strong coupling region, i.e. the spontaneous breaking of chiral symmetry and trace anomaly. The results suggest that a system in deconfined phase develops gradually with increasing temperature/density toward weakly-interacting quark-gluon matter composed of almost massless quarks and gluons. Our model improves the standard linear sigma model by introducing missing gluons and EoS, energy density in particular, shows a good agreement with the expected high-temperature (see Fig. 1 left).

The condensates of the sigma and dilaton fields are dynamically linked via their gap equations. How strong they are correlated depends crucially on the sigma-meson mass m_σ chosen in vacuum (see Fig. 1 right). We found that a large $m_\sigma \sim 1$ GeV is consistent with the lattice result regarding the thermal behavior of the gluon condensate. This further leads to the chiral phase transition which takes place almost simultaneously with the deconfinement transition at $\mu \sim 0$. At finite μ these two transitions are expected to be separated.

The present model can also be applied to a non-equilibrium system, where the time evolution of the gluon condensate is described by the equation of motion for the dilaton. On the other hand, in several models with Polyakov loops it is unclear how the kinetic term of the Polyakov loop dynamically emerges since the Polyakov loop by itself does not represent a field but a character of the SU(3) color group. It would be interesting to explore non-equilibrium dynamics along this line.

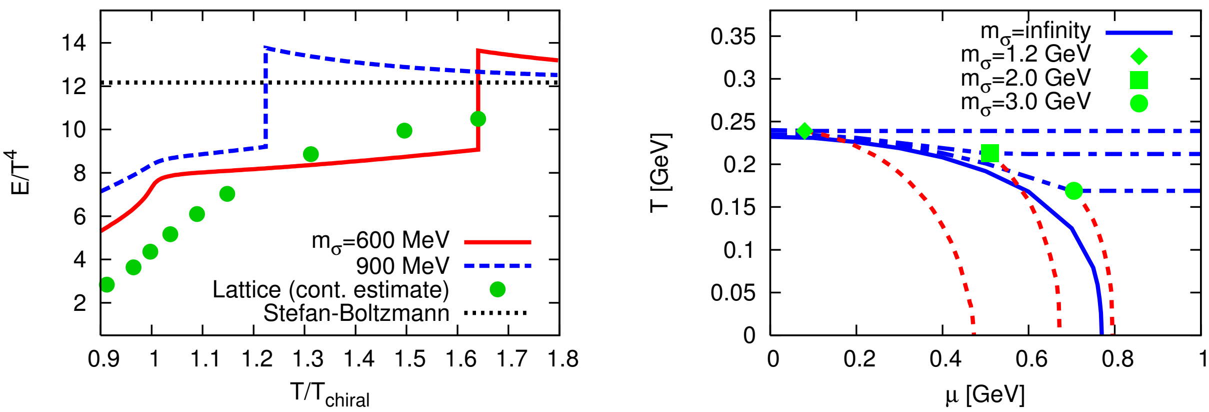


Figure 1: (Left) The scaled energy density at $\mu = 0$. (Right) The phase diagram of our model for several m_σ.

Related publication in 2011:

1) C. Sasaki and I. Mishustin, *The phase structure of a chiral model with dilatons in hot and dense matter*, arXiv:1110.3498 [hep-ph], accepted for publication in Physical Review C.

Trace anomaly and the vector coupling in dense matter

Collaborators: C. Sasaki[1], H.K. Lee[2], W.-G. Paeng[2], M. Rho[2,3]

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In nuclear physics, a scalar meson plays an essential role as known from Walecka model that works fairly well for phenomena near nuclear matter density. On the other hand, at high density, the relevant Lagrangian that has correct symmetry is the linear sigma model, and the scalar needed there is the fourth component of the chiral four-vector $(\vec{\pi},\sigma)$. Thus in order to probe highly hot/dense matter, we have to figure out how the chiral scalar at low temperature/density transmutes to the fourth component of the four-vector.

In this work we have presented how an effective theory near chiral symmetry restoration emerges from the dilaton-implemented HLS Lagrangian as illustrated in Fig. 1, and discussed its phenomenological implications at high baryon density. The soft dilaton is responsible for the spontaneous breaking of the scale symmetry and its condensate vanishes when the chiral symmetry is restored. In fact, topological stability of the half-skyrmion phase has been observed. This is a strong indication that the configuration is robust and it could be associated with the scale symmetry restoration at high density in continuum theories.

Our main observation on the suppressed repulsive interaction is a common feature in the two different assignments, "naive" and mirror, of chirality. The nucleon mass near chiral symmetry restoration exhibits a striking difference in the two scenarios. How the suppression of the repulsion at the dilaton limit – which seems to be universal independent of the assignments but may manifest itself differently in the two cases – will affect the EoS for compact stars is an interesting question to investigate.

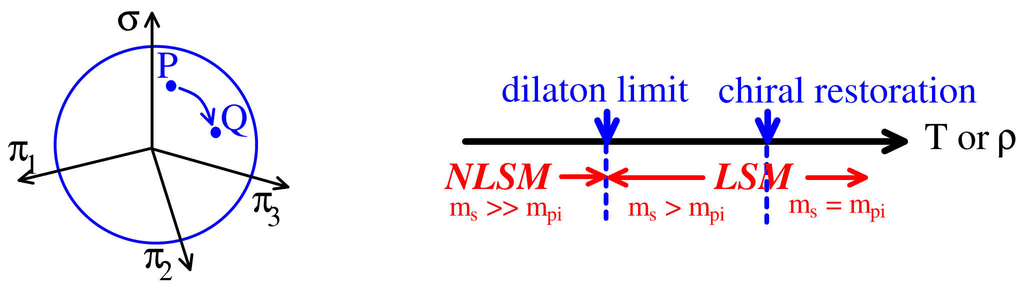

Figure 1: (Left) A chiral sphere in $(\vec{\pi},\sigma)$ space. P on the sphere is mapped to another point Q via chiral transformations. (Right) Expected changeover of effective theories near chiral symmetry restoration.

Related publications in 2011:

1) C. Sasaki, H. K. Lee, W. -G. Paeng and M. Rho, *Conformal anomaly and the vector coupling in dense matter*, Phys. Rev. D84, 034011 (2011), arXiv:1103.0184 [hep-ph].
2) W. -G. Paeng, H. K. Lee, M. Rho and C. Sasaki, *Dilaton-limit fixed point in hidden local symmetric parity doublet model*, arXiv:1109.5431 [hep-ph], submitted to Physical Review D.

Dynamical equilibration of the strongly-interacting parton matter

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

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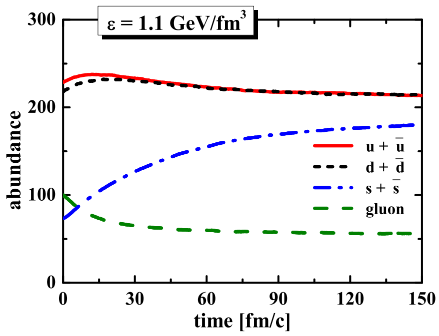
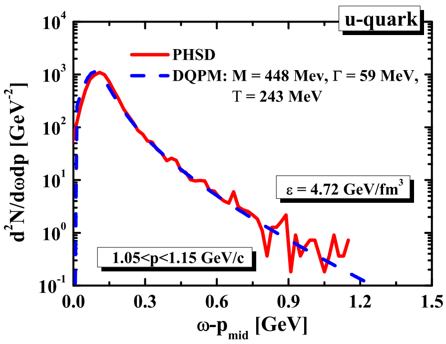
We study kinetic and chemical equilibration in 'infinite' parton-hadron matter within the Parton-Hadron-String Dynamics (PHSD) transport approach, which is based on generalized transport equations on the basis of the off-shell Kadanoff-Baym equations for Green's functions in phase-space representation. The basis of the partonic phase description is the dynamical quasiparticle model (DQPM) matched to reproduce lattice QCD results – including the partonic equation of state – in thermodynamic equilibrium. The transition from partonic to hadronic degrees of freedom is described by covariant transition rates for fusion of quark-antiquark pairs or three quarks (antiquarks), obeying flavor current conservation, color neutrality as well as energy-momentum conservation.

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. We start with light (u,d) and strange quarks, antiquarks and gluons with random space positions and the momenta distributed exponentially, but *not with equilibrium* distribution.

A sign for chemical equilibration is the stabilization of the numbers of partons of the different species in time for $t \to \infty$. In Fig. 1(a) we show the particle abundances of the u,d,s quarks+antiquarks and gluons as functions of time for system initialized at energy density of 1.1 GeV/fm^3.



(a)



(b)

(a) Abundances of the u (solid red), d (short-dashed black), s (dash-dotted blue) quarks+antiquarks and gluons (dashed green) as a function of time for system initialized at energy density of 1.1 GeV/fm^3. (b) The spectrum of u quarks (antiquarks) for system initialized at energy density of 4.72 GeV/fm^3 from the PHSD simulations (solid red) in comparison to the DQPM model (dashed blue).

Choosing the momenta of the partons in the narrow interval $|\mathbf{p}| \in [p_-, p_+]$, we construct the distribution of partons with given energy and momentum as

$$\frac{dN_{g(q,\bar{q})}}{d\omega dp} = \frac{V d_{g(q,\bar{q})}}{2\pi^3} |p_{mid}|^2 \omega \rho_{g(q,\bar{q})}(\omega, p_{mid}) n_{B(F)}(\omega/T), \quad (1)$$

where $p_{mid} = (p_+ - p_-)/2$. In Fig. 1(b) we show $d^2N/d\omega dp$ for u quarks obtained by the PHSD simulations of infinite partonic system as initialized at energy density of 4.72 GeV/fm^3. For comparison, we present on the same plot the DQPM assumption for the respective distribution. We find a good agreement between the DQPM distribution and the result of the microscopic simulations.

Related publication in 2011:

V. Ozvenchuk, E. Bratkovskaya, O. Linnyk, M. Gorenstein, W. Cassing, arXiv:1101.0218v1 [nucl-th].

Dileptons from the strongly interacting quark-gluon plasma (sQGP)

Collaborators: O. Linnyk[1,3], E. L. Bratkovskaya[1,2], V. Ozvenchuk[2], J. Manninen[1,3], W. Cassing[3], C.M. Ko[4]

[1] Institut für Theoretische Physik, Goethe Universität Frankfurt am Main, Germany, [2] Frankfurt Institute for Advanced Studies, Germany, [3] Institut für Theoretische Physik, Justus Liebig Universität Gießen, Germany [4] Cyclotron Institute and Department of Physics and Astronomy, Texas A&M University, College Station, Texas, USA

We address dilepton production in Au+Au collisions at $\sqrt{s_{NN}} = 200$ GeV by employing the parton-hadron-string dynamics (PHSD) off-shell transport approach [3,4,6]. Within the PHSD one solves generalized transport equations and consistently describes the full evolution of a relativistic heavy-ion collision [2]. We calculated the dilepton radiation from partonic interactions through the reactions $q\bar{q} \to \gamma^*$, $q\bar{q} \to \gamma^* + g$ and $qg \to \gamma^* q$ ($\bar{q}g \to \gamma^* \bar{q}$) in the early stage of relativistic heavy-ion collisions with the differential cross sections for electromagnetic radiation calculated with the same propagators as those incorporated in the PHSD transport approach [1]. By comparing our calculated results [3,4] to the data, we have studied the relative importance of different dilepton production mechanisms and addressed in particular the 'PHENIX puzzle' of a large enhancement of dileptons in the mass range from 0.15 to 0.6 GeV as compared to the emission of hadronic states. Similar to our findings at SPS energies [5], we find that the partonic dilepton production channels are visible in the intermediate-mass region between the ϕ and J/Ψ peaks [3,4,6,9]. Our studies have demonstrated that the observed excess in the low mass dilepton regime cannot be attributed to partonic productions as expected earlier. Thus the 'PHENIX puzzle' still has no explanation from the theoretical approaches so far. The solution has to be relegated to the experimental side. In fact, the STAR collaboration has taken independent dilepton data for centralities different from the PHENIX measurements and also with different detector acceptances. Our calculations allow to match with the different experimental conditions and thus to provide a 'theoretical link' between the different measurements. To this extent, we have provided our predictions for the conditions of the STAR experiment, which happen to be in a rough agreement with the preliminary data [4].

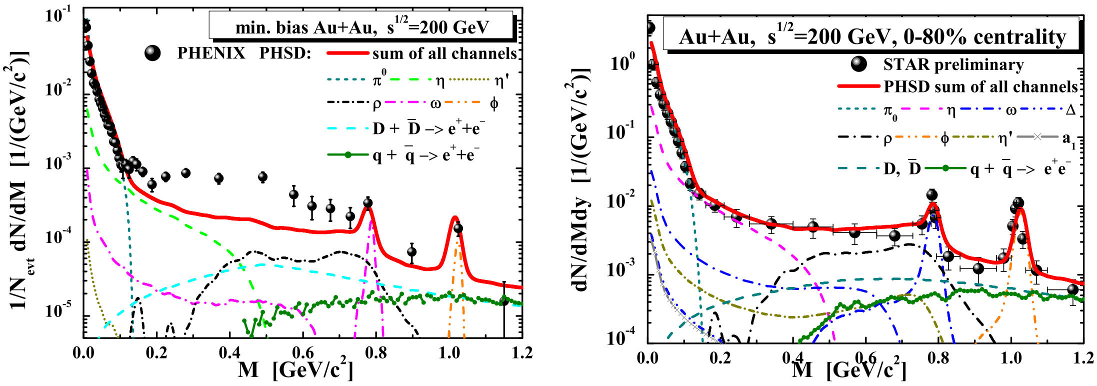


Figure 1: The PHSD results for the mass differential dilepton spectra in case of inclusive $Au+Au$ collisions at $\sqrt{s} = 200$ GeV in comparison to the data from PHENIX (left pannel) and STAR (right pannel) Collaborations.

Related publications in 2011:

1) O. Linnyk, J. Phys. G38 (2011) 025105.
2) E.L. Bratkovskaya, W. Cassing, V.P. Konchakovski, O. Linnyk, Nucl. Phys. A856 (2011) 162.
3) O. Linnyk, W. Cassing, E.L. Bratkovskaya, J. Manninen, Nucl. Phys. A855 (2011) 273.
4) O. Linnyk, W. Cassing, J. Manninen, E.L. Bratkovskaya, C.M. Ko, arXiv:1111.2975, Phys. Rev. C (in print).
5) O. Linnyk, E.L. Bratkovskaya, V. Ozvenchuk, W. Cassing, C.M. Ko, Phys. Rev. C84 (2011) 054917.
6) J. Manninen, E.L. Bratkovskaya, W. Cassing, O. Linnyk, Eur. Phys. J. C71 (2011) 1615.
7) O. Linnyk, E.L. Bratkovskaya, W. Cassing, J. Phys. Conf. Ser. 316 (2011) 012028.
8) O. Linnyk, E.L. Bratkovskaya, J. Manninen, W. Cassing, J. Phys. Conf. Ser. 312 (2011) 012010.
9) J. Manninen, E.L. Bratkovskaya, W. Cassing, O.Linnyk, J. Phys. Conf. Ser. 270 (2011) 012039.
10) O. Linnyk, E.L. Bratkovskaya, W. Cassing, PoS BORMIO2011 (2011) 029.

Rise of v_2 as a signature of the Quark-Gluon-Plasma

Collaborators: E. L. Bratkovskaya[1], W. Cassing[2], V. P. Konchakovski[2], V. D. Toneev[1,3], V. Voronyuk[1,3]

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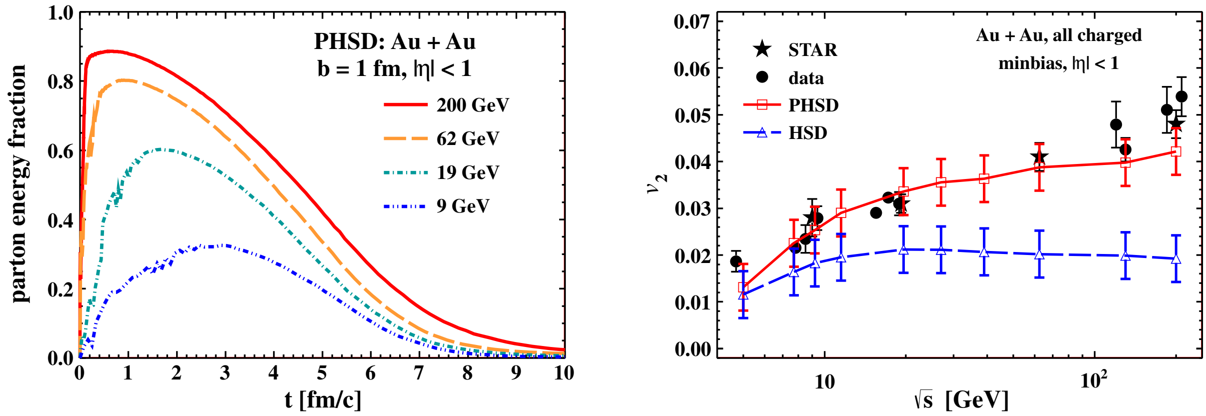
A large number of anisotropic flow measurements have been performed by many experimental groups at SIS, AGS, SPS and RHIC energies over the past 20 years. Very recently the azimuthal asymmetry has also been measured at the Large Hadron Collider (LHC) at CERN. The Beam Energy Scan (BES) program proposed at RHIC covers the energy interval from $\sqrt{s_{NN}} = 200$ GeV, where partonic degrees of freedom (DOF) play a decisive role, down to the AGS energy $\sqrt{s_{NN}} \approx 5$ GeV.



Left: The evolution of the parton fraction of the total energy density at the mid-pseudorapidity for different collision energies. *Right:* Average elliptic flow v_2 of charged particles at midrapidity calculated within the PHSD (solid curves) and HSD (dashed curves) approaches in comparison to the STAR data compilation for minimal bias collisions.

The increase of elliptic flow v_2 on the right panel is clarified on the left panel of the figure where the partonic fraction of the energy density at mid-pseudorapidity with respect to the total energy density in the same pseudorapidity interval is shown. We recall that the repulsive scalar mean field potential $U_s(\rho_s)$ for partons in the PHSD model leads to an increase of the flow v_2 as compared to that for HSD calculations without partonic mean fields. As seen from the Figure, the energy fraction of the partons substantially grows with increasing bombarding energy while the duration of the partonic phase is roughly the same.

The elliptic flow v_2 is reasonably described within the PHSD model in the whole transient energy range naturally connecting the hadronic processes at moderate bombarding energies with ultrarelativistic collisions at RHIC energies where the quark-gluon DOF become dominant due to a growing number of partons. The smooth growth of the elliptic flow with collision energy demonstrates the increasing importance of partonic DOF This feature is reproduced by neither explicit hadronic kinetic models like HSD or UrQMD nor the AMPT model treating the partonic phase on the basis of pQCD with massless partons and a noninteracting equation-of-state for the partons. Further signatures of the transverse collective flow, the higher-order harmonics of the transverse anisotropy v_3 and v_4 change only weakly from $\sqrt{s_{NN}} \approx 7$ GeV to the top RHIC energy $\sqrt{s_{NN}} = 200$ GeV, roughly in agreement with preliminary experimental data.

Related publication in 2011:

1) V. P. Konchakovski, E. L. Bratkovskaya, W. Cassing, V. D. Toneev and V. Voronyuk, *Rise of azimuthal anisotropies as a signature of the Quark-Gluon-Plasma in relativistic heavy-ion collisions*, arXiv:1109.3039 [nucl-th].

Space-time evolution of the magnetic field in relativistic heavy-ion collisions

V. P. Konchakovski[1], E. L. Bratkovskaya[2,3], W. Cassing[1], V. D. Toneev[3,4], and V. Voronyuk[3,4]
[1]ITP, Uni-Giessen, Germany; [2]ITP, Uni-Frankfurt, Germany; [3]FIAS, Frankfurt, Germany; [4]JINR, Dubna, Russia

In dense QCD matter in the presence of an external magnetic field and/or topological defects, a spontaneous creation of axial currents may happen. The presence of a magnetic field also favors the formation of spatially inhomogeneous spiral-like quark condensate configurations at low temperatures and non-zero chemical potentials. The influence of a constant magnetic field on possible color-superconducting phases (the color Meissner effect) has also actively been discussed. A clarification of such phenomena by experimental observations requires e.g. the production of QCD matter in relativistic heavy-ion collisions where in non-central reactions strong electromagnetic fields are created by the charged four-current of the spectators.

We study the space-time evolution of electromagnetic fields formed in relativistic heavy-ion collisions. The Hadron String Dynamics (HSD) transport approach, which solves Kadanoff-Baym equations and treats the nuclear collisions in terms of quasiparticles with a finite width, is used as a basis of our considerations. In our approach the dynamical formation of the electromagnetic field, its evolution during a collision and influence on the quasiparticle dynamics as well as the interplay of the created electromagnetic field and back-reaction effects are included simultaneously. The set of transport equations is solved in a quasiparticle approximation by using the Monte-Carlo parallel ensemble method. To find the electromagnetic field, a space-time grid is used. The quasiparticle propagation in the retarded electromagnetic field is calculated as:

$$\frac{d\mathbf{p}}{dt} = e\mathbf{E} + \frac{e}{c}\mathbf{v} \times \mathbf{B} \,. \qquad (1)$$

The time evolution of $eB_y(x, y = 0, z)$ for Au+Au collisions for the colliding energy $\sqrt{s_{NN}}$ =200 GeV at the impact parameter $b = 10$ fm is shown in Fig. 1. If the impact parameter direction is taken as the x axis (as in the present calculations), then the magnetic field will be directed along the y-axis perpendicularly to the reaction plane $(z - x)$. The geometry of the colliding system at the moment considered is demonstrated by points in the $(z-x)$ plain where every point corresponds to a spectator nucleon. It is seen that the largest values of $eB_y \sim 5m_\pi^2$ are reached in the beginning of a collision for a very short time corresponding to the maximal overlap of the colliding ions. Note that this is an extremely high magnetic field, since $m_\pi^2 \approx 10^{18}$ gauss. The first panel in Fig. 1 is taken at a very early compression stage with $t = 0.01$ fm/c. The next panel shows configuration of the magnetic field at the time $t = 0.2$ fm/c. Then, the system expands (note the different z-scales in the different panels of Fig. 1) and the magnetic field decreases. For $b = 0$ the overlap time is maximal and roughly given by $2R/\gamma_c$ which for our case is about 0.15 fm/c. For peripheral collisions this time is even shorter.

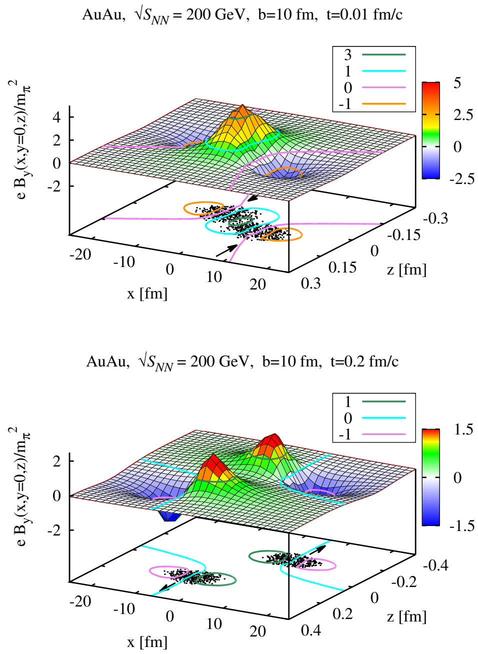


Figure 1: Time dependence of the spatial distribution of the magnetic field B_y at times t created in Au+Au ($\sqrt{s}$=200 GeV) collisions with the impact parameter b =10 fm. The location of spectator protons is shown by dots in the $(x-z)$-plane. The level $B_y = 0$ and the projection of its location on the $(x - z)$ plane is shown by the solid lines.

Globally, the spatial distribution of the magnetic field is evidently inhomogeneous and Lorentz-contracted along the z-axis. At the compression stage there is a single maximum which in the expansion stage is splitted into two parts associated with the spectators. In the transverse direction the bulk magnetic field is limited by two minima coming from the torqued structure of the single-charge field. See references [1,2] for more details.

Related publications in 2011:

1) V. Voronyuk, V. D. Toneev, W. Cassing, E. L. Bratkovskaya, V. P. Konchakovski and S. A. Voloshin, Phys. Rev. C83, 054911 (2011).
2) V. D. Toneev, V. Voronyuk, E. L. Bratkovskaya, W. Cassing, V. P. Konchakovski and S. A. Voloshin, arXiv:1112.2595 [hep-ph].

Research Projects of Prof. Reinhard Stock

Project 1: Investigation of hadronic fluctuations in relativistic nuclear collisions

Collaborators: Tim Schuster[1], Thosten Kollegger[1], Reinhard Stock[1] with the CERN NA49 Collaboration
[1] Frankfurt Institute for Advanced Studies

We have investigated the event-by-event-fluctuation of hadrons produced in central collisions of Pb+Pb at five energies at the CERN SPS. More precisely: the ratios of Kaon to Pion and Kaon to Proton eventwise fluctuation, which are predicted to be sensitive to the existence of a "critical point" of QCD that was recently conjectured in lattice QCD calculations at finite baryochemical potential. The CERN SPS energy interval covered by our investigation coincides with the energy domain of critical point occurence, envisioned in the Lattice calculations. The analyzed data were gathered by our NA49 experiment in 2002. We indeed observe small amplitude fluctuations of these hadron ratios. For the Kaon to Pion event by event fluctuation this fluctuation could be traced to finite number statistics effects inherent in the studied observable, However, the Kaon to Proton ratio fluctuation exhibits a steep rise toward the low energy end of the studied interval, for which no such "trivial" explanation could be found. The theoretical discussion is still going on.

Project 2: Hadronization, and the hadronic freeze-out curve in relativistic nuclear collisions

Collaborators: Marcus Bleicher[1], Thosten Kollegger[1], Tim Schuster[1], Reinhard Stock[1], Francesco Becattini[2], Michael Mitrovski[3]
[1] Frankfurt Institute for Advanced Studies, [2] University of Florence, Italy, [3] Brookhaven National Laboratory, NY, USA

One of the outstanding open questions of relativistic nuclear collision research consists of the observation of a global statistical equilibrium among all produced hadron/resonance species. This "hadro-chemical" equilibrium is captured within the Grand Canonical Gibbs ensemble. Its principal parameters, temperature T and baryochemical potential μ_B, as determined at a multitude of different incident energies, establish the so-called "hadronic freeze-out curve". Its most spectacular aspect: it merges, closely, with the confinement/deconfinement line (between partons and hadrons) predicted by recent Lattice QCD, at temperature of about 165 MeV. Have we thus located, semi-experimentally, this main quantity of QCD matter: the "critical temperature"? We investigate the question of how such a hadronic species equilibrium can survive the final expansion cascade of hadrons that is characteristic for a nucleus-nucleus-collision. To this end we employ the microscopic hadron transport model UrQMD that was developed in the Frankfurt Theory Group. We propose certain corrections to the freeze-out curve but confirm its relevance indicated above.

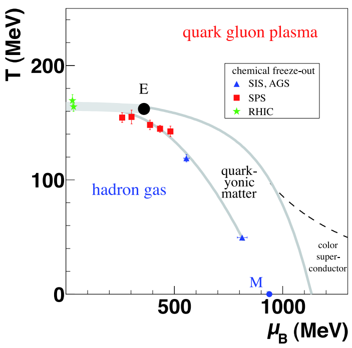


Figure: Sketch of the QCD phase diagram, showing the parton-hadron coexistence boundary line, inferred from lattice QCD at low μ_B, and from chiral restoration theory at high μ_B and, second, the hadronic freeze-out curve of the statistical model.

Related publications in 2011:

1) T. Schuster and NA49 Collaboration, *New results on event-by-event ratio fluctuations in Pb+Pb collisions at CERN SPS energies*, J. Phys. G 38, 124096 (2011)
2) T. Anticic et al. (NA49 Collaboration), *Energy dependence of kaon-to-proton ratio fluctuations in central Pb+Pb collisions from* $\sqrt{s_{NN}} = 6.3$ *to 17.3 GeV*, Phys. Rev. C 83, 061902 (2011)
3) F. Becattini, M. Bleicher, Th. Kollegger, M. Mitrovski, T. Schuster and R. Stock, *Validity of the hadronic freeze-out curve*, J. Phys. G 38, 124075 (2011)
4) F. Becattini, M. Bleicher, Th. Kollegger, M. Mitrovski, T. Schuster and R. Stock, *Hadronization and hadronic freeze-out in relativistic nuclear collisions*, submitted to Phys. Rev. C

Extreme isospin in heavy nuclei

Collaborators: S. Schramm[1], D. Gridnev[1], W. Greiner[1], D. V. Tarasov[2], V. N. Tarasov[2]

[1] Frankfurt Institute for Advanced Studies, [2] NSC, Kharkov Institute of Physics and Technology, Ukraine

The focus of many experimental and theoretical efforts in nuclear physics are focused on exploring extreme states of strongly interacting matter. One aspect of these efforts is the study of very neutron rich nuclei, as they will be measured extensively in the upcoming FAIR facility at GSI, the FRIB facility in Michigan, and a number of other laboratories around the world. In addition to the fundamental issues of nuclear stability involved in this research, the properties of neutron-rich nuclei are crucial input for the nucleosynthesis in supernovae, and the isospin dependence of the nuclear interactions has direct impact on the properties and stability of neutron stars.

In order to study this region of large isospin we investigated the stability of heavy nuclei around Uranium and studied the maximum amount of neutrons the different elements can contain. We calculated nuclear properties for a variety of non-relativistic Skyrme forces as well as relativistic and chiral effective nuclear models. We could observe a huge difference of this maximum neutron number depending on the model adopted (as can ben seen in Fig. 1), where differences in the maximum neutron number exceed 70 neutrons (!) in specific cases. Following the isotope chain, a change of nuclear deformation from spherical to prolate, then oblate, and back to spherical shape could be observed (Fig. 2).

The results show that there are still huge theoretical uncertainties in the properties of nuclei with large neutron excess. In the future, performing combined calculations of the neutron drip line, phase structure of strong interactions, as well as neutron star phenomenology will help to correlate model predictions over a larger range of observables, helping to constrain models to a much bigger extent.

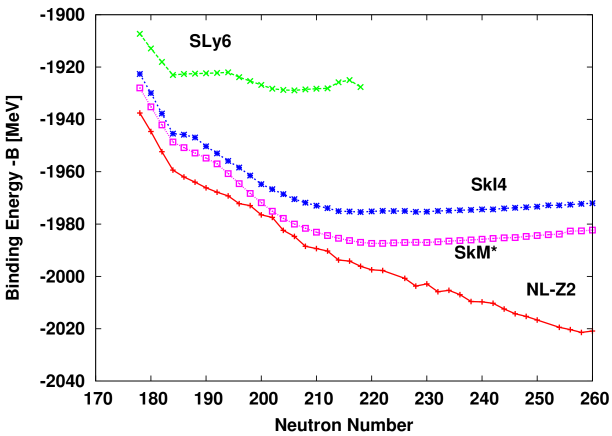


Figure 1: Total binding energy of Uranium isotopes for different parameterizations. The curves show the result for a relativistic mean-field (NL-Z2) and Skyrme models (SkM*, SkI4, SLy6). The chiral model χ_M (not shown) has its minimum at N = 184.

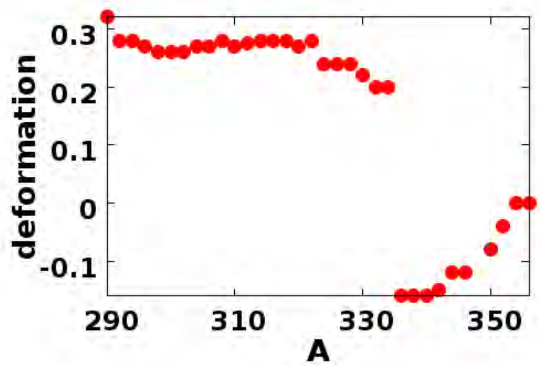


Figure 2: Deformation β_2 for different Californium isotopes for the Skyrme parameter set SkM*.

Related publications in 2011:

S. Schramm, D. Gridnev, D. V. Tarasov, V. N. Tarasov and W. Greiner, *The quest for the heaviest uranium isotope*, arXiv:1107.1055 [nucl-th].

V. N. Tarasov, K. A. Gridnev, D. K. Gridnev, D. V. Tarasov, S. Schramm, X. Vinas and W. Greiner, *Stability peninsulas on the neutron drip line*, arXiv:1106.5910 [nucl-th].

Cluster radioactivities of superheavy nuclei

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

Calculations of half-lives of superheavy nuclei (SH) show an unexpected result: for some of them cluster radioactivity (CR) dominates over alpha decay — the main decay mode of the majority of discovered SHs with atomic numbers $Z \leq 118$. The result is important for theory and future experiments producing heavier SHs with a substantial amount of funding. The standard identification technique by alpha decay chains will be impossible for these cases.

CR had been predicted in 1980 (see http://www.britannica.com/EBchecked/topic/465998/). A parent nucleus produces an emitted particle and a daughter. All measured half-lives on ^{14}C, ^{20}O, ^{23}F, $^{22,24-26}$Ne, ^{28,30}Mg, ^{32,34}Si radioactivities are in agreement with predicted values within our analytical superasymmetric fission (ASAF) model. The shortest half-life of $T_c = 10^{11.01}$ s corresponds to ^{14}C radioactivity of ^{222}Ra and the largest branching ratio relative to alpha decay $b_\alpha = T_\alpha/T_c = 10^{-8.9}$ was measured for the ^{14}C radioactivity of ^{223}Ra. Consequently CR in the region of transfrancium nuclei is a rare phenomenon in a strong background of α particles.

In the present work we changed the concept of CR to allow emitted particles with atomic numbers $Z_e > 28$ from parents with $Z > 110$ and daughter around ^{208}Pb. A new table of measured masses AME11 (G. Audi and W. Meng, private communication, 2011) and the theoretical KTUY05 (H. Koura et al. Prog. Theor. Phys. 113 (2005) 305) and FRDM95 (P. Möller et al. Atomic Data Nucl. Data Tables 59 (1995) 185) tables are used to determine Q-value. Calculations for SH nuclei with $Z = 104-124$ are performed within the ASAF model. All superheavy nuclei present on the AME11 mass table are proton-rich nuclides with neutron numbers smaller than N_β on the line of beta stability.

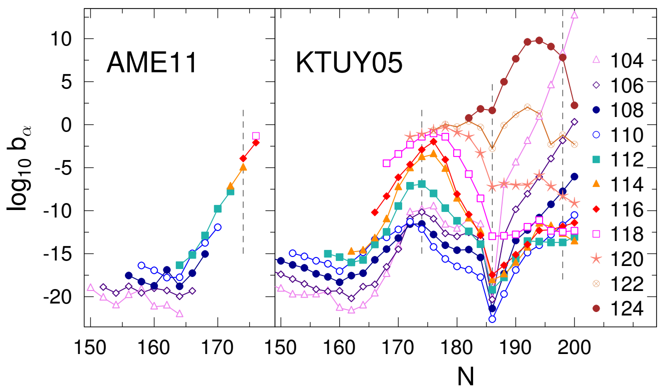


Figure: Branching ratio relative to α decay for cluster emission from even-even superheavy nuclei versus the neutron number of the parent nucleus.

The general trend of a larger branching ratio relative to α decay, b_α, when the atomic and mass numbers of the parent nucleus increases may be seen on the left hand side of the figure obtained within ASAF model by using the AME11 mass tables to calculate the Q values.

One can advance toward neutron-rich nuclei by using the KTUY05 calculated mass tables, as shown in the right panel of this figure. The pronounced minimum of the branching ratio at $N = 186$ is the result of the strong shell effect of the assumed magic number of neutrons $N = 184$ present in the KTUY05 masses. It can be seen that branching ratios higher than unity may exist for some isotopes of SHs with $Z = 122, 124$.

Related publications in 2011:

1) D. N. Poenaru, R. A. Gherghescu, W. Greiner, *Heavy-particle radioactivity of superheavy nuclei*, Phys. Rev. Lett. 107 (2011) 062503.

2) D. N. Poenaru, R. A. Gherghescu, W. Greiner, *Single universal curve for cluster radioactivities and α decay*, Phys. Rev. C 83 (2011) 014601.

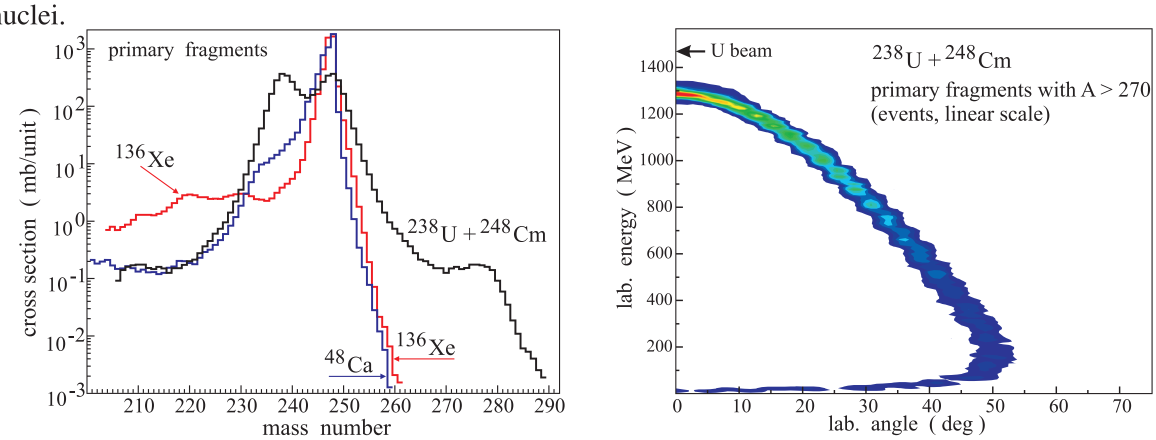
Production of heavy and superheavy neutron-rich nuclei in transfer reactions

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

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

The problem of production and study of heavy neutron-rich nuclei has been intensively discussed during recent years. The multi-nucleon transfer reactions can be used for the production of new neutron-rich isotopes in the superheavy (SH) mass area. Additional enhancement of the corresponding cross sections at low collision energies may originate here due to shell effects. We called it "inverse quasi-fission" process. In this process one of the heavy colliding partners, say ^{238}U, transforms to lighter doubly magic nucleus ^{208}Pb while the other one, say ^{248}Cm, transform to the complementary superheavy nucleus. The role of these shell effects in damped collisions of heavy nuclei is still not absolutely clear and was not carefully studied experimentally. However very optimistic experimental results were obtained recently [W. Loveland, et al., Phys. Rev. C (2011)] confirming such effects in the ^{160}Gd + ^{186}W reaction for which the similar "inverse quasi-fission" process (^{160}Gd→^{138}Ba while ^{186}W→^{208}Pb) has been predicted earlier [V. Zagrebaev and W. Greiner, J. Phys. G (2007)].

In multi-nucleon transfer reactions the yields of SH elements with masses heavier than masses of colliding nuclei strongly depend on the reaction combination. The cross sections for the production of neutron-rich transfermium isotopes in reactions with ^{248}Cm target change sharply if one changes from medium mass (even neutron-rich) projectiles to the uranium beam. In figure the mass distributions of heavy primary reaction fragments are shown for near barrier collisions of ^{238}U, ^{136}Xe and ^{48}Ca with a curium target. The "lead shoulder" manifests itself in all these reactions. For ^{136}Xe+^{248}Cm and ^{48}Ca+^{248}Cm collisions it corresponds to the usual (symmetrizing) quasi-fission process in which nucleons are transferred mainly from the heavy target (here ^{248}Cm) to the lighter projectile. Contrary to this ordinary quasi-fission phenomena, for the ^{238}U + ^{248}Cm collisions we may expect an inverse process in which nucleons are predominantly transferred from the lighter partner to heavy one (U transforms to Pb and Cm to element 106). In this case, besides the lead shoulder in the mass and charge distributions of the reaction fragments, there is also a pronounced shoulder in the region of SH nuclei.



(left panel): Mass distributions of heavy primary reaction fragments formed in collisions of ^{238}U, ^{136}Xe and ^{48}Ca with ^{248}Cm at $E_{c.m.}$=750, 500 and 220 MeV, correspondingly.) (right panel): Energy-angular distribution of primary heavy fragments (A> 270) in the laboratory system in collisions of ^{238}U with ^{248}Cm target at 750 MeV center-of-mass energy.

The figure also shows the laboratory-frame energy-angular distribution of SH nuclei produced in ^{238}U+ ^{248}Cm collisions at 750 MeV center-of-mass beam energy. The angular distribution of the desired SH nuclei formed in transfer reactions does not reveal any grazing features, it is just forward directed. However this angular distribution is rather wide. Thus, an appropriate separator (which is currently designed only) needs to collect and separate SH reaction fragments ejected within a wide angular range of at least ±20°. This is a very difficult problem because these fragments have in addition rather wide energy distribution.

Related publications in 2011:

1) V.I. Zagrebaev and Walter Greiner, *Production of heavy and superheavy neutron-rich nuclei in transfer reactions*, Physical Review **C83** (2011) 044618.

Production of heavy and superheavy neutron-rich nuclei in neutron capture processes

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

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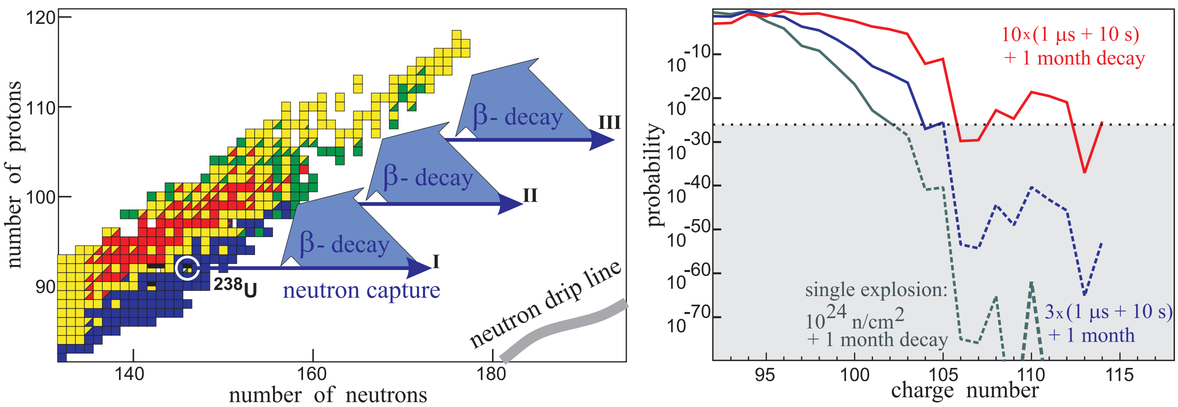
The neutron capture process is an alternative (to the fusion and multinucleon transfer reactions) and oldest method for the production of new heavy elements. Strong neutron fluxes might be provided by nuclear reactors and nuclear explosions under laboratory conditions and by supernova explosions in nature. All these three possibilities were studied. The "Fermium gap", consisting of the short-living Fermium isotopes $^{258-260}$Fm located at the β-stability line and having short half-lives for spontaneous fission, impedes formation of nuclei with $Z > 100$ by the weak neutron fluxes realized in existing nuclear reactors. Another region of short-lived nuclei is located at $Z = 106 - 108$ and $A \sim 270$. In nuclear and supernova explosions (rapid neutron capture) these gaps may be bypassed. The same may be done in pulsed reactors of the next generation.

In figure the probabilities of heavy element formation are shown for one, three and ten subsequent short-time (1 μs) neutron explosions of 10^{24} n/cm^2 each following one after another with time interval of 10 seconds with final one month waiting. These results demonstrate that multiple (rather "soft") nuclear explosions could be really used for the production of noticeable (macroscopic) amount of neutron rich long-lived superheavy nuclei (the region above the dotted line in figure). We studied the same process of multiple neutron exposures realized in pulsed nuclear reactors. The pulse duration here could be much longer than in nuclear explosions (up to few milliseconds). In spite of that, the neutron fluence usually does not exceed 10^{16} n/cm^2 in existing nuclear reactors. Thus, the multi-pulse irradiation here corresponds to "slow" neutron capture process, in which new elements with larger charge numbers are situated close to the line of stability and finally reach the Fermium gap where the process stops. We have formulated requirements for the pulsed reactors of the next generation which could be also used in future for the production of long-lived superheavy nuclei. We found that an increase of the neutron fluence in an individual pulse by about 3 orders of magnitude compared with existing pulsed reactors, i.e., up to 10^{20} n/cm^2, could be quite sufficient to bypass both gaps.



Schematic picture for multiple neutron irradiation of initial ^{238}U material (left) and probability for formation of heavy nuclei (right) in such process (one, three and ten subsequent explosions). The dotted line denotes the level of few atoms.

We estimated also the possibility for formation of SH nuclei during astrophysical *r*-process of neutron capture. The found probability for production of SH elements (namely, the neutron-rich copernicium isotopes ^{291}Cn and ^{293}Cn, with half-lives longer than several tens of years) is not very pessimistic: the yield of these nuclei relative to lead could be about 10^{-12} if one assumes initial natural abundance of all the elements (including thorium and uranium) at the beginning of *r*-process. This ratio is not beyond the experimental sensitivity of a search for SH elements in nature. The question is how long are their half-lives? In accordance with our estimations, the half-lives of most long-living copernicium isotopes, ^{291}Cn and ^{293}Cn, do not exceed several hundred years. Even this short time provides hope of finding relatively long-living SH nuclei in nature, for example, in cosmic rays.

Related publication in 2011:

1) V.I. Zagrebaev, A.V. Karpov, I.N. Mishustin, and Walter Greiner, *Production of heavy and superheavy neutron-rich nuclei in neutron capture processes*, Physical Review **C84** (2011) 044617.

The phase diagram in T-μ_B-N_c space

Collaborators: G. Torrieri[1], I.N. Mishustin[1], S. Lottini[2]

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

Research in this project has been devoted to exploring the QCD phase diagram in varying number of colors. This follows from work done the year before, explaining the quantitative smallness of the critical point in the nuclear liquid-gas phase transition by an interplay of the number of colors and the number of neighbours in a densely packed system [1].

Such an interplay suggests that a percolation transition arises when the density and the number of colors are varied. In [2] we have explored this transition for a general class of quark-quark propagators in a confined phase at finite density. We show that typically percolation occurs at $N_c \sim O(10)$ when the chemical potential is of order Λ_{QCD}. Fig. 1 shows the critical number of colors as a function of the parameter space of the quark-quark propagator in such a confined but high-density system.

This paper has left a number of questions open: How does this percolation transition interplay with deconfinement when both density and number of colors are varied? Are there phenomenological consequences of percolation, on the lattice or in real heavy ion collisions? And what is the relationship between percolation and the widely studied quarkyonic phase transition? Answering some of these questions will be a main target of my research in 2012.

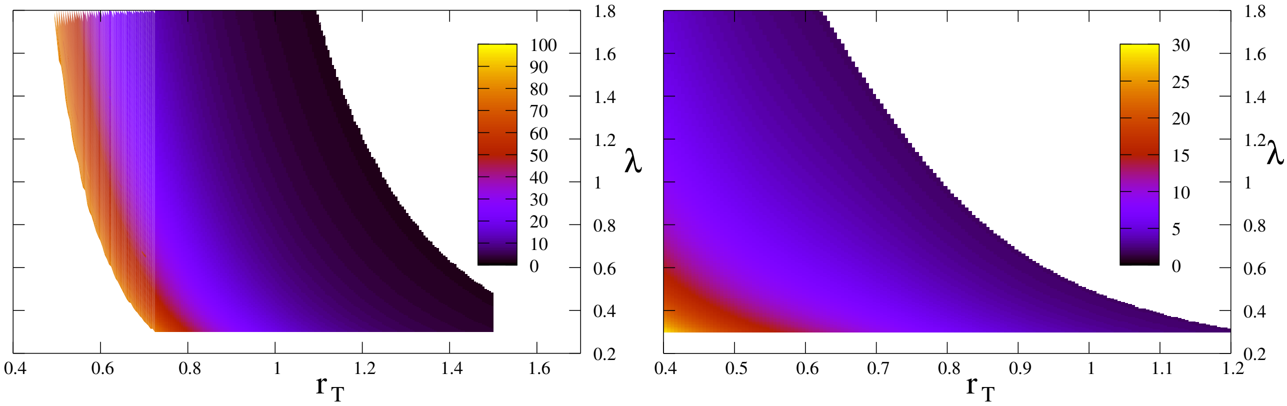


Figure 1: Contour plot of the critical N_c vs coupling constant λ and propagator range r_T, assuming the quark-quark propagator is a Θ-function in momentum space (left panel) and position space (right panel). See [2] for further details.

Related publications in 2011:

1) G. Torrieri, S. Lottini, I. Mishustin, P. Nicolini, *The phase diagram in T-μ-N_c space*, arXiv:1110.6219 [nucl-th].

2) S. Lottini and G. Torrieri, *A percolation transition in Yang-Mills matter at finite number of colours*, Phys. Rev. Lett. 107, 152301 (2011). arXiv:1103.4824 [nucl-th].

3) G. Torrieri, *Strange quark matter: Business as usual or phase transition?*, arXiv:1111.6122 [nucl-th].

Fourier analysis of jets abundances as a probe of the initial state and jet suppression mechanism

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

[1] Frankfurt Institute for Advanced Studies, [2] Columbia University, New York, USA

Jet suppression remains one of the signatures in the study of heavy ion collisions which has aroused most theoretical and experimental interest. The phenomenological interpretation of jet suppression, however, remains somewhat controversial: We have not been able to use jets as a tomographic tool which can conclusively determine the initial density of the system (in particular, distinguishing between the popular "Glauber" and "Color glass" models of the initial state), nor do we know whether the jet-medium interaction is characterized by weak coupling (and is best studied by perturbative QCD) or strong coupling (amenable to be described by Gauge-string duality).

In [1] we attempt to examine these issues in a systematic way. We use both Glauber and color glass initial conditions, making sure event-by-event fluctuations and hotspots are included in the description. We then assume a completely general energy loss, constrained only by dimensional analysis

$$\frac{dE}{dx}(\vec{x}_0, \phi, \tau) = -\kappa P^a \tau^z T^{z-a+2}[\vec{x}_0 + \hat{n}(\phi)\tau, \tau]$$

and estimate the effect of the different z, a have on the Fourier coefficients of jet abundance (the zeroth coefficient, the absolute jet suppression, has been fit to experimental data to determine the parameter κ).

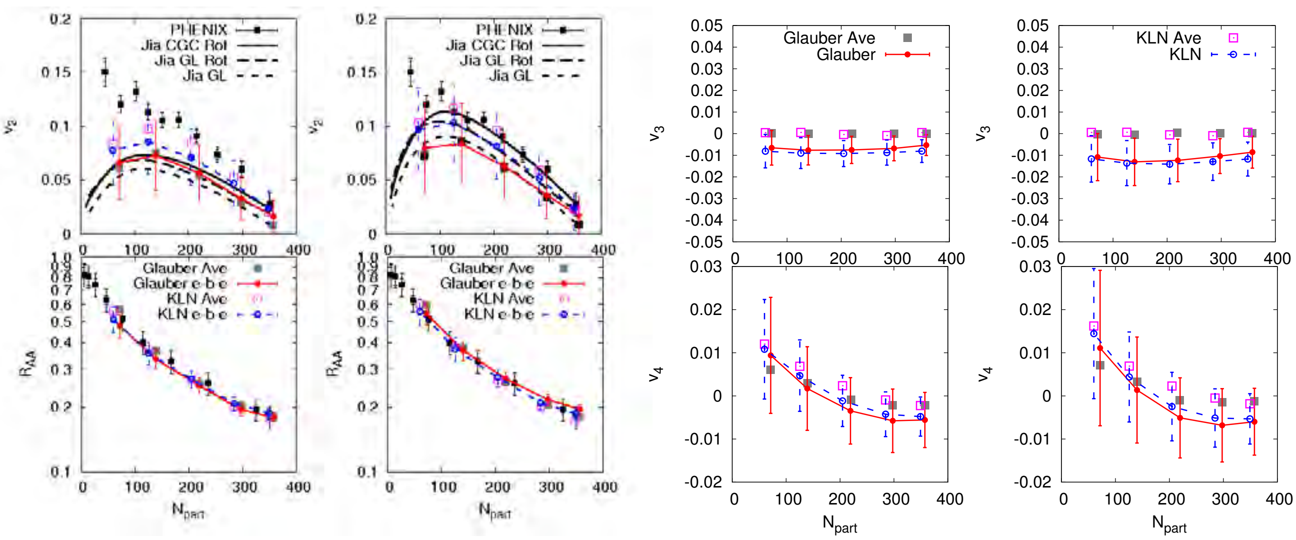


Figure 1: Different Fourier components of jet abundance in different initial state models and jet-medium interactions

The results are shown in Fig. 1. We see that while higher order Fourier components are more sensitive to jet-medium interaction, they are also more affected by initial state fluctuations, making an overall disentangling of the two problematic. In the next year, we aim to see if heavy-quark Fourier harmonics could help in this respect.

Related publications in 2011:

1) B. Betz, M. Gyulassy and G. Torrieri, *Fourier harmonics of high-p_T particles probing the fluctuating initial condition geometries in heavy-ion collisions*, Phys. Rev. C84, 024913 (2011). arXiv:1102.5416 [nucl-th].

Critical Zeeman Fields for Unitary Fermi Superfluids and Dilute Neutron Matter

Collaborators: Lianyi He[1,2,3], Pengfei Zhuang[3]

[1] Frankfurt Institute for Advanced Studies, [2] Institute for Theoretical Physics, Frankfurt University, [3] Department of Physics, Tsinghua University, Beijing, China

We determine the critical Zeeman energy splitting of a homogeneous Fermi superfluid at unitary in terms of the Fermi energy ε_F according to recent experimental results at ENS of LKB-Lhomond Paris. Based on the universal equations of state for the superfluid and normal phases, we show that there exist two critical fields H_{c1} and H_{c2}, between which a superfluid-normal mixed phase is energetically favored. Universal formulae for the critical fields and the critical population imbalance P_c are derived. We have found a universal relation between the critical fields and the critical imbalances: $H_{c1} = \gamma\xi\varepsilon_F$ and $H_{c2} = (1+\gamma P_c)^{2/3}H_{c1}$ where ξ is the universal constant and γ is the critical value of the chemical potential imbalance in the grand canonical ensemble. Since ξ, γ and P_c have been measured in the experiments, we can determine the critical Zeeman fields without the detail information of the equation of state for the polarized normal phase. Using the experimental data from LKB-Lhomond, we have found $H_{c1} \simeq 0.37\varepsilon_F$ and $H_{c2} \simeq 0.44\varepsilon_F$. Our result of the polarization P as a function of the Zeeman field H/ε_F is in good agreement with the data extracted from the experiments. Since the neutrons carry a tiny magnetic moment $\mu_n \simeq 6.03\times10^{-18}$MeV·G^{-1} (in natural units), the superfluid state in dilute neutron matter can be destroyed when the magnetic field reaches a critical value and the matter becomes spin-polarized. Since the effective interaction in dilute neutron matter is quite close to unitary, the experimental data from cold atoms can help us determine the critical magnetic field for dilute neutron matter. We give an estimation of the critical magnetic field for dilute neutron matter at which the matter gets spin polarized, assuming the properties of the dilute neutron matter are close to those of the unitary Fermi gas. It was found that the critical magnetic fields are in the range of $10^{16}-10^{18}$Gauss for neutron density of $(10^{-3}-10^{-1})n_0$, where n_0 is the nuclear saturation density.

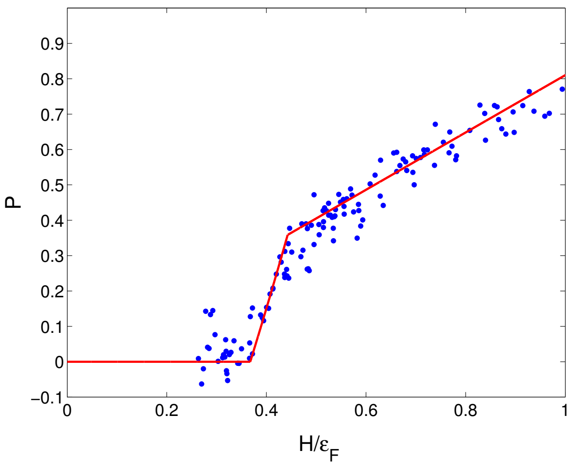


Figure: The spin polarization $P = (N_\uparrow - N_\downarrow)/(N_\uparrow + N_\downarrow)$ as a function of the external Zeeman field H (divided by ε_F) for a homogeneous Fermi gas at unitary. The blue dots are data extracted from the ENS experiments. The red solid line is the theoretical prediction. We use the data $\gamma = 0.897$, $\xi = 0.41$ from ENS and $H_{c1} = 0.368\varepsilon_F$. For the normal phase $H > H_{c2}$, we use the linear fit $P = \frac{3}{2}\tilde{\chi}H/\varepsilon_F$ with $\tilde{\chi} = 0.54$. In between, the formula $P = \gamma^{-1}[(H/H_{c1})^{3/2}-1]$ from our theory is adopted. The value of P_c is self-consistently determined as $P_c = 0.359$.

Related publications in 2011:

1) Lianyi He and Pengfei Zhuang, *Critical Zeeman splitting of a unitary Fermi superfluid*, Phys. Rev. B83, 174504 (2011).

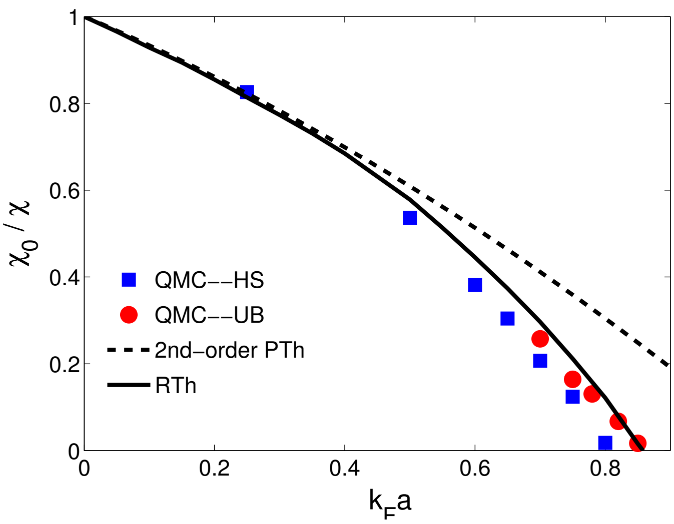
Nonperturbative Prediction of the Ferromagnetic Transition in Repulsive Fermi Gases

Collaborators: Lianyi He[1,2], Xu-Guang Huang[2]

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

It is generally believed that a dilute spin-1/2 Fermi gas with repulsive interactions can undergo a ferromagnetic phase transition to a spin-polarized state at a critical gas parameter. Previous theoretical predictions of the ferromagnetic phase transition are based on the perturbation theory which treats the gas parameter as a small number. On the other hand, Belitz, Kirkpatrick, and Vojta (BKV) have argued that the phase transition in clean itinerant ferromagnets is generically of first order at low temperatures, due to the correlation effects that lead to a nonanalytic term in the free energy. The second-order perturbation theory predicts a first order phase transition at a critical gas parameter 1.054, consistent with the BKV argument. However, since the critical gas parameter is expected to be of order $O(1)$, perturbative predictions may be unreliable.

In this work we study the non-perturbative effects on the ferromagnetic phase transition by summing the particle-particle ladder diagrams to all orders in the gas parameter. We consider a universal repulsive Fermi gas where the effective range effect can be neglected, which can be realized in a two-component Fermi gas of ^{6}Li atoms by using a nonadiabatic field switch to the upper branch of a Feshbach resonance with a positive s-wave scattering length. The resummation of particle-particle ladder diagrams predicts a second order phase transition, which indicates that ferromagnetic transition in dilute Fermi gases is a possible counter example of the BKV argument. The predicted critical gas parameter 0.858 is in good agreement with recent Quantum Monte Carlo result 0.86 for a nearly zero-range potential [S. Pilati, *et al.*, Phys. Rev. Lett. 105, 030405 (2010)]. We also compare the spin susceptibility with the Quantum Monte Carlo result and find good agreement.



The dimensionless inverse spin susceptibility χ_0/χ vs. the dimensionless gas parameter $k_F a$. The blue squares and red circles are the Quantum Monte Carlo (QMC) data for the hard sphere (HS) potential and upper branch (UB) of a zero range attractive potential, respectively. The solid line is the result calculated from our resummation theory (RTh). The dashes line is result from the 2nd-order perturbation theory (PTh). At a critical gas parameter $k_F a = 0.858$ the spin susceptibility χ diverges, indicating a ferromagnetic transition.

Related publications in 2011:

1) Lianyi He and Xu-Guang Huang, *Non-perturbative prediction of the ferromagnetic transition in repulsive Fermi gases*, arXiv: 1106.1345, submitted to Phys. Rev. A.

BCS-BEC Crossover in 2D Fermi Gases Induced by Synthetic Spin-Orbit Coupling

Collaborators: Lianyi He[1,2], Xu-Guang Huang[1,2]

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

It has been widely believed for a long time that a smooth crossover from Bardeen–Cooper–Schrieffer (BCS) superfluidity to Bose–Einstein condensation (BEC) of molecules could be realized in an attractive Fermi gas. This BCS-BEC crossover phenomenon has been successfully demonstrated in ultracold fermionic atoms by means of the Feshbach resonance. Recent experimental breakthrough in generating synthetic non-Abelian gauge field has opened up the opportunity to study the spin-orbit coupling (SOC) effect in cold atomic gases. For fermionic atoms, it provides an alternative way to study the BCS-BEC crossover according to the theoretical observation that novel bound states in three dimensions can be induced by a non-Abelian gauge field even though the attraction is weak. This is analogous to the catalysis of the dynamical mass generation by an external non-Ablelian field in quantum field theory.

Recently, the anisotropic superfluidity in 3D Fermi gases with Rashba SOC has been intensively studied. Two-dimensional (2D) fermionic systems with Rashba SOC is more interesting for condensed matter systems and topological quantum computation. By applying a large Zeeman splitting, a non-Abelian topologically superconducting phase and Majorana fermionic modes can emerge in spin-orbit coupled 2D systems. In the absence of SOC, the BCS-BEC crossover and Berezinskii-Kosterlitz-Thouless (BKT) transition temperature in 2D attractive fermionic systems were investigated long ago, which provide a possible mechanism for pseudogap formation in high-temperature superconductors.

In this work we have presented a systematic study of 2D attractive Fermi gases in the presence of Rashba SOC. The main results are summarized as follows:
(A) The SOC enhances the difermion bound states in 2D. At large SOC, even for weak intrinsic attraction, the many-body ground state is a Bose-Einstein condensate of bound molecules. In the presence of a harmonic trap, the atom cloud shrinks with increased SOC.
(B) The BKT transition temperature is enhanced by the SOC at weak attraction, and for large SOC it tends to the critical temperature for a Bose gas with an effective mass determined by the exact two-body problem. The SOC effect therefore provides a new mechanism for pseudogap formation in 2D fermionic systems.
(C) In the presence of SOC, the superfluid ground state exhibits both spin-singlet and -triplet pairings, and the triplet one has a non-trivial contribution to the condensate density. In general, the condensate density is enhanced by the SOC due to the increase of the molecule binding. However, the superfluid density has entirely different behavior: it is suppressed by the SOC due to the increasing molecule effective mass.

Related publications in 2011:
1) Lianyi He and Xu-Guang Huang, *BCS-BEC crossover in 2D Fermi gases with Rashba spin-orbit coupling*, arXiv: 1109.5577, Phys. Rev. Lett. (2012), in press.

Supernova dynamics and explosive nucleosynthesis

Collaborators: K. Langanke[1,2,3], G. Martinez-Pinedo[2,3], T. Fischer[2,3], Q. Zhi[2,3], L. Huther[3]

[1] Frankfurt Institute for Advanced Studies, [2] GSI Helmholtzzentrum für Schwerionenforschung, Darmstadt, Germany, [3] Technische Universität Darmstadt, Darmstadt, Germany

Reactions mediated by the weak interaction play an important role for the dynamics of core-collapse supernovae. During the collapse phase, the capture of electrons on protons in nuclei are particularly important. Some years ago we have pointed out that this process dominates over the capture on free protons, changing the then-accepted paradigm. Our argument was built on the observation that nucleonic correlations across the $N = 40$ shell gap are strong enough to overcome the unblocking of the Gamow-Teller (GT) strength. We have now confirmed our argument by large-scale shell model calculations performed for the nucleus ^{76}Se (with 34 protons and 42 neutrons). Our calculations agree well with recent measurements of the ground state GT strength and with nucleon occupation numbers for the orbitals across the shell gap as determined from transfer measurements. We are now planning to extend our studies to other neutron-rich nuclei. These studies are also important for the crust evolution of mass-accreting neutron stars in binary systems.

Supernovae are the site of explosive nucleosynthesis when hot material is ejected from the surface of the newly born proto-neutron star. This matter, originally free protons and neutrons, is resembled into nuclei upon reaching cooler regions at larger distances. The nucleosynthesis depends strongly on the proton-to-neutron ratio which is determined by the interaction of neutrinos and antineutrinos with the free nucleons. The early phase of the explosive nucleosynthesis is the site of the recently discovered νp process, while the later phase might be the origin of the r-process which produces half of the heavy elements in nature, including all of the transactinides.

We have studied the influence of collective neutrino oscillations on νp nucleosynthesis. We observe that the production of the light p-nuclides is noticeably enhanced if the electron and muon neutrino spectra are switched due to collective oscillations above a certain energy (the split energy).

The astrophysical r-process runs through nuclei with extreme neutron excess the properties of which are experimentally mostly unknown (until facilities like FAIR become operational) and must be modelled. We have calculated neutron capture cross sections for such nuclei within the framework of the statistical model using M1 strength distributions calculated in the shell model rather than adopting simple parametrizations. Furthermore we have calculated individual distributions for the excited states in this way, for the first time, testing the Brink hypothesis. Finally we have studied the influence of the M1 scissors mode on the capture cross sections.

We have performed r-process nucleosynthesis studies using a recently developed code which also allows detailed consideration of various fission modes and their associated yield distributions. In particular we studied whether long-lived superheavy elements might be produced by the r-process using input from different nuclear models. We have also explored the production of the cosmochronometers ^{232}Th and ^{238}U which are observed in old stars and, due to their lifetimes which are compatible with the age of the Universe, are used to determine the age of the stars.

Related publications in 2011:

1) G. Martinez-Pinedo, B. Ziebarth, T. Fischer, and K. Langanke, *Effect of collective neutrino flavor oscillations on νp-process nucleosynthesis*, Eur. Phys. J. A47, 98 (2011)
2) Q. Zhi, K. Langanke, G. Martinez-Pinedo, F. Nowacki, and K. Sieja, *The ^{76}Se Gamow-Teller strength distribution and its importance for stellar electron capture rates*, Nucl. Phys. A859, 172 (2011)
3) K. Langanke, G. Martinez-Pinedo, I. Petermann, and *F. K. Thielemann, Nuclear quests for supernova dynamics and nucleosynthesis*, Prog. Part. Nucl. Phys. 66, 319 (2011)
4) L. Huther, H. P. Loens, G. Martinez-Pinedo, and K. Langanke, *s-process stellar enhancement factors obtained within the statistical model with parity-dependent level densities*, Eur. Phys. J. A 47, 1 (2011)

Applications of a chiral SU(3) model for the binding energies of nuclei, driplines of nuclei and hyper-nuclei, and the mass-radius relation of neutron stars

Collaborators: T. Schürhoff[1,2], S. Schramm[1], C. Samanta[3,4]

[1] Frankfurt Institute for Advanced Studies, [2] Institute for Theoretical Physics (ITP), Goethe University, Frankfurt, [3] Saha Institute of Nuclear Physics, Kolkata, India, [4] Department of Physics, Virginia Commonwealth University, Richmond, VA, USA

One of the major goals in contemporary nuclear physics is the determination of the equation of state of hadronic matter. This will allow for a great many applications, both on the experimental and theoretical side, for example in supernova simulations. In order to theoretically study hadrons, we look at the binding energies of nuclei and compare the results of our model with experimental results. We can reproduce the binding energies of nuclei over the whole nuclide chart up to 0.7 % and work to improve our fitting parameters.

We also study the driplines of normal and hyper-nuclei and extrapolate to regions not experimentally accessible at the moment. This is of interest for upcoming experiments at GSI. We find that the extrapolation of drip-lines is very much model dependent.

In addition, we study the effect of the change of the fitting parameters of our model for the mass-radius relation of neutron stars. There, parameter changes only have a very marginal effect.

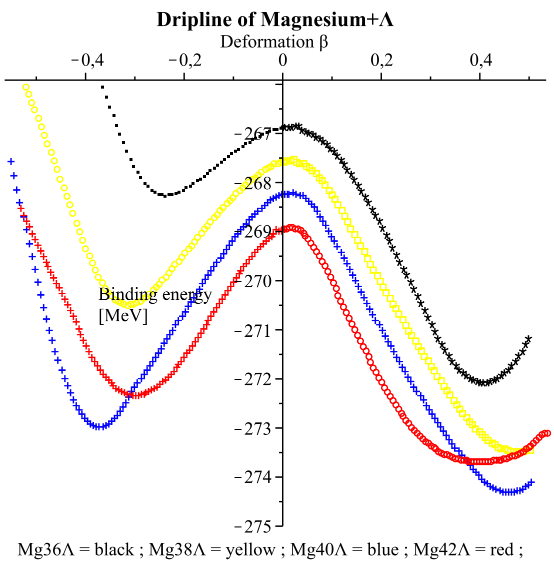


Figure 1: The dripline determination of the hyper-nucleus Magnesium 40 containing one Λ hyperon. Plotted is the the deformation β versus the total binding energy in MeV. The nucleus will move to the deformation with the lowest binding energy, i.e. the minimum. The dripline is that nucleus for which the addition of further particles, here neutrons, will no longer yield an increase in binding energy.

Related publications in 2011:

1) S. Schramm, V. Dexheimer, R. Negreiros, T. Schürhoff, *Nuclear matter, nuclei and neutron stars in hadron and and quark-hadron models*, in Symposium on Advances in Nuclear Physics in our time, Goa, India, 28. Nov. - 2. Dec. 2010, 2011. arXiv:1102.2325 [nucl-th].

2) S. Schramm, R. Negreiros, J. Steinheimer, T. Schürhoff, V. Dexheimer, *Properties and stability of hybrid stars*, in Strangeness in Quark matter (SQM2011), Krakow, Poland, 18.-24. Sept. 2011. arXiv:1112.1853 [astro-ph.SR].

A new approach to the thermal evolution of neutron stars

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

[1] Frankfurt Institute for Advanced Studies, [2] San Diego State University, USA, [3] Gettysburg College, USA

Neutron stars are the extraordinarily compact remnants of massive stars that blew apart in violent supernova explosions. Due to their extreme properties, compact stars are superb astrophysical laboratories, that present a wealth of physical phenomena that may provide insight in the overlapping areas of nuclear physics, particle physics and relativistic astrophysics. Currently, the equation of state (EoS) that describes ultra-dense matter is widely unknown because of the very complicated mathematical structure of the many-body equations that govern matter at extreme pressures. Understanding the equation of state of matter, under extreme conditions of pressure/density and temperature, is of key importance for correctly understanding the phase diagram of baryon matter. One of the most prominent methods of probing the inner composition of a neutron star is by investigating its thermal evolution, since its thermal behaviour depends intrinsically on its microscopic composition. Following this, we have used state-of-the-art microscopic models to simulate the cooling of compact stars. Our results were then compared with a wealth of observed data, allowing us to obtain key information about the microscopic composition of these objects. Furthermore we have proposed a new study that challenges the traditional neutron star cooling paradigm. With our sophisticated simulations we were able to explain comfortably the observed thermal behaviour of the neutron star in supernova remnant Cassiopeia A.

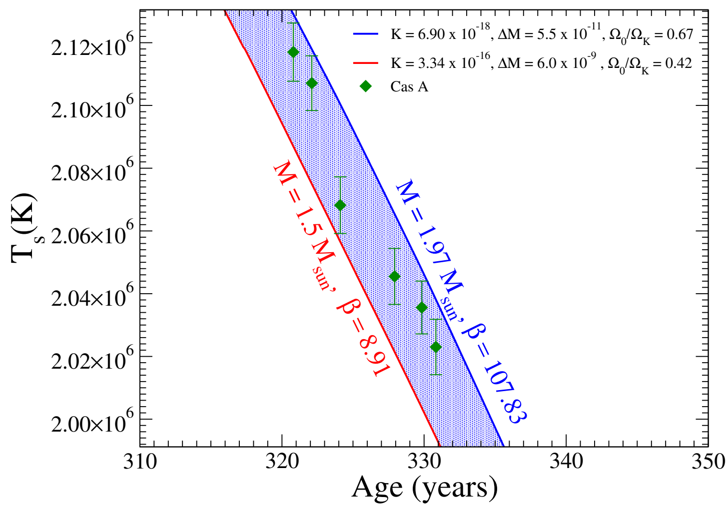


Figure: Predicted thermal evolution of spinning-down neutron stars of different masses and observed data of Cas A

Related publications in 2011:

1) R. Negreiros, S. Schramm, F. Weber, *Impact of Rotation-Driven Particle Repopulation on the Thermal Evolution of Pulsars*, arXiv:1103.3870.

2) V. Dexheimer, R. Negreiros, S. Schramm, *Quark Deconfinement Under the Influence of Strong Magnetic Fields*, arXiv:1108.4479.

3) M. Malheiro, R. Negreiros, F. Weber, V. Usov, *The effects of charge on the structure of strange stars*, J. Phys. Conf. Ser. 312 (2011) 042018.

4) R. Negreiros, S. Schramm. F. Weber, *The Crust of Spinning Down Neutron Stars*, chapter contribution to book: *The Crust of Neutron Stars*, edited by C.A. Bertulani and J. Piekarewicz, Nova Publishers.

5) R. Negreiros, R. Ruffini, C. Bianco, J. Rueada, *Cooling of young neutron stars in GRB associated to Supernova*, accepted for publication in Astronomy and Astrophysics, arXiv:1112.3462.

6) S. Schramm, V. Dexheimer, R. Negreiros, J. Steinheimer, *Dense Matter and Neutron Stars in Parity Doublet Models*, arXiv:1110.0609.

The phase diagram of black holes in AdS space and Gauge-string duality

Collaborators: G. Torrieri[1], P. Nicolini[1], M. Sprenger[1], M. Kaminski[2]

[1] Frankfurt Institute for Advanced Studies, [2] University of Washington, Seattle, USA

As we have long known, deconfinement is a phase transition in the large number of colors limit, but is a cross-over at 3 colors and 2 flavors. Thus, there must be a critical point for confinement when temperature and $N_{flavors}/N_{colors}$ are varied. While this can not of course be studied experimentally, it can be studied numerically on the lattice, and analytically using Gauge-String duality.

We generally believe that deconfinement is dual to the Hawking-Page phase transition, the transition from a stable black-hole phase to an unstable black hole in Anti DeSitter space. The critical point mentioned in the previous paragraph, therefore, must have a counterpart within the Hawking-Page framework.

In [1] we show that, given a commonly used ansatz to describe quantum corrections to black hole physics (see references in [1]), for a certain ratio of the Planck length to the black hole radius the Hawking-Page transition exhibits a critical point and becomes a cross-over. The phase diagram, in Planck length-Temperature, resembles the Van der Waals phase diagram in density-temperature (see Fig. 1).

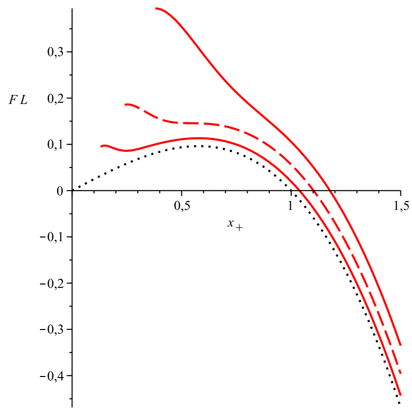


Figure 1: Free energy vs Schwarzschild radius for a black hole in AntideSitter space given the “mean field” ansatz described in [1].

We conjecture, therefore, that these two phenomena (deconfinement critical point in $T-N_f/N_c$ and Hawking-Page critical point in $T-l_p$) are related via Gauge-string duality. This is a natural relation, since in the AdS/CFT dictionary $1/N_c$ is dual to the string coupling constant on the AdS side, and the effect of string loops is to introduce a limit on space resolution which could well be similar to that used in the ansatz of [1].

In the coming year, we aim to test this conjecture by expanding the use of this ansatz to new backgrounds (including those relevant for AdS/condensed matter phenomenology) and calculating the critical exponents around the critical point. We also aim to link this research with the one described in the previous section. Since one of the parameters driving the critical point is $1/N_c$, it is natural to look for percolation-type signatures in the dual gravity theory.

Related publication in 2011:

1) P. Nicolini and G. Torrieri, *The Hawking-Page crossover in noncommutative anti-deSitter space*, JHEP 1108, 097 (2011). arXiv:1105.0188 [gr-qc].

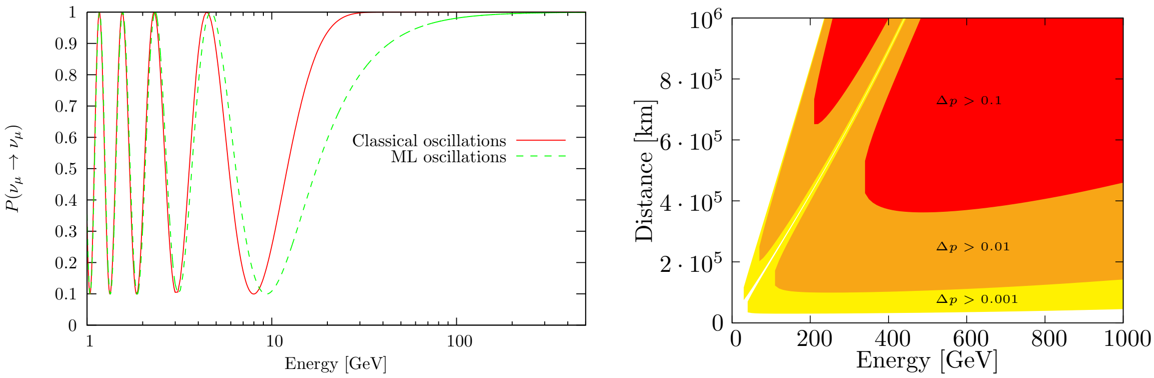
The quest for quantum gravity signals

Collaborators: P. Nicolini[1], M. Bleicher[1,2], R. Garattini[3], M. Rinaldi[4], M. Sprenger[1,2]

[1]Frankfurt Institute for Advanced Studies, [2]Institut für Theoretische Physik, Johann Wolfgang Goethe-Universität, [3]Università di Bergamo, Italy, [4]Université de Gèneve, Switzerland.

Research in quantum gravity is often associated to attempts of describing in an efficient and self consistent way the gravitational field at quantum level. Even if this is certainly true, it is just a narrow view. Before embarking in the formulation of sophisticated theories, a crucial point is to understand whether quantum gravity signals might be detected in current experiments or in a near future. This task is mandatory but challenging for two reasons: first, it is hard to foresee quantum gravity effects without a widely accepted theory of quantum gravity; second, we conventionally expect quantum gravity effects at a scale, the Planck scale, something like 15 orders of magnitude higher than the highest energy particle physics experiments.

Despite this background in 2011 we succeeded to determine a detectable signature of quantum gravity effects. To achieve this, we showed that neutrinos can be the privileged probe to detect the sought signals: even if neutrino energies do not reach the Planck scale, they propagate without interactions over very large distances allowing a non-negligible accumulation of small effects. Specifically we showed that the highest-energetic neutrinos emitted by active galactic nuclei would not oscillate during their propagation towards the Earth, a fact that opens the possibility of their detection in the original flavor eigenstate at telescopes like IceCube and ANTARES. A key point of this work has been the implementation of quantum gravity effects in the neutrino propagation. Along the lines of what already obtained in several other contexts like the Unruh effect and the quantum vacuum energy, we adopted a string theory induced model of noncommutative geometry to reproduce the emergence of quantum spacetime graininess in an effective way.



On the left: classical and modified (ML) oscillations for the two-flavour case with baseline $L = 5000$ km.
On the right: departures from classical oscillations for different values of probability deviation Δp.

Related publications in 2011:

1) P. Nicolini and M. Rinaldi, *A minimal length versus the Unruh effect*, Physics Letters B 695 (2011) 303.
2) R. Garattini and P. Nicolini, *A Noncommutative approach to the cosmological constant problem*, Physical Review D 83 (2011) 064021.
4) M. Sprenger, P. Nicolini and M. Bleicher, *Neutrino oscillations as a novel probe for a minimal length*, Classical and Quantum Gravity 28 (2011) 235019.
5) M. Sprenger, P. Nicolini and M. Bleicher, *Quantum Gravity signals in neutrino oscillations*, International Journal of Modern Physics E 20S2 (2011) 1.

Black holes in short scale modified theories

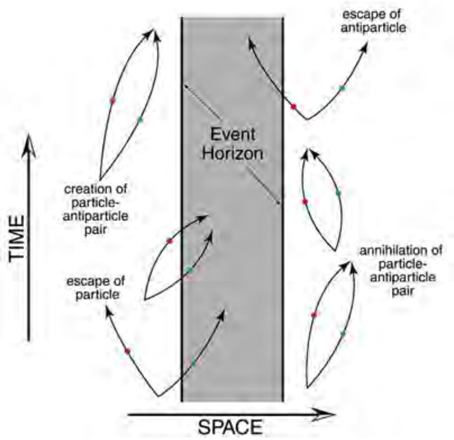
Collaborators: P. Nicolini[1], M. Bleicher[1,2], L. Modesto[3], J. W. Moffat[3], J.R. Mureika[4], M. Sprenger[1,2], E. Winstanley[5]

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

A curvature singularity in general relativity represents the breakdown of the description of the gravitational field in classical terms. However, contrary to the other interactions, gravity escapes a direct quantization for the appearance of an uncontrolled number of divergences in the perturbation theory at all orders. This fact prevents to consistently apply any regularization scheme to gravity. To circumvent the problem we have followed another route, namely the formulation of an ultraviolet finite quantum gravity by considering nonlocal terms in the graviton Lagrangian.

As a test for the new theory, we studied nonlocal gravity as a static interaction emerging from the virtual graviton exchange. We found relevant short scale modifications which provide an asymptotic safe character of the gravitational field: the classical black hole curvature singularity is replaced by a regular deSitter core accounting for the quantum vacuum energy of virtual gravitons. On the thermodynamics side the Hawking emission is characterized by a maximum black hole temperature and a phase transition towards a positive heat capacity cooling down even for the neutral non-rotating case. At the end of the evaporation a black hole remnant forms corresponding to the extremal, zero temperature configuration.

Given this background we studied the repercussions of the new metric on the phenomenology of microscopic black holes in particle detectors. By considering the case of additional spatial dimensions we showed that a maximum temperature determines an emission of soft particles mostly on the brane. This result is in marked contrast to previous findings based on inadequate classical metrics and opens the route to potentially distinctive signatures for the black hole production in particle detectors.



The Hawking radiation as a quantum vacuum effect in the presence of an event horizon.

Related publications in 2011:

1) L. Modesto, J. W. Moffat and P. Nicolini, *Black holes in an ultraviolet complete quantum gravity*, Physics Letters B 695 (2011) 290.
2) J. R. Mureika and P. Nicolini, *Aspects of noncommutative (1+1)-dimensional black holes*, Physical Review D 84 (2011) 044020.
3) P. Nicolini and E. Winstanley, *Hawking emission from quantum gravity black holes*, JHEP 1111 (2011) 075.
4) M. Bleicher, P. Nicolini, M. Sprenger and E. Winstanley, *Micro black holes in the laboratory*, International Journal of Modern Physics E 20S2 (2011) 7.

Noncommutative black holes in non-asymptotically flat backgrounds and gauge-gravity duality

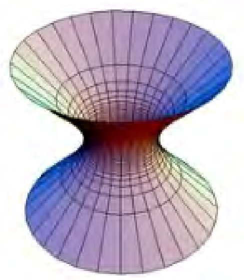
Collaborators: P. Nicolini[1], R.B. Mann[2,3], G. Torrieri[1], S. Lottini[4], I. Mishustin[1]

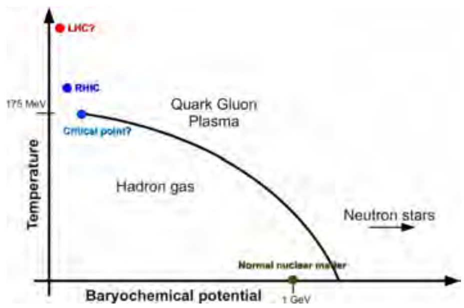
[1]Frankfurt Institute for Advanced Studies, [2]Perimeter Institute for Theoretical Physics, Canada, [3]University of Waterloo, Canada, [4]Institut für Theoretische Physik, Johann Wolfgang Goethe-Universität.

In 2011 we faced the problem of regular noncommutative black holes in non-asympotically flat backgrounds. Specifically we considered two cases: a deSitter background and an Anti-deSitter one. The two cases have relevance respectively in early Universe cosmology and in the context of the gauge-gravity duality paradigm.

In inflationary epochs, the Universe is well described by the deSitter geometry, which is known to be stable under classical perturbations. However at quantum mechanical level, the deSitter space exhibits instability due to the spontaneous nucleation of black holes. The standard semiclassical formalism for pair creation is based on the study of instantons, *i.e.* stationary points of the gravitational action which permit the evaluation of amplitudes within the Euclidean quantum gravity path integral formalism. We showed that noncommutative black holes would have plentifully been produced during inflationary times for Planckian values of the cosmological constant. However, as a special result we found that, in these early epochs of the universe, Planck size black holes production would have been largely disfavoured. We remark that noncommutative black holes are longer-lived with respect to conventional black holes, since they do not completely evaporate. Thus their production could have potential repercussions for Planck-scale inflation as well as for the production of primordial black holes.

A radiating black hole in Anti-deSitter space corresponds to a heat source in a reflecting box of finite volume. Thermodynamically these black holes are dual to systems described by particular kinds of gauge field theory in one dimension fewer. In this spirit we considered noncommutative black holes as a model for a ultraviolet completion of the conventional Anti-deSitter black hole geometry. As a consequence of the profile of their temperature, we showed that the phase structure of the solution is modified: the conventional Hawking-Page phase transition extends into a van der Waals-like phase diagram, with a critical point and a smooth crossover thereafter. This result has profound and intriguing repercussions: one may think to exploit such a new black hole phase transition to describe, via the gauge-gravity duality paradigm, the nuclear matter transition from the "classical" skyrme crystal to a phase where quantum effects weaken the bond between baryons and eventually melt the crystal into a nuclear gas with consequent switch of the deconfinement phase into a cross over.





On the left: a representation of the Anti-deSitter space. On the right: the phase diagram of nuclear matter.

Related publications in 2011:

1) R. B. Mann and P. Nicolini, *Cosmological production of noncommutative black holes*, Physical Review D 84 (2011) 064014.
2) P. Nicolini and G. Torrieri, *The Hawking-Page crossover in noncommutative anti-deSitter space*, JHEP 1108 (2011) 097.
3) G. Torrieri, S. Lottini, I. Mishustin and P. Nicolini, *"The Phase diagram in T–μ–N_c space"*, arXiv:1110.6219 [nucl-th].

Fractal dimensions and micro-structure of a quantum universe

Collaborators: P. Nicolini[1], B. Niedner[2], E. Spallucci[3]

[1]Frankfurt Institute for Advanced Studies, [2]University of Oxford, UK, [3]University of Trieste, Italy.

Spacetime is expected to change its nature when probed at high energies/short scales. Roughly speaking spacetime is like a surface which from afar (low energies) appears smooth, while it turns out to be rough at close distance (high energies). As a result, instead of the classical description in terms of a smooth differential manifold, spacetime in such extreme regime can be accurately modeled by a fractal surface. There exist two major indicators of the fractal character of a manifold: the Hausdorff dimension and the spectral dimension.

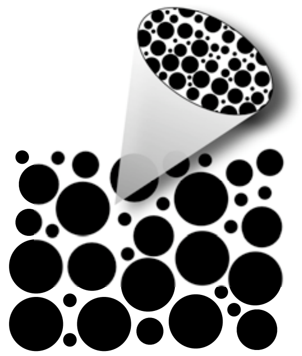
To discolse further features of quantum spacetimes, in 2011 we have introduced another indicator namely the *un-spectral dimension*. The latter consist in the spectral dimension due to the propagation of an *un-particle probe*. Un-particles are a conjectured new sector of the standard model of particle physics which is supposed to show up at energies higher than 1 TeV. The main feature of un-particles is the possibility of generalizing to the massive case the concept of neutrino: un-particles are supposed to be weakly interacting with other particles and have a scale-invariant mass spectrum controlled by a non-integer scaling dimension.

When considering the simplest realization of the un-particle diffusion equation, we found that the problem is equivalent to that of a one-dimensional heat conduction along a bar subject to a time dependent heat source. On the gravity side we considered the diffusion on a black hole event horizon: by taking into account the curvature effects we found a complete fractalization of the horizon, corresponding to the geometry built up by un-gravitons (*i.e.* the un-particle analogue of bosons that mediate the gravitational force) trapped at the Schwarzschild radius.

We also showed that the spacetime manifold undergoes a new "trans-Planckian" regime characterized by an un-spectral dimension lower than two. This new phase we can dub "spacetime vapor" to be consistent with the thermal interpretation of the diffusion process cannot be probed by any sort of ordinary matter.

a)

b)

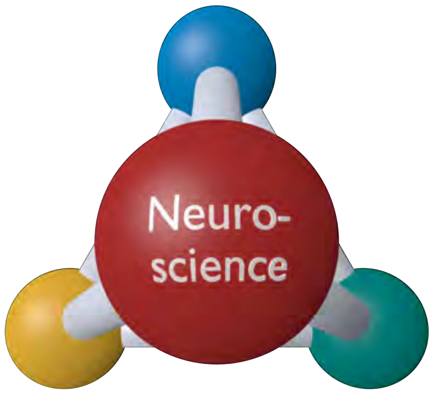


In (a) we have a Cantor set, i.e. a fractal surface which resembles the quantum spacetime.
In (b), there is an artistic picture of the spacetime, whose holed structure shows a fractal self-similarity.

Related publications in 2011:

1) P. Nicolini and E. Spallucci, *Un-spectral dimension and quantum spacetime phases*, Physics Letters B 695 (2011) 290.
2) P. Nicolini and B. Niedner, *Hausdorff dimension of a particle path in a quantum manifold*, Physical Review D 83 (2011) 024017.

4.2 Neuroscience



Untangling the interactions between brain waves of different frequencies

Collaborators: Raul Vicente[1,2], Juhan Aru[3], Jaan Aru[1,2], Michael Wibral[4], Viola Priessemann[5], Gordon Pipa[6], Luiz Lana[1], Wolf Singer[1,2]

[1] Dept. Neurophysiology, Max-Planck Institute for Brain Research, Frankfurt, [2] Frankfurt Institute for Advanced Studies, [3] Center for Research and Interdisciplinarity, Faculty of Medicine, Paris Descartes University, Paris, France [4] MEG Unit, Brain Imaging Center, Goethe University, Frankfurt, [5] Neural Systems and Coding, Max-Planck Institute for Brain Research, Frankfurt, [6] Institute of Cognitive Science, University of Osnabrück

One of the central questions in neuroscience is how neural activity is organized across different spatial and temporal scales. Brain waves of slow frequencies extend over large regions of cortex as opposite to faster oscillations which are coherent over smaller patches. Thus, the interaction between oscillations at different frequencies has been proposed to facilitate flexible coordination of neural activity simultaneously in time and space. Although various experiments have revealed amplitude-to-amplitude and phase-to-phase coupling, the most common and most celebrated result is that the phase of the lower frequency component modulates the amplitude of the higher frequency component. Over the recent 5 years the amount of experimental works finding such phase-amplitude and associating it to behavioral and pathological states has been tremendous.

In this research project, we evaluate the mathematical foundations of cross frequency analysis and provide evidence that current methods might overestimate physiological cross-frequency coupling (CFC) actually evident in the signals of LFP, ECoG, EEG and MEG. In particular, we have pointed out three conceptual problems in assessing the components and their correlations of a time series. Although we focus on phase-amplitude coupling, most of our argument is relevant for any type of coupling. Our results are based on mathematical considerations, numerical simulations, and analysis of neurophysiologic data.

The problems are associated with: 1) the ambiguous identification of physiological oscillatory components via filtering and Fourier decomposition, 2) the origin of the correlation between oscillatory components (effects of non-linearity and non-stationarity), and 3) the statistical evaluation of the measures of CFC.

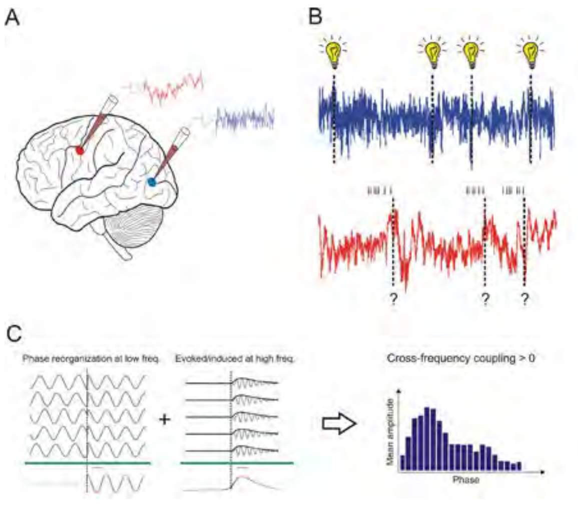


Figure 1: A) Recordings at early sensory (blue), and higher (red) cortical areas. B) While inputs to the early cortical areas can be easily controlled or monitored, inputs to higher areas are difficult to evaluate. C) The non-stationarities associated to input arrival can generate patterns that can be confounded with cross-frequency interactions. Unfortunately, without control of inputs the ambiguity between oscillatory interactions and input-related patterns cannot be easily disentangled.

Thus, in this research project we study which conditions need to be tested to solve some of the ambiguities with the hope that knowing such conditions will be helpful for the advancing of cross-frequency analysis of brain activity.

[1] J. Aru, J. Aru, M. Wibral, V. Priesemann, G. Pipa, L. Lana, W. Singer, R. Vicente, *Untangling cross-frequency analysis in neuroscience*, submitted.

The neural correlates of motion-in-depth perception in human and non-human primates

Collaborators: H. S. Lee[1,2], S. van Stijn[3], R. Deichmann[4], W. Singer[1,2,3], A. Kohler[5]

[1] Frankfurt Institute for Advanced Studies, [2] Max-Planck Institute for Brain Research,
[3] Ernst Strüngmann Institute, [4] Brain imaging Center Frankfurt, [5] University of Münster

Perceiving motion in depth would require processing of both depth information and motion information. Numerous studies focused on one of the two mechanisms – either processing of static depth or processing of frontoparallel motion – but not both in one. To understand the inter-play between these two processes, we devised a stereoscopic stimulus (random-dot stereogram) that differentiates the processing stages of depth and motion in the brain; and then applied state-of-art brain mapping techniques to identify these areas.

From a human fMRI study, we found that the area V3A/B in the intraparietal sulcus is involved in process of forming a surface in depth, and the area MST in the inferior temporal sulcus is responsible for seeing motion of the surface in depth.

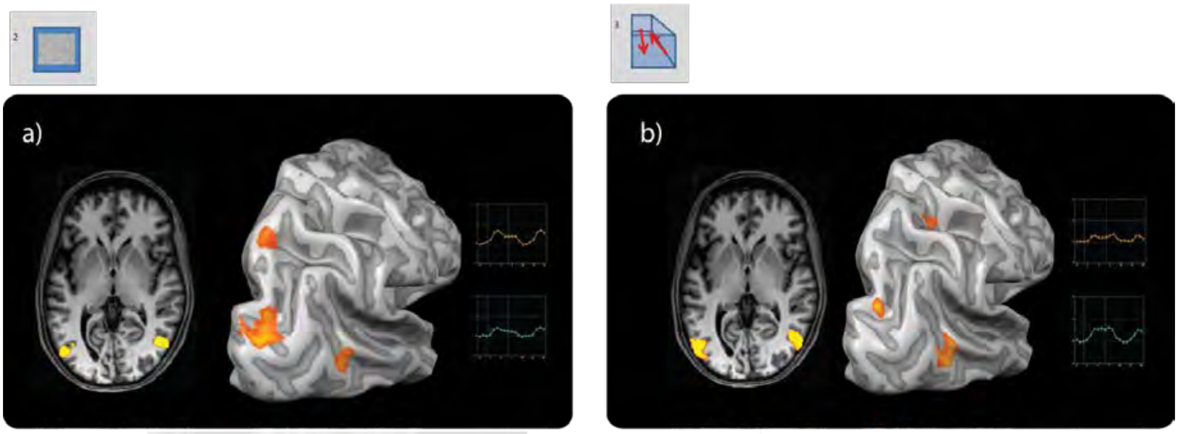


Figure: Whole brain analysis of an exemplary subject. Transversal view (left) and reconstructed right hemisphere (middle) showing the activations clusters of contrasting motion component in the stimulus (a) and contrasting depth component (b). The averaged BOLD time courses for orange and green region on the right in each panel.

These areas were previously defined in monkey studies and better understood from the electrophysiology of awake monkeys. To find the homologues in non-human primates we are currently repeating the identical paradigm with awake moneys doing the identical task. The results will guide us to identify matching brain regions in two species (human and monkey) and bridge the gap between human fMRI findings and the more prevalent data from monkey electrophysiology.

Stimulus information coded by spike timing

Collaborators: M. N. Havenith, S. Yu, J. Biederlack, N-H. Chen, W. Singer, D. Nikolić

The synchronized activity of cortical neurons often features spike delays of several milliseconds. Usually, these delays are considered too small to play a role in cortical computations. We used simultaneous recordings of spiking activity from up to 12 neurons to show that, in the cat visual cortex, the pairwise delays between neurons form a preferred order of spiking, called firing sequence. This sequence spans up to 15 ms and is referenced not to external events but to the internal cortical activity (e.g., beta/gamma oscillations). Most importantly, the preferred sequence of firing changed consistently as a function of stimulus properties. During beta/gamma oscillations, the reliability of firing sequences increased and approached that of firing rates. This suggests that, in the visual system, short-lived spatio-temporal patterns of spiking defined by consistent delays in synchronized activity occur with sufficient reliability to complement firing rates as a neuronal code.

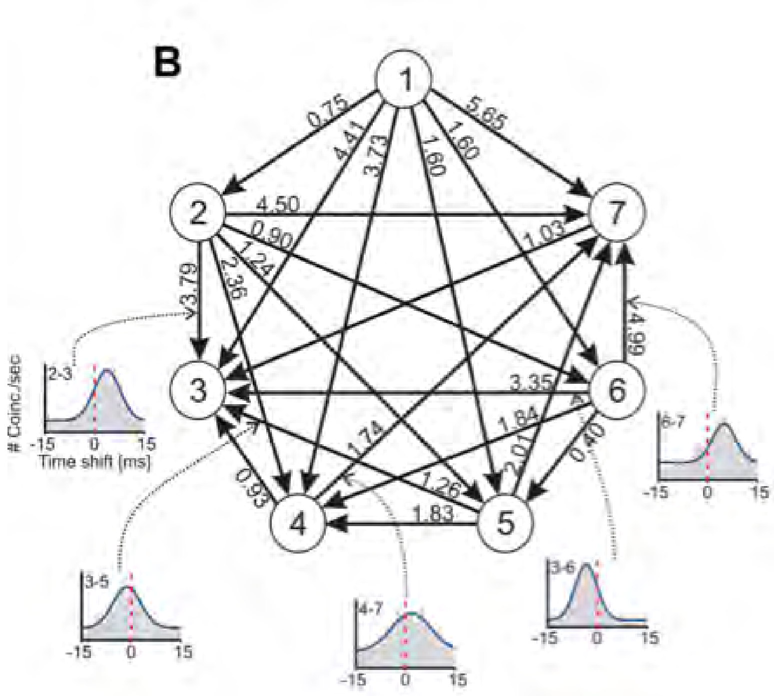


Figure: A network of time delays extracted from all possible pairwise cross correlations computed for seven multi-units. Example cross-correlo-grams are shown on the bottom. The time delays on the edges are in milliseconds and have the property of additivity.

Related publication in 2011:

M. N. Havenith, S. Yu, J. Biederlack, N-H. Chen, W. Singer and D. Nikolić, *Synchrony makes neurons fire in sequence – and stimulus properties determine who is ahead*, Journal of Neuroscience, 31, 8570-8584 (2011).

The structure and origin of higher order correlations in the brain

Collaborators: S. Yu, H. Yang, H. Nakahara, G.S. Santos, D. Nikolić, D. Plenz

In the cortex, the interactions among neurons give rise to transient coherent activity patterns that underlie perception, cognition, and action. Recently, it was actively debated whether the most basic interactions, i.e., the pairwise correlations between neurons or groups of neurons, suffice to explain those observed activity patterns. So far, the evidence reported is controversial. Importantly, the overall organization of neuronal interactions and the mechanisms underlying their generation, especially those of high-order interactions, have remained elusive. We showed that higher-order interactions are required to properly account for cortical dynamics such as ongoing neuronal avalanches in the alert monkey and evoked visual responses in the anesthetized cat. A Gaussian interaction model that utilizes the observed pairwise correlations and event rates and that applies intrinsic thresholding identifies those higher-order interactions correctly, both in cortical local field potentials and spiking activities. This allows for accurate prediction of large neuronal population activities as required, e.g., in brain–machine interface paradigms. Our results demonstrate that higher-order interactions are inherent properties of cortical dynamics and suggest a simple solution to overcome the apparent formidable complexity previously thought to be intrinsic to those interactions.

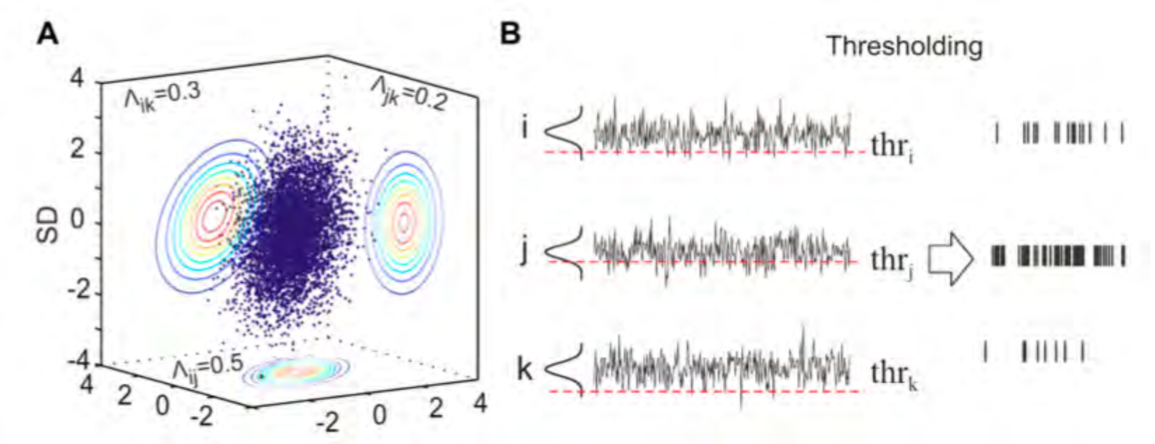


Figure: Distributed Gaussian model. A. An example 3D data set. B. Time series with indicated thresholding procedure (red horizontal line) and the resulting spike trains (far right).

Related publication in 2011:

S. Yu, H. Yang, H. Nakahara, G.S. Santos, D. Nikolić and D. Plenz, *Higher–order interactions characterized in cortical activity*, Journal of Neuroscience, 31, 17514-17526 (2011).

Non-stationarity of neuronal activity
(LOEWE Neuronale Koordination Forschungsschwerpunkt Frankfurt (NeFF))

Collaborators: D. Nikolić, R.C. Mureşan, W. Feng, W. Singer

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 developed 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 defined by the scale. Scaled correlation analysis has several advantages over traditional filtering approaches based on computations in the frequency domain. Among its other applications, the method can assist the studies of precise neuronal synchronization.

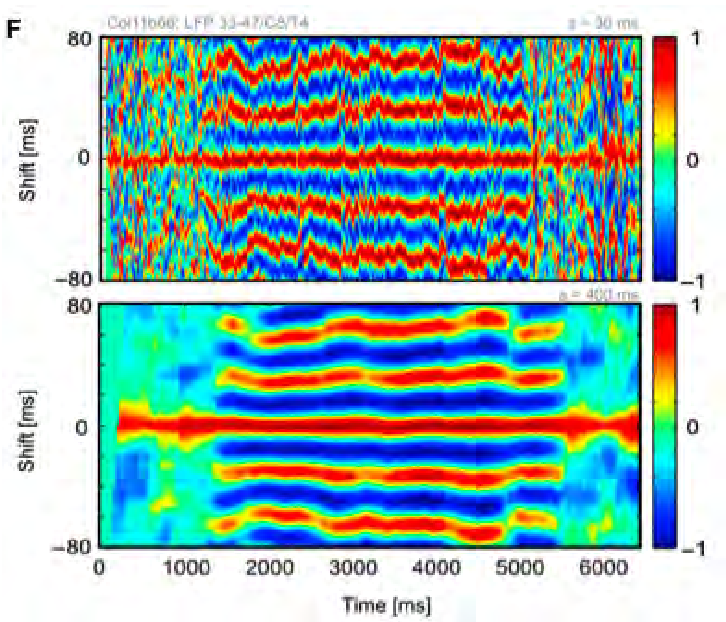


Figure: Time resolved auto-correlation of local field potentials computed with (top) and without scaled correlation (bottom).

Related publication:

D. Nikolić, R.C. Mureşan, W. Feng and W. Singer, *Scaled correlation analysis: A better way to compute a cross-correlogram.* European Journal of Neuroscience (to appear)

The semantic component of synesthesia

Collaborators: D. Nikolić, U.M. Jürgens, N. Rothen, B. Meier, A. Mroczko

The traditional and predominant understanding of synesthesia is that a sensory input in one modality (inducer) elicits sensory experiences in another modality (concurrent). Recent evidence suggests an important role of semantic representations of inducers. We reported the cases of two synesthetes, experienced swimmers, for whom each swimming style evokes another synesthetic color. Importantly, synesthesia is evoked also in the absence of direct sensory stimulation, i.e., the proprioceptive inputs during swimming. To evoke synesthetic colors, it is sufficient to evoke the concept of a given swimming style e.g., by showing a photograph of a swimming person. A color-consistency test and a Stroop-type test indicated that the synesthesia is genuine. These findings imply that synesthetic inducers do not operate at a sensory level but instead, at the semantic level at which concepts are evoked. Hence, the inducers are not defined by the modality-dependent sensations but by the "ideas" activated by these sensations.

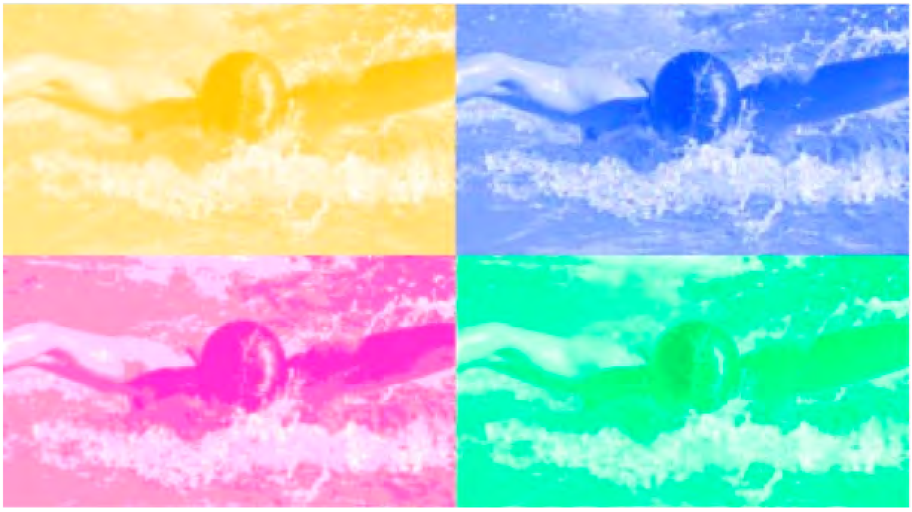


Figure: Stimuli used in the study. A person using a certain swimming style was shown either in synesthetic color or in a different color. The task for the subjects was to name the color as quickly as possible.

Related publications in 2011:

D. Nikolić, U.M. Jürgens, N. Rothen, B. Meier and A. Mroczko, *Swimming-style synesthesia*, Cortex, 47, 874-879 (2011).

D. Nikolić und U. M. Jürgens, *Sinfonie in Rot*, Gehirn & Geist, 6/2011: 58-63.

Timescale of information processing in visual cortex

Collaborators: Ovidiu Jurjuț[1,2], Cătălin Rus[1], Luiz Lana[1,2], Danko Nikolić[1,2], Raul Mureșan[3], Wolf Singer[1,2]

[1] Frankfurt Institute for Advanced Studies, [2] MPI for Brain Research, Frankfurt, [3] Coneural, Romanian Institute of Science and Technology, Cluj-Napoca

Our project investigates how information is processed in the cortex by means of spatiotemporal spike patterns, i.e. constellations of spikes distributed across multiple neurons over a given time window. We are particularly interested in identifying the temporal scale(s) on which patterns that are informative about the environment occur.

To address this issue, we used multielectrode spiking data recorded from the primary visual cortex of anesthetized cats and awake behaving monkeys, while the animals were presented artificial and natural visual stimuli with different temporal dynamics. To analyze such data we developed a method that is able to quantify the occurrence of spike patterns on arbitrary timescales and determine which timescale is most informative for discriminating between stimuli at different moments in time (Jurjut et al. 2011).

In the cat data we found that slow changing stimuli, such as drifting gratings, can be distinguished best by using spike patterns with longer timescales (~100 ms), while fast changing stimuli, such as briefly flashed graphemes, are better distinguished by spike patterns with short timescales (~10 ms). For stimuli with mixed dynamics, such as movies containing natural images, we found that short and longer timescales were both informative, but at different moments in time. Thus, informative spike patterns appear on a continuum of coexisting timescales, which strongly relate to the temporal dynamics of the stimuli (Jurjut et al. 2011). Moreover, preliminary results from monkey data indicate that information flow on short timescales is enhanced during awake states.

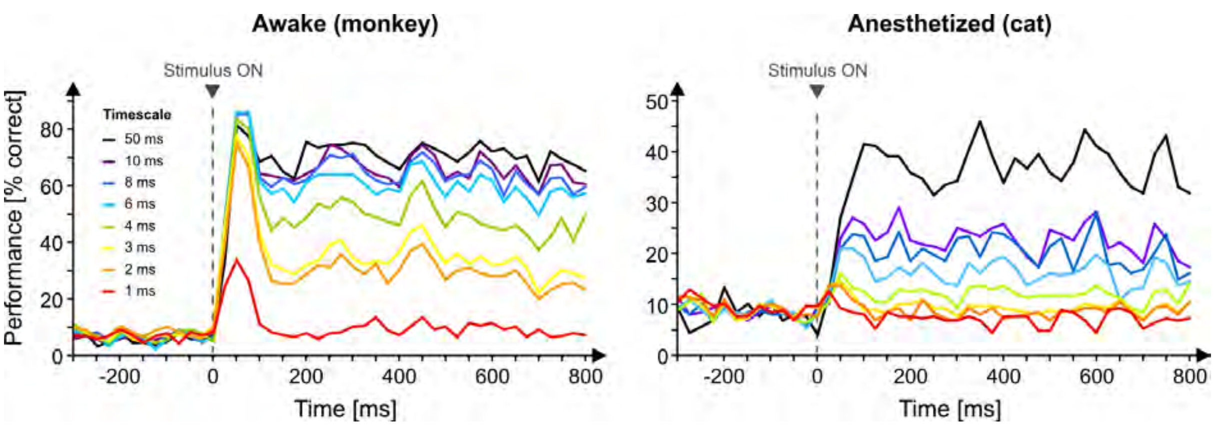


Figure: Classification performance of stimuli at different timescales, in awake and anesthetized brain states. Stimuli were gratings, drifting in different directions (16 – monkey, 12 – cat).

Related publication in 2011:

O. F. Jurjuț, D. Nikolić, W. Singer, S. Yu, M. N. Havenith, R. C. Mureșan, *Timescales of multi-neuronal activity patterns reflect temporal structure of visual stimuli*. PLoS ONE 6(2): e16758, doi:10.1371/journal.pone.0016758 (2011)

Beta/gamma oscillations increase neural complexity

Collaborators: Peng Wang[1], Bruss Lima[2], Wolf Singer[1], Sergio Neuenschwander[3], Danko Nikolić[1]

[1]FIAS and MPIH, Frankfurt, Germany, [2]Department of Neuroscience, Columbia University, New York, USA, [3]Brain Institute, Universidade Federal do Rio Grande do Norte, Natal, Brazil

High complexity of an information processing system is thought to reflect enhanced computational capacity, while the reverse is true if complexity is reduced. Currently, it is unclear how the synchronous oscillations in the beta/gamma range affect the complexity of brain activity and hence, which implications they have for the computational capabilities of neuronal networks.

According to Tononi, Sporns, and Edelman, (1994), neural complexity is maximal when the system is able to perform simultaneously both integration and segregation. Thus, both fully synchronized and totally uncorrelated states (e.g. white noise) have minimal complexity. The formal definition of neural complexity by Tononi et al. permits estimating computational capabilities of a system without having to specify the actual computational mechanisms.

We investigated neural complexity in the visual cortex of both anesthetized cats and awake monkeys by analyzing in parallel the responses of up to 17 neurons to visual stimuli. Unexpectedly, higher complexity was found when the cortical network engaged in synchronous gamma oscillations. This was the case in both preparations and irrespective of whether oscillations were induced by manipulating stimulus properties or occurred spontaneously following changes in cortical states. Importantly, the changes in complexity could not be explained by variations in firing rates.

In conclusion, when cortical networks engage in gamma oscillations, their dynamics becomes richer. This suggests that during states characterized by gamma synchrony, the cortex exhibits higher computational and coding capacities.

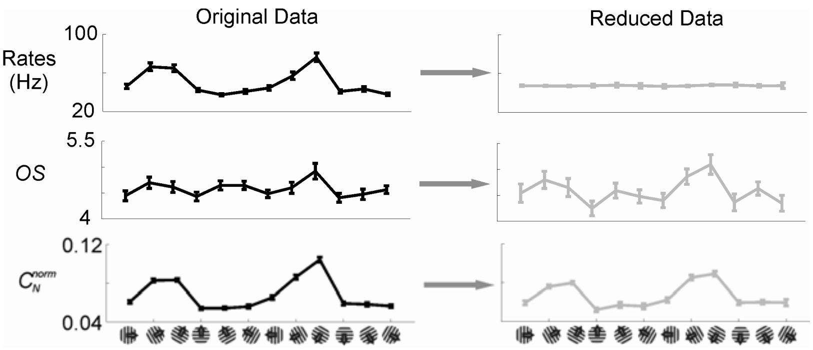


Figure: Neural complexity has similar tuning as oscillation score, even in a subset of data when tuning of firing rates disappears.

Related publication in 2011:

P. Wang, B. Lima, W. Singer, N. Neuenschwander and D. Nikolić, *Beta/gamma oscillations increase neural complexity*, Conference abstract: Society of Neuroscience 2011, 483.16.

Discovery of agency in 6 and 8-month-old human infants

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

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

As an infant tries to make sense of the vast array of signals from its sense organs 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, in other words, to discover agency. It has been difficult shedding light on this ability in infants because of their limited motor repertoires. Fortunately, however, infants reach accurate control over their eyes comparatively early, suggesting that eye movements could be used as a window into their ability to discover novel action outcomes. Using a newly-developed gaze-contingent (GC) paradigm employing automated eye-tracking, we here show 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. Such gaze-contingent paradigms based on eye-tracking have been explored with adult subjects before, but only recently it has become possible to apply eye tracking to infants. The ability of infants to quickly discover new ways of controlling their environment that we demonstrate here, paves the way for truly interactive new paradigms for studying infant learning and cognition and may provide a basis for novel training and medical intervention strategies.

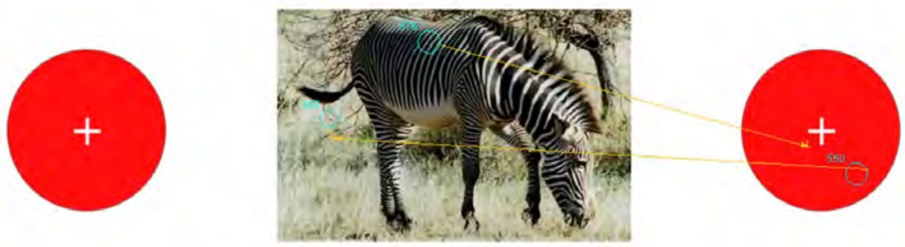


Figure: By looking at one of the two red buttons, infants can trigger the appearance of a new animal picture. Our results show that they quickly start to anticipate the appearance of these pictures with their eyes. Circles indicate fixation locations, numbers give their durations in milliseconds.

Related publications:

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, in press.

Unifying procedural memory consolidation and structure learning in a recurrent network model of motor control

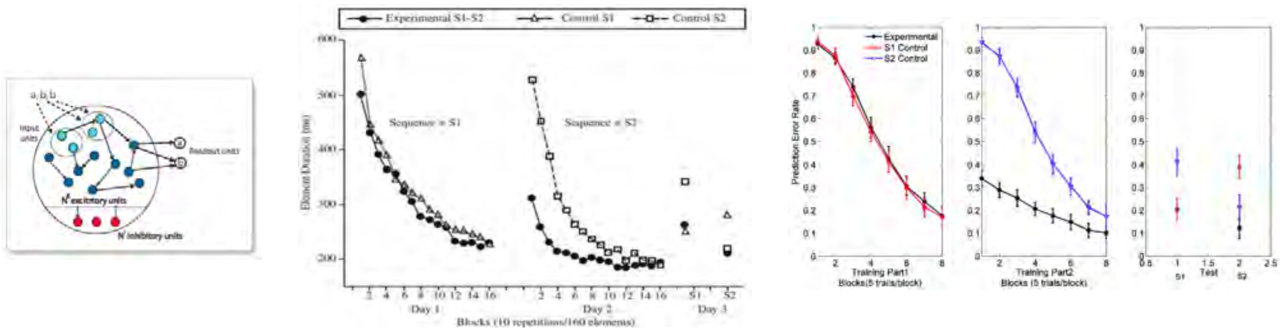
Collaborators: Q. Wang[1], C.A. Rothkopf[1], J. Triesch[1]

[1] Frankfurt Institute for Advanced Studies

Humans can improve their performance in movement sequence tasks through practice, but such motor learning has shown a wide variety of puzzling and partly contradictory effects. Blocked training of multiple sequences has been shown to lead to reduced retention compared to interleaved training and a wide variety of proactive and retroactive facilitation and interference effects have been observed. Furthermore, recent studies have shown that transfer of learning between different tasks is based on structural task similarities. Here we address the question of how these phenomena can be understood in terms of the shaping of neuronal representations through different plasticity mechanisms in a recurrent network model.

We use a sparsely connected recurrent network whose connectivity is shaped by STDP, intrinsic plasticity, and synaptic scaling. Additionally, this network is connected to a layer of motor neurons mediating the movement sequence. We apply this network to a series of experiments about movement sequence learning and use a single set of parameters in all simulations. The network learns to carry out the correct movement sequences over trials and shows striking similarity to the human behavior in a variety of training schedules over different sequence similarities.

We show how psychophysical performance measures are reflective of the underlying neuronal representations in the recurrent network. These results are interpreted in terms of the changes in the neuronal sequence representations and testable predictions for further experiments are derived. Specifically, we show how sequence similarity and training schedule interact to produce a rich set of interference and facilitation effects thereby unifying structure learning and procedural consolidation.



Left: Illustration of reservoir computing with recurrent network. *Center:* Empirical data (Panzer et al., 2006). *Right:* Simulation results showing facilitation for sequence 2 and retroactive interference for sequence 1.

Related publications in 2011:

1) Q. Wang, C. A.Rothkopf, J. Triesch, *Unifying procedural memory consolidation and structure learning in motor control*, COSYNE - Computational and Systems Neuroscience, February 24-27, 2011, Salt Lake City, Utah, USA.

Power spectra of the natural input to the visual system explain retinal coding

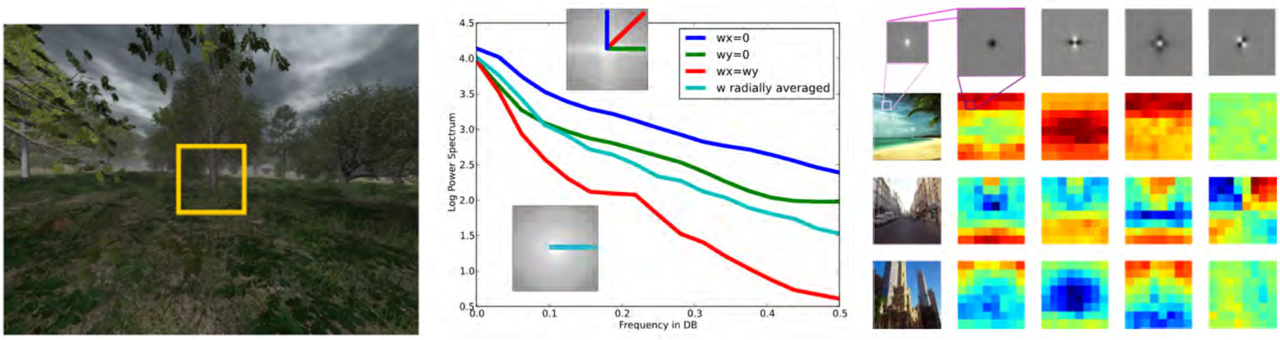
Collaborators: D. Pamplona[1], J. Triesch[1], C. A. Rothkopf[1]

[1] Frankfurt Institute for Advanced Studies

The statistics of the natural environment have been characterized to gain insight in the processing of natural stimuli based on the efficient coding hypothesis. The statistical regularities present in these images have been measured and neurons have been shown to reduce the redundancy present in these stimuli. This analysis reveals that retinal Ganglion cells' properties can be related to the second order dependencies present in natural images. While such analysis has used the convenient assumption that natural image data is isotropic across the visual field, giving up on this assumption has reveal important dependencies reflected by their neuronal coding. Here we consider and quantify precisely the second order dependencies in images of natural environments due to the imaging properties of a model eye.

First, we generated artificial scenes with three-dimensional edge elements and quantified the resulting distributions of orientations by applying the perspective projection onto a spherical surface. These distributions show a strong influence of the imaging process on the statistics of the input to the visual system. Secondly, image data from a naturalistic virtual environment was obtained. The second order statistics were computed as a function of eccentricity and radial distance from the center of projection. This analysis confirms strong dependencies of the second order statistics on the position across the visual field. Finally, we repeated the analysis to commonly used natural image databases including the van Hateren database and quantified the second order dependencies as function of the position across the visual field using a new generalized parameterization of the power spectra.

We conclude by providing a detailed quantitative analysis of the second order statistical dependencies of the natural input to the visual system and making novel predictions of the retinal Ganglion cells' profiles as function of their position across the visual field.



Left: Naturalistic virtual reality image covering 120 degrees of field of view and a region corresponding to 26 degrees of eccentricity. *Center:* Profile power spectra for different directions across the visual field. *Right:* Distribution of the projections on the principal components of power spectra depending on the position and scene. On the left column are the first four principal components, the rows are average coefficients of projection of three scenes categories: coast, street and tall building.

Related publication in 2011:

1) D. Pamplona, J. Triesch, C. A. Rothkopf, *Predicting Ganglion Cells Variability*, COSYNE - Computational and Systems Neuroscience, February 24-27, 2011, Salt Lake City, Utah, USA.

Modeling the effect of transcranial magnetic stimulation on cortical circuits

Collaborators: 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, Goethe University Frankfurt

The goal of this research is to better understand how brain activity might be directly controlled from outside the head through magnetic stimulation. Specifically, transcranial magnetic stimulation (TMS) and other non-invasive stimulation techniques have been hypothesized to improve learning, facilitate stroke rehabilitation, treat depression, schizophrenia, chronic pain, or addictions such as alcoholism. Despite recent success in clinical treatments little is known about the cellular mechanisms underlying such stimulation techniques or the nature of the high-frequency repetitive responses (I-waves) they induce along descending motor pathways. Moreover, assessing the nature of I-waves or establishing the biophysical basis underlying the magnetic stimulation in purely experimental settings remains difficult given the scarce recording opportunities and high variability of results across healthy subjects. Models incorporating anatomically detailed neurons could overcome these limitations and provide valuable insight into the effects of TMS at the cellular level. Our model reproduces I-waves similar to those observed in epidural responses during *in vivo* experiments on conscious humans and explains their formation, frequency, and timing. Furthermore, our model reproduces findings from a range of experiments with different stimulation protocols and pharmacological interventions. We view this as an important first step towards designing optimized protocols for specific clinical purposes.

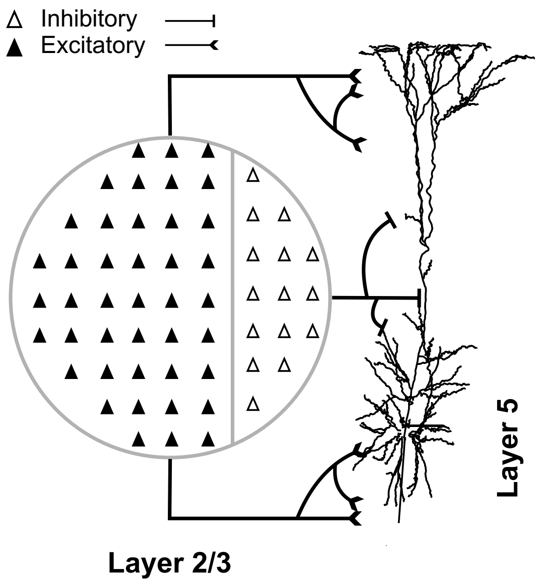


Figure: The model we have developed includes a reconstructed dendritic tree of a L5 pyramidal cell. A total of 300 excitatory and inhibitory L2/3 cells (ratio 4:1) project synapses on to the L5 cell.

Related publications:

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

Self-organization in recurrent neural networks with multiple forms of plasticity

Collaborators: P. Zheng[1], C. Dimitrakakis[1,2], A. Lazar[1,3], G. Pipa[1,4], D. Krieg[1], P. Sterne[1], L. Aitchison[5], J. Triesch[1]

[1] Frankfurt Institute for Advanced Studies, [2] EPFL, Switzerland, [3] Max-Planck Institute for Brain Research Frankfurt, [4] University of Osnabrück, [5] Gatsby Computational Neuroscience Unit, UK

Understanding the network structure of cortical circuits is of fundamental importance for understanding cortex function. 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. At present it is unclear, however, how the measured distribution of synaptic strengths and the pattern of synaptic fluctuations arise. Our explanation is based on concepts from self-organization. We show 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 self-organization produces a network with irregular activity patterns consistent with cortical recordings, lognormal-like weight distributions, and patterns of synapse fluctuations closely matching experimental data (see Figure). This self-organization is very robust to parameter changes in the network but critically depends on the presence of the different homeostatic plasticity mechanisms. Our findings have far reaching implications for the development, structure, and function of cortical circuits. First, it reveals the fundamental importance of different homeostatic plasticity mechanisms for the organization of cortex. Second, it sheds light on the structure of spontaneous activity in the cortex, which has traditionally been treated as noise. Our work suggests that this activity is in fact highly organized and essential for shaping network structure and function.

In a second line of research we study these self-organizing networks from the viewpoint of information theory and try to understand their learning mechanisms as approximations to the maximization of mutual information. In a similar vein, we have developed a theory of spike-timing dependent plasticity and other forms of synaptic long-term plasticity that tries to bridge biophysical and computational levels of description.

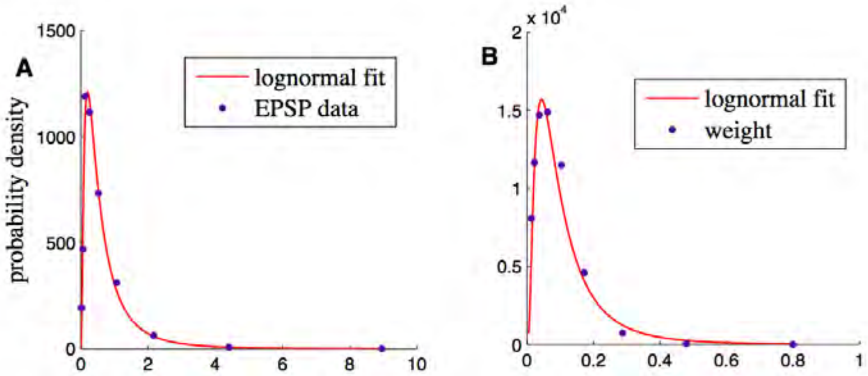


Figure: Distribution of synaptic weights in our model matches lognormal distribution of EPSPs in cortex. A: distribution of EPSP sizes from Song et al. (2005) and lognormal fit. B: distribution of weight strength in our model and lognormal fit.

Related publications:

1) P. Zheng, C. Dimitrakakis, J. Triesch, *Network Self-organization Explains the Statistics and Dynamics of Synaptic Connection Strengths in Cortex*, in preparation.

2) A. Lazar, G. Pipa, J. Triesch, *Emerging Bayesian Priors in a Self-Organizing Recurrent Network*, Proc. of the International Conference on Artificial Neural Networks (ICANN), 2011.

3) D. Krieg, J. Triesch, *A unifying theory of synaptic long-term plasticity based on a sparse synaptic strength*, submitted.

4) P. Sterne, L. Aitchison, J. Triesch, *SORN network dynamics approximately maximise mutual information*, in preparation.

Developmental robotics

Collaborators: P. Chandrashekhariah[1] , G. Spina[1], D. Krieg[1] , D. Pamplona[1], C. Rothkopf[1] , J. Triesch[1] , B. Shi[2], Z. Yu[2]

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

In this line of research we investigate how principles of learning and development from biological organisms can be exploited to build autonomously learning robots. 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 learning of disparity tuning and vergence eye movements. Concretely, a generative model is learning to jointly encode the left and right images. At the same time, the system 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 a the ability to properly align the two eyes and lean a representation of binocular disparity can develop and self-calibrate completely autonomously on the basis of efficient coding principles.

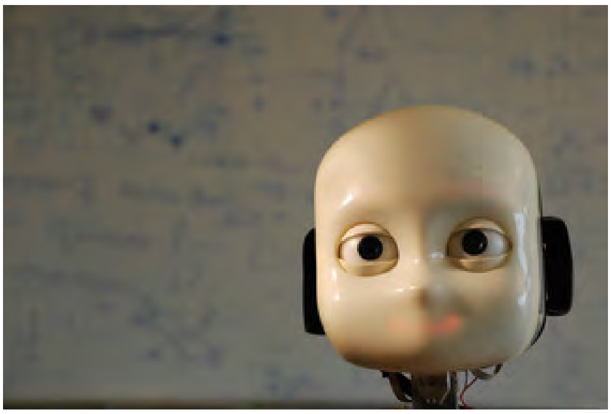


Figure: The iCub robot head used in our studies. Its degrees of freedom and appearance are modeled after a 2-year-old child.

Related publications in 2011:
1) P. Chandrashekhariah, Q. Wang, G. Spina, *Familiarity-to-novelty shift driven by learning: a conceptual and computational model*, IEEE Int. Conference on Development and Learning and Epigenetic Robotics (ICDL-EpiRob), 2011.
2) P. Chandrashekhariah, G. Spina, J. Triesch, *Let it learn: A curious vision system for autonomous object learning*, in preparation.

Learning mechanisms underlying visual orienting and other coordinated motor behaviors

Collaborators: S. Saeb[1], C. Weber[2], J. Triesch[1], T. Weisswange[1,3], C. Rothkopf[1], T. Rodemann[3], L. Lonini[1], C. Dimitrakakis[1,4]

[1] Frankfurt Institute for Advanced Studies, [2] Dept. of Computer Science, University of Hamburg, [3] Honda Research Institute Europe, Offenbach, [4] EPFL, Switzerland

Orienting movements are a fundamental class of motor behaviors that most animals must perform. In this line of research we study the learning principles and mechanisms that may give rise to coordinated orienting movements. On the one hand we are interested in how multiple sensory modalities such as vision and audition are integrated for successful orienting movements. On the other hand we investigate how we learn to coordinate multiple motor pathways such as eye and neck for successful orienting. More generally, we are asking how motor control can be organized hierarchically and what this implies for learning complex behaviors, especially when multiple behaviors have to be learned by the same system.
Of particular interest are saccades – rapid gaze shifts through which Human beings and many other species redirect their gaze towards relevant targets. Saccades are made approximately three to four times every second, and larger saccades result from fast and concurrent movement of the animal's eyes and head. Experimental studies have revealed that during saccades, the motor system follows certain principles such as respecting a specific relationship between the relative contribution of eye and head motor systems to total gaze shift. Various researchers have hypothesized that these principles are implications of some optimality criteria in the brain, but it remains unclear how the brain can learn such an optimal behavior. We have proposed a new model that uses a plausible learning mechanism to satisfy an optimality criterion. We show that after learning, the model is able to reproduce motor behavior with biologically plausible properties. In addition, it predicts the nature of the learning signals.

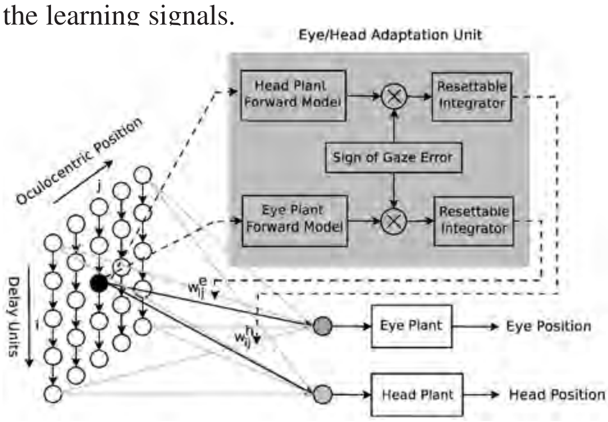


Figure: Architecture of our model learning coordinated eye and head movements.

Related publications in 2011:

1) S. Saeb, C. Weber, J. Triesch, *Learning the Optimal Control of Coordinated Eye and Head Movements*, PLoS Computational Biology, 7(11), doi:10.1371/ journal.pcbi.1002253, 2011.
2) H. Toutounji, C. A. Rothkopf, J. Triesch, *Scalable reinforcement learning through hierarchical decompositions for weakly-coupled problems*, IEEE 10th International Conference on Development and Learning (ICDL), August 24-27 (2011)
3) C. Karaoguz, T. H. Weisswange, T. Rodemann, B. Wrede, C. A. Rothkopf, *Reward-based learning of optimal cue integration in audio and visual depth estimation*, 15th International Conference on Advanced Robotics (ICAR), June 20-23 (2011)
4) T. H. Weisswange, C. A. Rothkopf, J. Triesch, *Bayesian cue integration as a developmental outcome of reward mediated learning*, PLoS ONE, (2011), doi: 10.1371/journal.pone.0021575
5) C. A. Rothkopf, D. H. Ballard, *Learning to coordinate repertoirs of behaviors: credit assignment and module activation*, submitted.
6) L. Lonini, C. Dimitrakakis, C. A. Rothkopf, J. Triesch, *Generalization and interference in human motor control*, submitted.

Visual working memory contents bias ambiguous perception

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

[1] Frankfurt Institute for Advanced Studies, [2] Justus Liebig University, Giessen

When we interact with our environment, we are often faced with partially degraded or even ambiguous sensory information. Under those conditions, what we perceive can be largely determined by the state of our cognitive system. In the present study we show that what we are holding in working memory (WM) can bias the way we perceive ambiguous stimuli. Holding in memory the percept of an unambiguously rotating sphere influenced the perceived direction of motion of an ambiguously rotating sphere presented shortly thereafter. This was not the case if observers attended to but did not memorize the unambiguous stimulus. Differences in the time-course of the percept in the two conditions indicate that WM and attention act in a qualitatively different way on visual perception: in the attention condition, the short-lived repulsive effect may be an example of fast adaptation to a briefly displayed stimulus. In the WM condition instead, the long-lived facilitation effect may be ascribed to a sustained top-down modulation of neural activity in early sensory areas, due to the voluntary maintenance of a visual representation in WM. The results suggest that the WM representation of visual motion is supported by early visual areas.

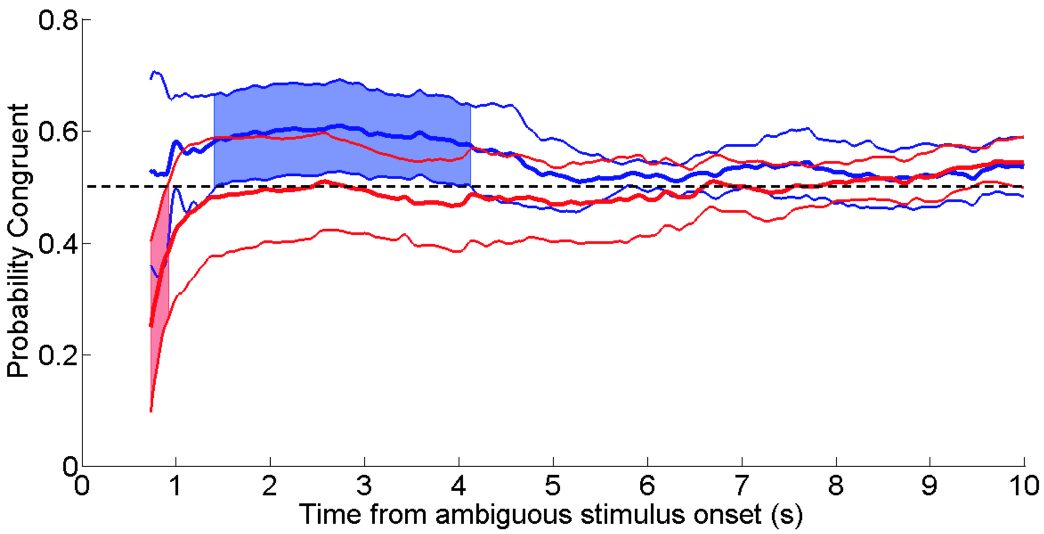


Figure: Average probability of seeing the ambiguous stimulus moving in the same direction as the unambiguous stimulus, expressed as a function of time from the ambiguous stimulus onset. Data are smoothed with a Gaussian filter of time constant 110 ms. Blue: Experiment 1, WM condition. Red: Experiment 2, control condition. Thick and thin lines represent group averages and 95% confidence intervals respectively. Colored insets represent periods where the probability of reporting a congruent percept is reliably above or below chance.

Related publications in 2011:

1. L. Scocchia, M. Valsecchi, K.R. Gegenfurtner, J. Triesch, *Working memory contents influence binocular rivalry*, Perception, 40, ECVP Abstract Supplement, 84 (2011).

2. L. Scocchia, M. Valsecchi, K.R. Gegenfurtner, J. Triesch, *Visual working memory contents bias ambiguous perception*, Psychological Science, 302415 (2011).

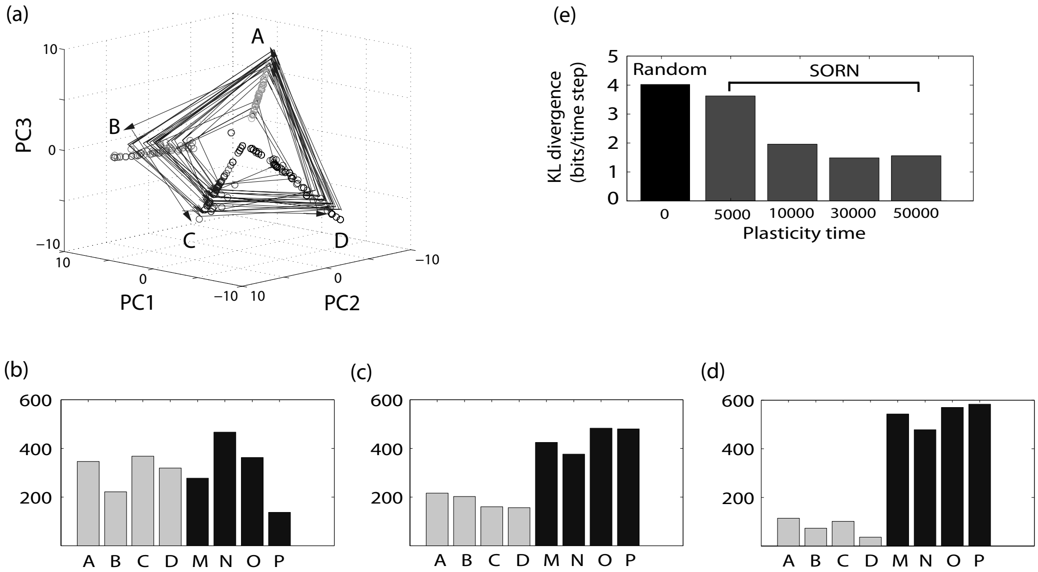
Emerging Bayesian priors in a self-organizing recurrent network

Collaborators: A. Lazar[1,2], G. Pipa[3], J. Triesch[1]

[1] Frankfurt Institute for Advanced Studies, [2] Max-Planck Institute for Brain Research, [3] Institute of Cognitive Science, University of Osnabrück

Convincing evidence supports the idea that cortical processing is efficiently adapted to the statistical properties of the environment and that perception and action arise on the basis of Bayesian statistical calculations. However, little is known about the neuronal correlates of statistical learning and inference. Specifically, it is not known how statistical priors are encoded by neurons in a dynamic setting and how they are combined with sensory information to generate an optimal percept.

In this study, we explore the role of local plasticity rules in incorporating priors that reflect the statistical properties of the stimuli. Our self-organizing recurrent neural network (SORN) receives input sequences composed of different symbols and learns the structure embedded in these sequences via a simple spike-timing-dependent plasticity rule, while synaptic normalization and intrinsic plasticity maintain a low level of activity. Following the repetitive presentation of a given set of stimuli, we omit the input and analyse the characteristics of spontaneous activity. We find that the network revisits states similar to those evoked by sensory input and that it follows similar trajectories through its high-dimensional state space. Furthermore, the network has learned the statistical properties of the data: during spontaneous activity the network preferentially visits states that are similar to evoked activity patterns for inputs with a higher prior probability. In several classification tasks, we show that the network's 'perception' of the current source of information is influenced by the learned prior probabilities.



Spontaneous and evoked activity become similar in SORNs: (a) Result of PCA on SORN's internal representations during evoked activity to a sequence of letters (circles), and spontaneous activity in the absence of input (lines). (b) Distribution of spontaneous states for random networks in the absence of plasticity. Distribution of spontaneous states is similar to the evoked responses to different input letters, when MNOP is presented two times more often (c) or three times more often (d) than ABCD during plastic self-organization in SORNs. (e) Divergence between the distributions of evoked and spontaneous activity as a function of plastic self-organization.

Related Publication 2011:

A. Lazar, G. Pipa and J. Triesch, *Emerging Bayesian priors in a self-organizing recurrent network*, Artificial Neural Networks and Machine Learning, ICANN 2011, Part II, Lecture Notes in Computer Science, Springer: 6792: 127-134.

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], C. Savin[2], P. Berkes[3]

[1] Frankfurt Institute for Advanced Studies, [2] Computational and Biological Learning Lab, Dept of Engineering, University of Cambridge, UK, [3] Visual Information Processing and Learning Lab, Life Science, Brandeis University, USA

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 neural brain circuits acquire 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.

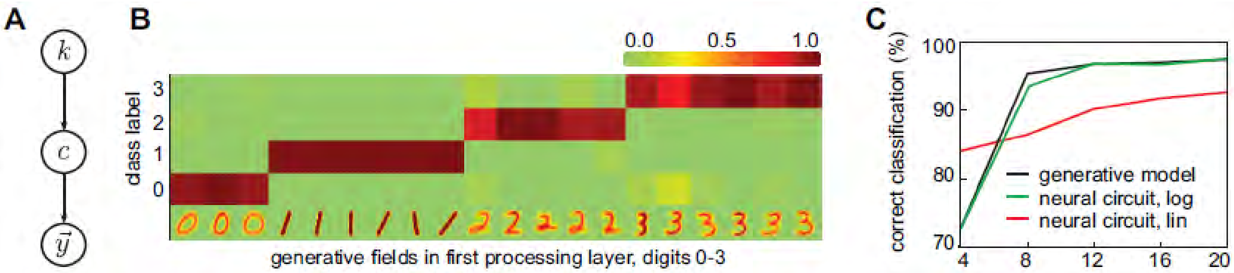


Figure *A:* Hierarchical graphic memory model for pattern classification. *B:* Assignment of autonomously learned hand-written digits (bottom row) to classes using few labelled examples. *C:* Classification results of a statistical generative model for classification compared to neural circuits. Both can be made almost equal (green and black line).

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) suggesting that neural response variability and spontaneous activity are a consequence of a probabilistic neural code that processes stimuli by stochastically activating neurons encoding possible stimulus interpretations. In the paper by Shelton et al. (2011) we made the high efficiency of neural processing and learning consistent with these experimental finding. Prior work on efficient learning (in collaboration with the Honda Research Institute, Europe; Lücke, Eggert, 2010) has, furthermore, allowed for the development of several new learning algorithms.

In the project by Keck et al. (2012) we go a step further and study concrete neural interaction rules that allow for optimal learning in an information theoretical sense. We could thus show that well-known neural interaction rules and mechanisms such as feed-forward inhibition and synaptic scaling can result in a statistically optimal learning of pattern memories (see figure).

All our approaches exploit the hardware for massively parallel computing available at the FIAS and the CSC Frankfurt (compare Dai et al., 2011).

Related publications in 2011:

Keck, C., Savin, C., and Lücke, J. Input normalization and synaptic scaling – two sides of the same coin? PLoS Computational Biology, submitted 2011, accepted 2012.

Shelton, J. A., Bornschein, J., Sheikh, A. S., Berkes, P., and Lücke, J. Select and sample – A model of efficient neural inference and learning. Advances in Neural Information Processing Systems 24, 2618-2626, 2011.

Dai, Z., Shelton, J. A., Bornschein, J., Sheikh, A. S., and Lücke, J. Combining approximate inference methods for efficient learning on large computer clusters. NIPS Workshop: Big Learning - Algorithms, Systems, and Tools for Learning at Scale, 2011.

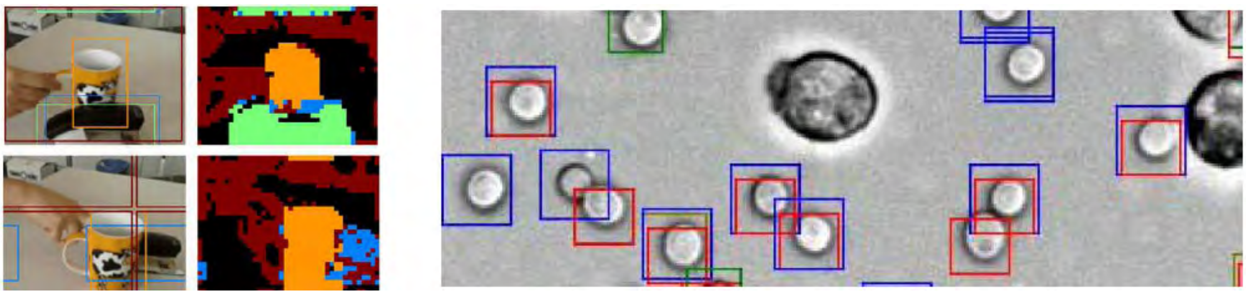
Non-linear generative models and their applications

Collaborators: J. Lücke[1], M. Henniges[1], A. S. Sheikh[1], J. Bornschein[1], Z. Dai[1], J. Eggert[2], R. Turner[3], M. Sahani[4], Marc-Thilo Figge[5]

[1] Frankfurt Institute for Advanced Studies, [2] Honda Research Institute, Europe, [3] Dept of Engineering, University of Cambridge, UK, [4] Gatsby Computational Neuroscience Unit, University College London, UK, [5] Applied Systems Biology, HKI, Friedrich-Schiller-Universität Jena, Germany

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. Based on the newly developed theoretical tools (Lücke, Eggert, 2010; Shelton et al., 2011; Lücke, Henniges, 2012) we developed algorithms reflecting the dicreteness of objects (Exarchakis et al., 2012; Lücke, Sheikh, 2012) and algorithms with explicit encoding of object location (Dai, Lücke, 2012). Furthermore, we continued the development and application of algorithms with non-linear component superposition (Lücke, Sahani, 2008; Lücke et al., 2009; Puertas et al., 2010) in the Bernstein Focus Neurotechnology Frankfurt.

In applications of the new algorithms to visual data, we could show that explicit representations of visual patterns can be learned autonomously. We have shown that representations can be learned from data with occluding objects, have demonstrated applicability to data from scanned text documents, and have started a collaboration with the Applied Systems Biology at Jena Univerity (Marc-Thilo Figge) to learn cell representations from microscopy images for image understanding in systems immunology (see Figure).



Left: Inferred objects after learning. *Right:* Inferred cell positions and types on microscopy images from immunological processes.

Related publications in 2011:

Lücke, J., and Sheikh, A. S. (2011). A Closed-Form EM Algorithm for Sparse Coding and Its Application to Source Separation (http://arxiv.org/abs/1105.2493).

Lücke, J. and Henniges, M. (2012). Closed-Form Entropy Limits – A Tool to Monitor Likelihood Optimization of Probabilistic Generative Models. Proceedings AISTATS, in press, accepted 2011.

Exarchakis, G., Henniges, M., Eggert, J., and Lücke, J. (2012). Ternary Sparse Coding. Proceedings ICA/LVA, LNCS 7191, 204–212, accepted 2011.

Dai, Z., and Lücke, J. (2012). Unsupervised Learning of Translation Invariant Occlusive Components. IEEE Conference on Computer Vision and Pattern Recognition, submitted 2011, accepted.

Dai, Z., and Lücke, J. (2012). Autonomous Cleaning of Corrupted Scanned Documents – A Generative Modeling Approach. IEEE Conference on Computer Vision and Pattern Recognition, accepted for oral presentation.

Optimally adapting heuristics: humans quickly abandon the constant bearing angle strategy

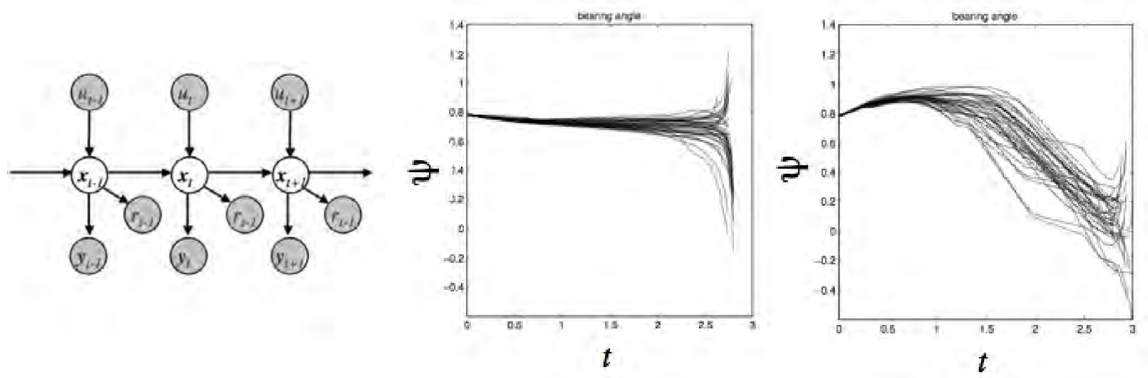
Collaborators: C.A. Rothkopf[1], P. Schrater[2]

[1] Frankfurt Institute for Advanced Studies, [2] University of Minnesota, Minneapolis, USA

Animals ranging from dragonflies through teleost fish to humans all intercept moving targets using the same strategy of adjusting their speed so as to hold the angle pointing towards their target constant over time. This constant-bearing-angle strategy has been suggested as a fundamental visuomotor heuristic and as an instance of Darwininan intelligence that overcomes the need for complex and expensive computations involving multiple sources of uncertainty.

We consider the task of intercepting a moving ball for which many previous studies have shown that humans use this constant bearing angle strategy. Here we manipulated the observation function in a virtual reality setup so as to change the uncertainty of the ball's position parametrically. Specifically, the contrast of the ball changes as a function of the heading angle towards the ball along the subject's momentary trajectory. Subjects adjusted their interception strategy within an average of 26 trials and were consistently able to catch these balls.

To gain insight into the adopted new interception strategy, we setup two approximate optimal control models, which know the observation function. In one case, an iterated signal dependent linear- quadratic-Gaussian controller was modified to handle non-linear observation models. The second approach utilizes a Monte Carlo sampling of smooth trajectories of increasing complexity in a low dimensional parameter space. These analyses show that the ideal actor modifies its trajectories by executing controls that increase information gain, and that these changes mirror human behavior. Thus, we provide evidence that humans quickly abandon the constant bearing angle strategy in favor of more informative action sequences, if this allows catching moving targets more reliably. The constant-bearing-angle-strategy is not an invariant heuristic of Darwinian intelligence as humans employ near-optimal information seeking actions that violate the constant bearing angle strategy, but produce less uncertainty in the interception.



Left: State space model used to model the interception task. *Center:* Bearing angle data from human subjects intercepting a moving ball of constant contrast demonstrating constant bearing angle strategy. *Right:* Bearing angle data from human subjects intercepting a moving ball of with variable contrast showing departure from constant bearing angle strategy.

Related publication in 2011:

1) C. A. Rothkopf, P. Schrater, *Coupling perception and action using probabilistic control*, COSYNE - Computational and Systems Neuroscience, February 24-27, 2011, Salt Lake City, Utah, USA.

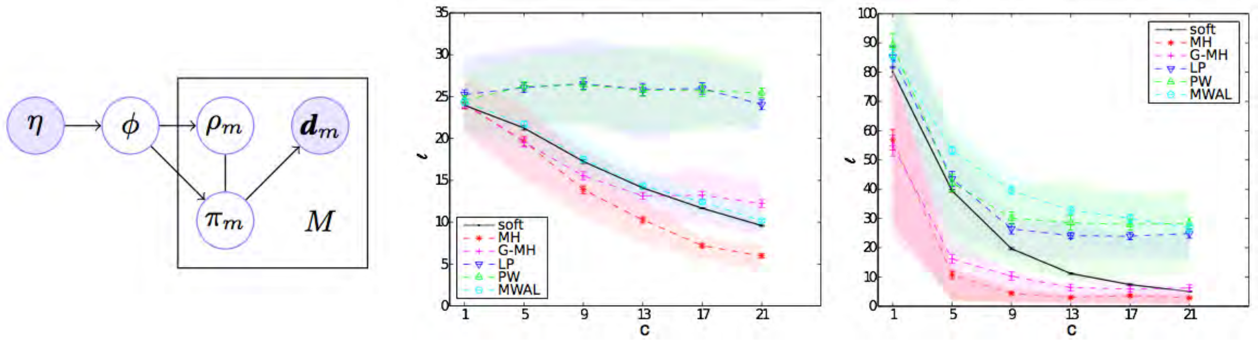
Preference elicitation and Bayesian inverse reinforcement learning

Collaborators: C.A. Rothkopf[1], C. Dimitrakakis[1,2]

[1] Frankfurt Institute for Advanced Studies, [2] EPFL, Lausanne, Switzerland

We state the problem of inverse reinforcement learning in terms of preference elicitation, resulting in a principled Bayesian statistical formulation. This generalizes previous work on Bayesian inverse reinforcement learning and allows us to obtain a posterior distribution on the agent's preferences, policy and optionally, the obtained reward sequence, from observations. We examine the relation of the resulting approach to other statistical methods for inverse reinforcement learning via analysis and experimental results. We show that preferences can be determined accurately via a Markov-Chain-Monte-Carlo sampling procedure, even if the observed agent's policy is sub-optimal with respect to its own preferences. In that case, significantly improved policies with respect to the agent's preferences are obtained, compared to both other methods and to the performance of the demonstrated policy.

Based on this formulation we generalize the problem of inverse reinforcement learning to multiple tasks, from multiple demonstrations. Each one may represent one expert trying to solve a different task, or as different experts trying to solve the same task. Our main contribution is to formalize the problem as statistical preference elicitation, via a number of structured priors, whose form capture our biases about the relatedness of different tasks or expert policies. In doing so, we introduce a prior on policy optimality, which is more natural to specify. We show that our framework allows us not only to learn to efficiently from multiple experts but to also effectively differentiate between the goals of each. Possible applications include analyzing the intrinsic motivations of subjects in behavioral experiments and learning from multiple teachers.



Left: Graphical model of general multitask reward-policy priors. Lighter color indicates latent variables. Here η is the hyperprior on the joint reward-policy prior ϕ while ρ_m and π_m are the reward and policy of the m-th task, for which we observe the demonstration $\mathbf{d}_m$. The undirected link between π and ρ represents the fact that the rewards and policy are jointly drawn from the reward-policy prior. *Center:* Total loss l with respect to the optimal policy, as a function of the inverse temperature c of the softmax policy of the demonstrator for the Random MDP, averaged over 100 runs. The shaded areas indicate the 80% percentile region, while the error bars the standard error. *Right:* Same as center plot but for random maze tasks.

Related publications in 2011:

1) C. A. Rothkopf, C. Dimitrakakis, *Preference elicitation and inverse reinforcement learning*, 22nd European Conference on Machine Learning (ECML), September 5-9, 2011.
2) C. Dimitrakakis, C. A. Rothkopf, *Bayesian multitask inverse reinforcement learning*, European Workshop on Reinforcement Learning (EWRL), September 9-11, 2011.

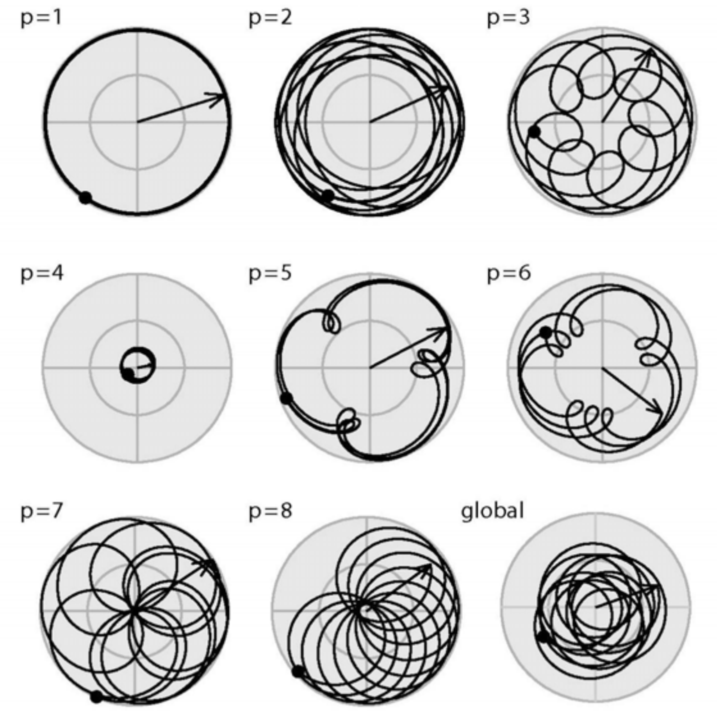
Patterned-Coherence-Mechanism (PCM): Temporal coding for recognition processes

Thomas Burwick

This work is part of a research program that studies the benefits of a recently discovered pattern recognition mechanism both for understanding the brain's information processing and for generating computational intelligence. In the following, we refer to this mechanism as Patterned Coherence Mechanism (PCM) and give a brief introduction to it and describe the current direction of research and steps taken in 2011.

The PCM uses the temporal structure of units in a neural network and adds a so-called acceleration mechanism to the synchronizing phase-based couplings in oscillatory networks (Burwick, Neural Computation, 2008). It turns out that including the acceleration mechanism has a profound and favorable effect on the recognition capabilities of the network. Based on the temporal structure of the activities of the neural units, the system introduces a competition for coherence among overlapping patterns. Neural assemblies are identified as (sets of) coherent (that is, synchronized or phase-locked) patterns that win the competition for coherence based on excitatory couplings that embody Hebbian memory.

Our recent work concentrated on further study the potential benefits of the PCM and to understand in how far it may describe aspects of the brain's information processing. In particular, the tasks cover including inhibitory couplings, going to asymmetric feedback relations, aspects of learning, interpretations with respect to neurophysiological observations of the role of cortical gamma oscillations. The latter aspect is followed with particular emphasis on the results obtained through the work of the Frankfurt-based research groups at the Ernst-Strüngmann-Institute (ESI) and Max-Planck-Institute for Brain Research. Our recent work concentrated on the inclusion of inhibitory couplings and interpretations with respect to attentional mechanisms. The latter serves a selection of incoming signals for representation of perceived objects.



Example for the PCM: Although the global network activity appears to be irregular, the decomposition into patterns reveals that pattern $p = 1$ wins the competition for coherence, leading to a partial coherence of the network that corresponds to the winning pattern. The figure shows the phenomenon of patterned coherence through displaying the decomposition of the global network activity (lower right corner) into the activities of the overlapping patterns $p = 1, ..., P$ ($P = 8$). For each pattern and global activity, the displayed trajectories are shown on the complex unit disk. Their magnitude correspond to the degree of collective activity times synchronization, while the phase describes the collective phase of the patterns. Simulation is for time $t = 0$ to $t = 8\tau = T$, the trajectories are shown from $t = 3\tau$ (thick dots) $t = T$ (indicated through arrows).

Related publications in 2011:

1) T. Burwick, *Pattern recognition through compatibility of excitatory and inhibitory rhythms*, Neurocomputing 74 (2011) 1315-1328.
2) T. Burwick, *Temporal coding is not only about cooperation - it is also about competition*, in A.R. Rao, G.A. Cecchi (eds.), "The Relevance of the Time Domain to Neural Network Models", Springer Series in Cognitive and Neural Systems 3 (2011) 33-56.

4.3 Biology, Chemistry, Molecules, Nanosystems

Structure and dynamics of clusters and fullerenes

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

[1] Frankfurt Institute for Advanced Studies, [2] St. Petersburg State Polytechnic University, Russia

A self-consistent Hartree-Fock calculation of electronic structure of noble gas endohedral fullerenes A@C_{60} was carried out for the first time [1,2]. All electrons of the encaged atom and 240 delocalized electrons of C_{60} were considered simultaneously within unified electronic configuration. It was shown [3,4] that the account of the non-local exchange interaction within the Hartree-Fock approximation leads to the significant modification of the 3p and 4d shells 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 shells 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.

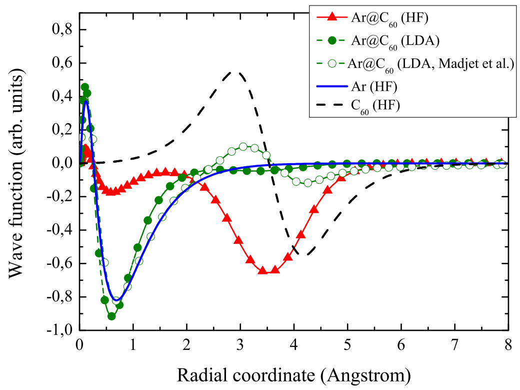


Figure: The 3p wave function in free Ar atom (solid line), in pristine C_{60} (dashed line) and in Ar@C_{60} calculated within the HF approximation (line with triangles) and the LDA (filled-circled line). Results of the LDA calculation performed by Madjet et al. (2007) are also presented (open-circled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

Related publications in 2011:

1. A.V. Verkhovtsev, R.G. Polozkov, V.K. Ivanov, A.V. Korol, A.V. Solov'yov, *Investigation of electronic structure of noble gas endohedral fullerenes*, Science and Technology Bulletin of Saint Petersburg State Polytechnic University, issue No 1(116), 61-70 (2011) (in Russian).

2. A.V. Verkhovtsev, R.G. Polozkov, V.K. Ivanov, A.V. Korol, A.V. Solov'yov, *Self-consistent Hartree-Fock approach to electronic structure of endohedral fullerenes*, International Conference 'Advanced Carbon Nanostructures (ACN 2011)' Book of Abstracts, p. 311 (St. Petersburg, Russia, July 4-8, 2011).

3. A.V. Verkhovtsev, R.G. Polozkov, V.K. Ivanov, A.V. Korol, A.V. Solov'yov, *Role of Exchange Interaction in Self-Consistent Calculations of Endohedral Fullerenes*, Nucl. Instrum. Meth. B, in press (2011) (see also arXiv:1108.0918).

4. A.V. Verkhovtsev, R.G. Polozkov, V.K. Ivanov, A.V. Korol, A.V. Solov'yov, *Self-consistent description of endohedral fullerenes' electronic structure within the Hartree-Fock and the local density approximations*, The Fifth International Symposium 'Atomic Cluster Collisions (ISACC 2011)' Book of Abstracts, p. 76 (Berlin, Germany, July 20-25, 2011).

DNA unzipping

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

[1] Bogolyubov Institute for Theoretical Physics, Ukraine, [2] Institute of Mathematical Problems of Biology RAS, Russia, [3] Frankfurt Institute for Advanced Studies

Short description:
All-atom molecular dynamics (MD) simulations of DNA duplex unzipping in a water environment were performed. The investigated DNA double helix consists of a Drew-Dickerson dodecamer sequence and a hairpin (AAG) attached to the end of the double-helix chain. The considered system is used to examine the process of DNA strand separation under the action of an external force. This process occurs in vivo and now is being intensively investigated in experiments with single molecules.

Main results:

- The DNA dodecamer duplex is consequently unzipped pair by pair by means of the steered MD. The unzipping trajectories turn out to be similar for the duplex parts with G·C content and rather distinct for the parts with A·T content.
- It is shown that during the unzipping each pair experiences two types of motion: relatively quick rotation together with all the duplex and slower motion in the frame of the unzipping fork. In the course of opening, the complementary pair passes through several distinct states: (i) the closed state in the double helix, (ii) the metastable preopened state in the unzipping fork and (iii) the unbound state.
- The performed simulations show that water molecules participate in the stabilization of the metastable states of the preopened base pairs in the DNA unzipping fork.

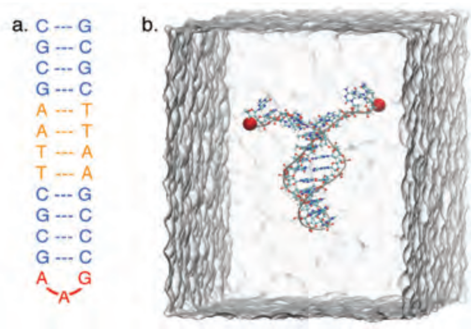


Figure 1. DNA duplex constructed from a Drew-Dickerson dodecamer with hairpin AAG: (a) nucleotide content in DD-h; (b) additional external force applied to the opposite phosphate groups of different strands (shown by red spheres) that drives the directed unzipping process of dsDNA.

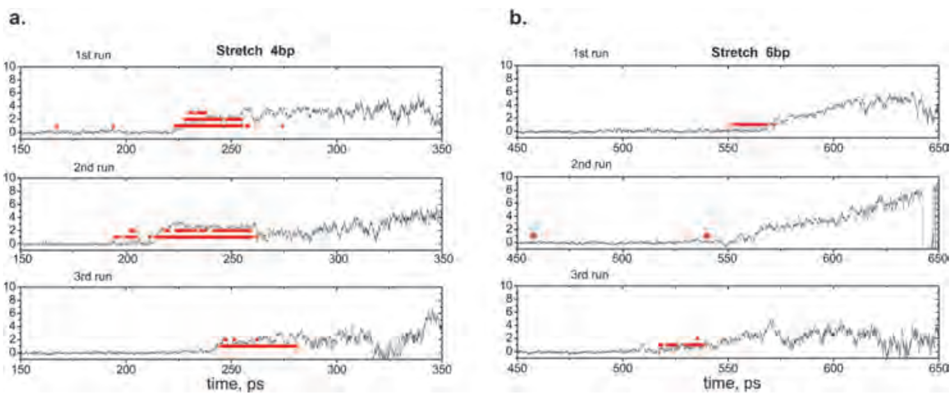


Figure 2. Base stretching coordinate (in angstrom) and the number of water molecules that link the bases in the unzipping pair.

Related publications in 2011:

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 (2012).

Laser-induced acoustic desorption

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

[1] Frankfurt Institute for Advanced Studies, [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:

- By means of molecular dynamics simulations we have investigated the desorption process of lysine amino acids from the surface of the nickel foil.
- The desorption rate of the amino acids as a function of the surface acceleration has been analysed. It was shown that the desorption rate has an exponential dependence on the value of the substrate acceleration.
- The final group velocities of the desorbed molecules were analysed. It was 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.

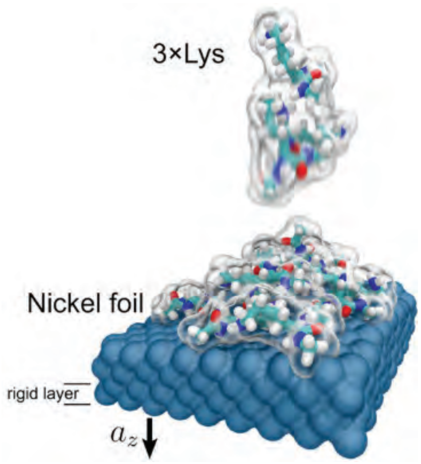


Figure 1. Evaporation of a cluster of several lysine residues from the surface of a nickel foil. The evaporation is caused by the foil acceleration.

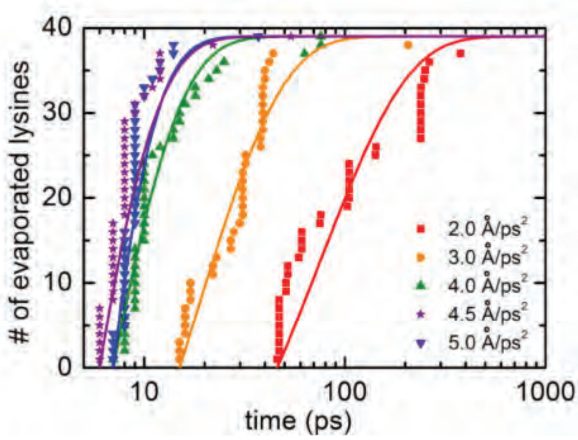


Figure 2. The number of evaporated lysine residues as a function of time after the start of nickel foil acceleration. Symbols show the results of molecular dynamics simulations corresponding to different values of foil acceleration. Solid lines show the theoretical curves corresponding to the results of molecular dynamics simulations. The legend indicates the values of acceleration used in the simulations.

Statistical mechanics of protein folding

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

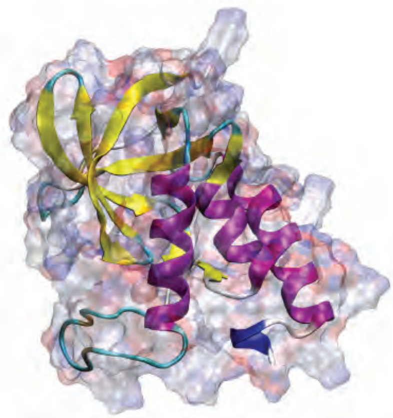
[1] Frankfurt Institute for Advanced Studies,[2] UIUC, Urbana, USA

Short description:
The important goal of numerous current investigations is to generate new, detailed knowledge about the nanoscale mechanisms leading to global conformational changes of single biomacromolecules. This goal is being tackled by different theoretical and experimental approaches and methods. Understanding such structural transformations reveals a tremendous amount of useful information about the properties of these systems, including how they function and how they are regulated. These transitions generally correspond to the finite system analogue of a phase transition.

Main results:

• We have developed theoretical framework which is based on an interdisciplinary approach combining the methods of molecular dynamics, statistical mechanics, computational chemical physics, and quantum mechanics aiming to provide a comprehensive description of phase transitions and cooperative dynamics in peptides, proteins, and other biomacromolecules [1].

• The accuracy of the developed theoretical formalism was validated by comparison with the results of experimental measurements of heat capacity profiles for a number of globular proteins.



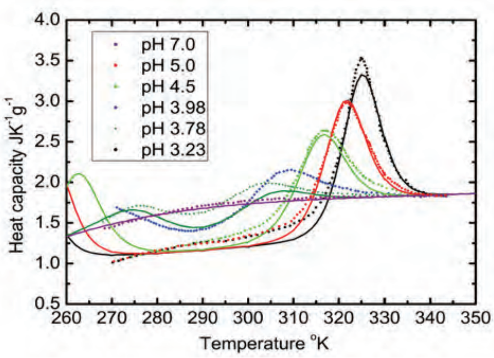


Figure: The 3D structure of protein staphylococcal nuclease (top) and the dependencies of the heat capacity of the protein on temperature (bottom). Symbols show the experimental results measured at different values of pH of the solvent. Solid lines present the results of our statistical mechanics model.

Related publications in 2011:

1. Alexander V. Yakubovich, *Theory of phase transitions in polypeptides and proteins*, Springer PhD Thesis series (Springer Heidelberg Dordrecht London New York, 2011) 121 pp.

Fractals on a surface

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

[1] Frankfurt Institute for Advanced Studies, [2] CNRS, France, [3] UIUC, Urbana, USA

Main results:
We developed a theoretical tool for studying post-growth processes occurring in nanofractals grown on a surface. A method was developed which accounts for the internal dynamics of particles in a fractal. We demonstrated that particle diffusion and detachment controls the shape of the emerging stable islands on a surface.

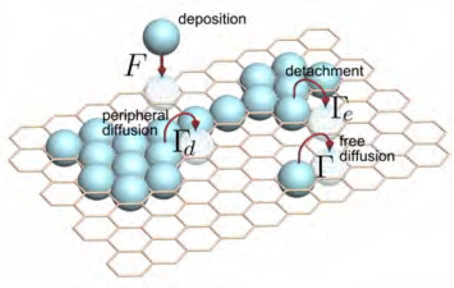


Fig. 1. Arrangement of deposited particles on a surface. The important processes which govern pattern formation on a surface are indicated by arrows: F is the particle deposition rate, Γ is the diffusion rate of a free particle, Γ_d is the diffusion rate of a particle along the periphery of an island, and Γ_e is the detachment rate of a particle from the island.

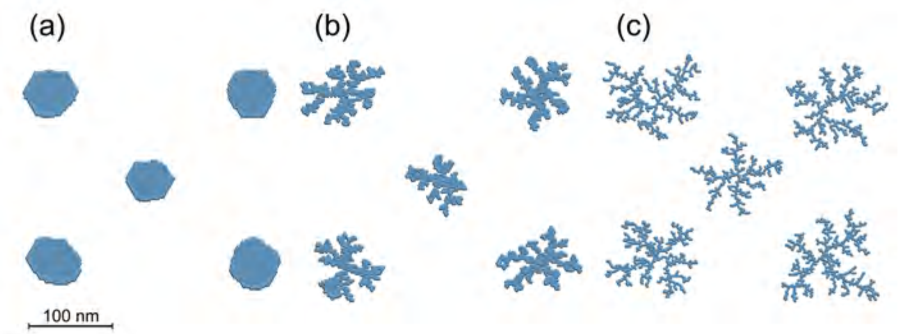


Fig. 2: Formation of islands with different morphologies on a surface during the particle deposition process: (a) formation of compact islands (low particle deposition rate); (b) formation of fractals with thick branches (intermediate particle deposition rate); (c) formation of the fractal structures with thin branches (fast particle deposition rate).

We demonstrated that the morphology of islands on a surface is mainly governed by the characteristic time needed for the newly deposited particles to reach the growth region (nucleation time) and by the characteristic time needed for a particle to find an optimum position within an island (rearrangement time). To get an in depth understanding of the self-organization and fragmentation processes on a surface we have investigated how various essential parameters of the system influence the diffusion of clusters on a surface. In particular, we considered the cluster size, the binding energy between clusters and the substrate and the temperature.

We considered different scenarios of fractal post-growth relaxation and analyzed the time evolution of the island's morphology. The result of calculations were compared with available experimental observations, and experiments in which the post-relaxation of deposited macrostructure can be probed were suggested.

Related publications in 2011:

1. V.V. Dick, I.A. Solov'yov and A.V. Solov'yov, *Fragmentation pathways of nanofractal structures on surfaces*, Phys. Rev. B84, 115408 (2011).

2. V.V. Dick, *Mechanism of nano-fractal structure formation and post-growth evolution*, Dissertation, Goethe-Universität Frankfurt am Main (2011).

Phase transitions in large clusters of transition metals

Collaborators: A.V. Yakubovich[1], A.V. Solov'yov[1], S.Schramm[1]

[1] Frankfurt Institute for Advanced Studies

Short description:
Nanoparticles of transition metals are utilized in various electronic and optical devices, serve as catalytic agents in chemical reactions. The aim of this project is to extend our knowledge on the phase transitions in the nanoparticles of the size of several nanometers. These transitions can be of the first order (melting) or the second order transitions associated with the change of the crystal symmetry. The finite size of the system adds an additional "degree of freedom" to the conventional thermodynamic equations – the number of particles in the cluster. We investigate thermodynamic properties of the clusters under the variation of temperature and cluster size. Better understanding of the properties of metallic clusters can provide additional insights into the understanding of one of the most intriguing processes of modern nanonechnology – the process of nanotube growth on catalytic nanoparticles.

Main results:

Using many-body Sutton-Chen, Gupta and Finnis-Sinclair potentials we perform the molecular dynamics simulations of the metallic clusters consisting of tens of thousands of atoms. We investigate the dependence of the phase transition properties of the cluster on their size. We investigate the evolution on the parameters of the phase transition (surface premelting, broad-with of the transition, latent heat) as the cluster size approaches the bulk limit. The calculations are performed on graphical processing units on the LOEWE-CSC cluster using a special version of the MBN Explorer software package.

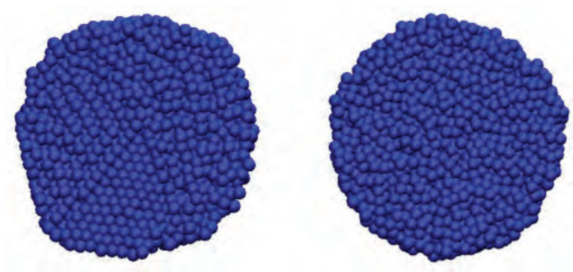


Figure 1. Structure of Ni_{8271} cluster just below (left) and above (right) phase transition temperature $\sim$ 1100K.

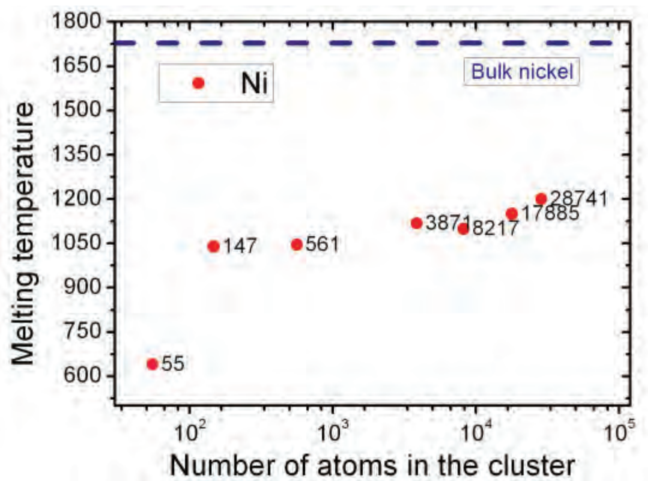


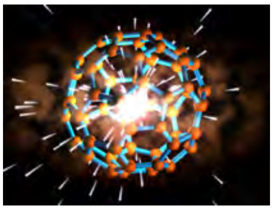
Figure 2: Melting temperatures of large nickel clusters calculated using many-body Sutton-Chen potential.

Photo-processes in clusters

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

[1] Frankfurt Institute for Advanced Studies, [2] St. Petersburg State Polytechnic University, Russia, [3] Imperial College, London, UK, [4] Justus-Liebig-Universität Giessen, Germany

Short description:
We study photo-processes (photoabsorption, bremsstrahlung, light scattering) in nanostructures. Special attention is paid to the role of collective electron excitations (plasmons) and mechanisms of their relaxation.



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^- and Na_{19}^- (R.G. Polozkov, V.K. Ivanov, A.V. Solov'yov, *Many-body theory for angular resolved photoelectron spectra of metal clusters*, Phys. Rev. A81, 021202 (2010)). In [1] we investigated the medium size sodium cluster, Na_{57}^-. The angular asymmetry parameter β was calculated within the single-particle Hartree-Fock (HF) approximation as well as with an account for many-electron correlations within the random phase approximation with exchange (RPAE). Both theoretical results were also compared with experimental data (von Issendorff et al., Science 323, 1323 (2009)). It was shown that the account for many-electron correlation leads to a good agreement with the experimental data.

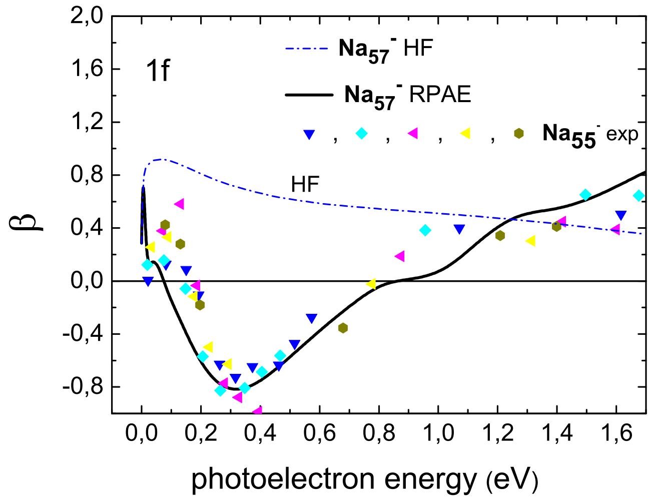


Figure: Angular anisotropy parameter β for the partial photionization cross section of Na_{57}^- versus photoelectron energy. Experimental data from von Issendorff et al. (2009).

Related publications in 2011:

1. V.K. Ivanov, R.G. Polozkov, A.V. Verkhovtsev, A.V. Korol, A.V. Solov'yov, *Photoionization processes with negative ions of atomic clusters*, Abstracts of the Fifth International Symposium 'Atomic Cluster Collisions (ISACC 2011)' Book of Abstracts, p.44 (Berlin, Germany, July 20-25, 2011).

Photo-processes in fullerenes and endohedral systems

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

[1] Frankfurt Institute for Advanced Studies, [2] St. Petersburg State Polytechnic University, Russia, [3] Imperial College, London, UK, [4] Justus-Liebig-Universität Giessen, Germany

Short description:
Within this project we study photo-processes (photoabsorption, bremsstrahlung, light scattering) in pristine and endohedral fullerenes. Special attention is paid to the influence of the fullerene on the encaged atom (molecule).

Main results:
We demonstrated, that the Auger decay rate in an endohedral atom is very sensitive to its location in the fullerene cage. Two additional decay channels appear in an endohedral system: (a) the one due to the change in the electric field at the atom caused by dynamic polarization of the fullerene electron shell by the Coulomb field of the vacancy, (b) the channel within which the released energy is transferred to the fullerene electron via the Coulomb interaction. The relative magnitudes of the correction terms are dependent not only on the position of the doped atom but also on the transition energy. Additional enhancement of the decay rate appears for transitions whose energies are in the vicinity of the fullerene surface plasmons energies of high multipolarity.

It is demonstrated that in many cases the additional channels can dominate over the direct Auger decay resulting in pronounced broadening of the atomic emission lines.

The case study, carried out for $Sc^{2+}@C_{80}$ (see Fig. 1), shows that narrow autoionizing resonances in an isolated Sc^{2+} are dramatically broadened if the ion is located strongly off-the-center. Using the developed model we carried out quantitative analysis of the photoionization spectrum for the endohedral complex $Sc_3N@C_{80}$ and demonstrate that the additional channels are partly responsible for the strong modification of the photoionization spectrum profile detected experimentally by Müller et al., J. Phys.: Conf. Ser. 88, 012038 (2007) (see Fig. 2).

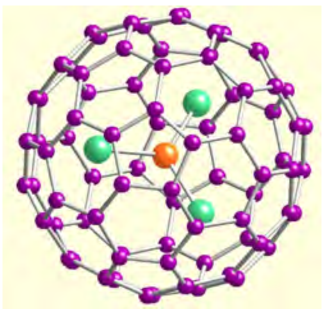


Figure 3: The structure of the $Sc_3N@C_{80}$ complex.

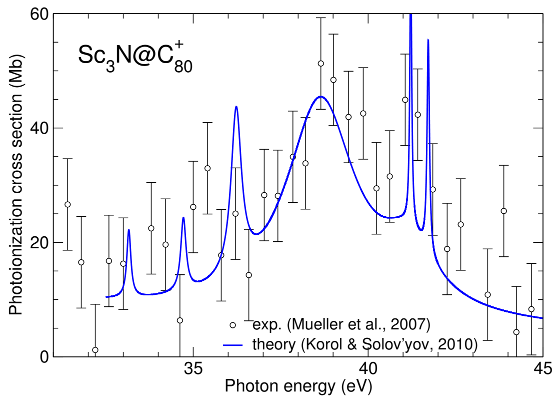


Figure 2: Photoionization of $Sc_3N@C_{80}$: Experiment (Müller et al., 2007) vs theory [1].

Related publications in 2011:

1. A.V. Korol, A.V. Solov'yov, *Vacancy decay in endohedral atoms: The role of an atom's non-central position*, J. Phys. B: At., Mol., Opt. Phys. 45, 085001 (1-17) (2011).

Multiscale approach to the physics of ion beam cancer therapy

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

[1] Oakland University, Michigan, USA, [2] Frankfurt Institute for Advanced Studies

Short description:
The multiscale approach to the radiation damage induced by irradiation with ions is aimed to the phenomenon-based quantitative understanding of the scenario from incidence of an energetic ion on tissue to the cell death. This approach joins together many spatial, temporal, and energetic scales involved in this scenario. The success of this approach will provide the phenomenological foundation for ion-beam cancer therapy, radiation protection in space, and other applications of ion beams. Main issues addressed by the multiscale approach are ion stopping in the medium, production and transport of secondary particles produced as a result of ionization and excitation of the medium, interaction of secondary particles with biological molecules, most important with DNA, the analysis of the induced damage, and evaluation of probabilities of subsequent cell survival or death. This approach is interdisciplinary, since it is based on physics, chemistry, and biology. Moreover, it spans over several areas within each of these disciplines.

Thermo-mechanical pathways of DNA damage

A number of different agents cause DNA damage as a consequence of irradiation. These include interactions of a DNA molecule with secondary electrons, holes and free radicals. Within this project we discuss the DNA damage due to thermal and mechanical effects which accompany the ion propagation.

• We have performed full-atom molecular dynamics simulations of the heat spike in the water medium caused by a heavy ion in the vicinity of its Bragg peak. High rate of energy transfer from an ion to the water molecules leads to the rapid increase of temperature in the vicinity of the ion trajectory. As a result of an abrupt increase of the temperature we observe the formation of the nanoscale shock wave propagating through the medium.

• We investigate the thermomechanical damage caused by the shock wave to the nucleosome located in the vicinity of heavy ion trajectory. We observe the substantial deformation of the DNA secondary structure. We show that the produced shock wave can lead to the thermomechanical breakage of the DNA backbone covalent bonds and present estimates for the number of such strand breaks per one cell nucleus.

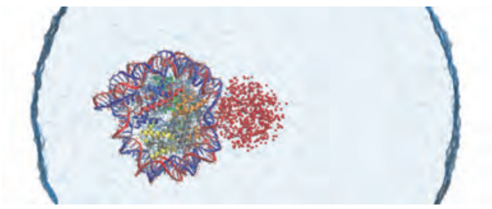


Figure: Structure of the nucleosome 150 fs after the carbon ion propagation. Water molecules initially located within 1 nm from the ion's track are shown by spheres. It is seen as substantial distortion of the nucleosome structure caused by the propagation of the shock wave.

Related publications in 2011:

1. A.V. Yakubovich, E. Surdutovich and A.V. Solov'yov, *Atomic and molecular data needs for radiation damage modeling: Multiscale approach*, AIP Conf. Proc. 1344, 230-238 (2011).

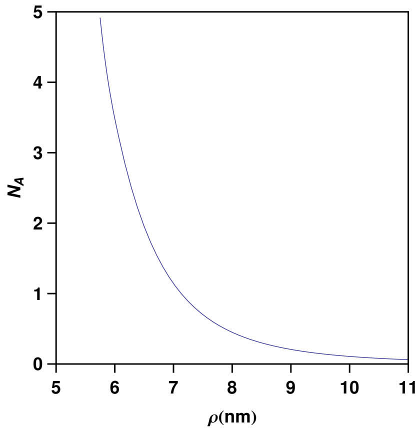
2. A.V. Yakubovich, E. Surdutovich, A.V. Solov'yov, *Thermomechanical damage of nucleosome by the shock wave initiated by ion passing through liquid water*, Nucl. Instrum. Meth. B, doi:10.1016/j.nimb.2011.10.069 (2011).

Assessment of complex DNA damage

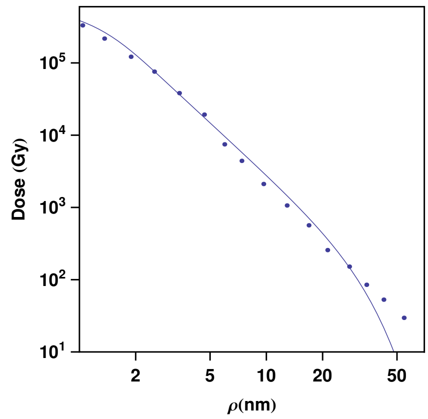
Collaborators: E. Surdutovich[1], A.V. Solov'yov[2], A.V. Yakubovich[2], W. Greiner[2]

[1] Oakland University, Michigan, USA, [2] Frankfurt Institute for Advanced Studies

In 2011, we have further explored approaches to the assessment of clustered or complex DNA damage[1]. The damage complexity is one of the most significant specific features of irradiation with ions. It arises from a high concentration of agents causing the damage. It is much more difficult to the repair mechanisms, present in the cell, to fix the complex damage and, as a result, such damage is more lethal than isolated DNA damage. We suggested ways to quantify the complex damage in ref. [1]. The fluence of secondary electrons through the DNA segment (two adjacent twists of DNA are the host of complex damage of DNA) is shown in Fig. 1. This fluence as well as the calculated radial dose, shown in Fig. 2, lead to the calculation of the distribution of clustered damage around the ion's path.

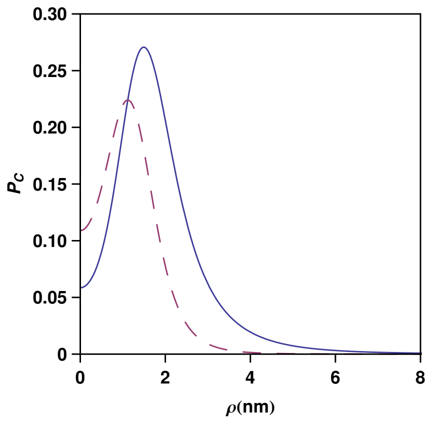


The dependence of number of secondary electrons hitting a two-twist-segment of DNA on the surface of a nucleosome on the distance of the nucleosome from the ion's path.

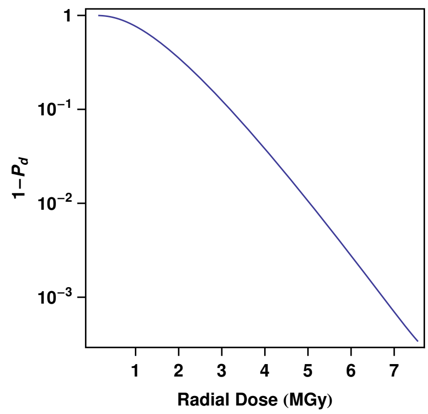


Comparison of the calculated (line) with the simulated (dots) radial dose for 25 MeV/u carbon ions.

Examples of radial distribution of complexity and cell survival on the radial dose based on damage complexity are shown in the figures below.



An example of radial distribution of clusters of two (solid line) and clusters of three lesions (dashed line).



The dependence of cell survival probability on the local radial dose per ion.

Related publications in 2011:

1. E. Surdutovich, D.C. Gallagher, and A.V. Solov'yov, *Calculation of complex DNA damage induced by ions*, Phys. Rev. E 84, 051918 (2011).

Mechanism of double strand breaking in DNA

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

[1] Oakland University, Michigan, USA, [2] Frankfurt Institute for Advanced Studies

Short description:

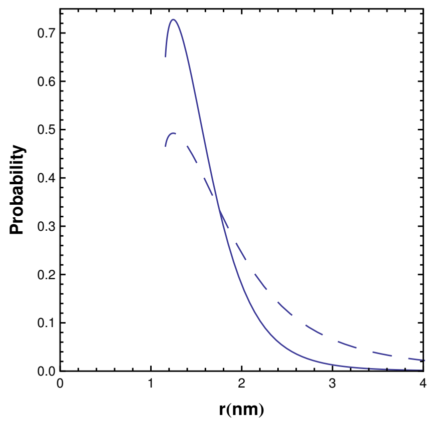
A mechanism of double strand breaking (DSB) in DNA due to the action of two electrons is considered. These are the electrons produced in the vicinity of DNA molecules due to ionization of water molecules with a consecutive emission of two electrons, making such a mechanism possible. This effect qualitatively solves a puzzle of large yields of DSBs following irradiation of DNA molecules.

Main results:

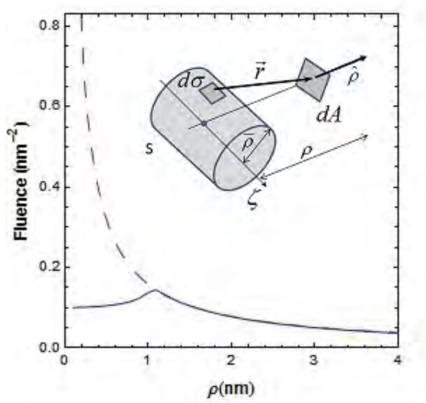
It is widely accepted that single strand breaks (SSBs) in DNA are due to direct action of low energy electrons. This, however, does not explain the mechanism of DSBs, since a single electron can only attach to one site causing dissociation. The number density of secondary electrons, produced on the ion's path, reduces rather steeply with the increasing distance from the path, so that the probability of two electrons incident on a single convolution of a DNA molecule, located a few nm from the track is very small. However, when ionization of a water molecule (cluster) producing an Auger electron occurs at a distance from the track, three electrons emerging from the same spot substantially boost the local number density of electrons and, hence, the probability of a nearby DNA convolution to be hit with two electrons.

Thus, due to the Auger mechanism, events in which two or more electrons interact with a single DNA convolution are not rare. DSB or other types of complex damage may result from these interactions. The dependence of probability of two electrons to hit the same DNA convolution on the distance of the convolution from the origin is shown in Fig. 1, where it is compared to the probability to be hit by the original secondary electron. It is remarkable, that for $r < 2$nm the probability of the impact of two electrons is comparable to that of one. A substantial quantity of this fluence makes the Auger-mechanism influence on DSB yield viable.

The contribution of Auger electrons to the fluence of secondary electrons was calculated. The additional fluence is compared to that of electron coming from the ion's path in Fig. 2. The calculation of the fluence of Auger electrons gives a framework for the calculation of the transport of free radicals formed due to an ion's traverse through a medium. This calculation, without the use of Monte Carlo simulations has long been desired.



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



The dependence of the fluence of an Auger electron from ionization by a secondary electron on the distance from the ion's path (solid line) compared to that of a single electron emitted from the path (dashed line).

Related publications in 2011:

1. E. Surdutovich and A.V. Solov'yov, *Double strand breaks in dna resulting from double-electron-emission events*, Phys. Rev. Lett. submitted for publication in 2011.

Novel light sources: Crystalline undulator and crystalline-undulator–based gamma-laser

Collaborators: A. Kostyuk[1], A.V. Korol[1], A.V. Solov'yov[1], W. Greiner[1], H. Backe[2], W. Lauth[2], U. Uggerhoj[3], V. Guidi[4]

[1] Frankfurt Institute for Advanced Studies, [2] Johannes Gutenberg-Universität Mainz, Germany [3] Aarhus University, Denmark, [4] Ferrara University, Italy

Short description:
Investigation of the feasibility of constructing a new 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:
• A patent for a hard x- and gamma-ray laser has been published [1]. It combines a CU with a conventional undulator. A beam of ultrarelativistic charged particles becomes spatially modulated in the conventional undulator so that it contains a harmonic with a period equal to the wavelength of the radiation of the CU. Due to this harmonic, the radiation process in the CU becomes coherent.

• A simulation of 855 MeV electron channeling of in Silicon has been performed with a new computer code. The dechanneling lengths for (100), (110) and (111) crystallographic planes have been estimated. The dependence of the intensity of the channeling radiation (ChR) on the crystal dimension along the beam has been calculated. A good agreement with recent experimental data is observed [2].

• The behaviour of a modulated positron beam in a planar crystal channel is investigated. The evolution of the particle distribution is described by means of the Fokker-Planck equation. A detailed analysis of the equation has been performed. It is demonstrated that the beam preserves its modulation at sufficiently large penetration depths which allows using a crystalline undulator as a coherent source of hard x- and γ-rays. This result is of crucial importance for the theory of the CU based γ-laser [3].

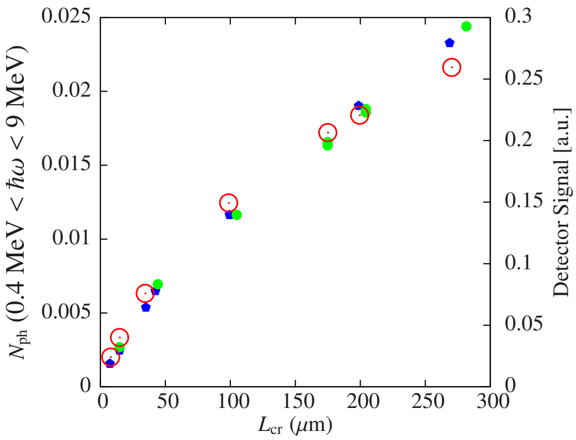


Figure: Intensity of ChR as function of the crystal thickness. Open circles – the simulation, filled circles – experimental data.

• Channelling of 855 MeV electrons along bent Si (110) crystallographic plane is studied within the Monte Carlo approach. The definitions of the dechanneling length and the asymptotic acceptance are formulated in a form suitable for the Monte Carlo procedure. The dependence of these quantities on the crystal bending is studied [4].

Related publications in 2011:

1. W. Greiner, A.V. Korol, A. Kostyuk, A.V. Solov'yov, *Vorrichtung und Verfahren zur Erzeugung elektromagnetischer Strahlung*, German patent, DE: 10 2010 023 632.2, published on Dec 15, 2011.

2. A. Kostyuk, A. Korol, A. Solov'yov, W. Greiner, *Planar channeling of 855 MeV electrons in silicon: Monte-Carlo Simulations*, J. Phys. B: At. Mol. Opt. Phys. 44, 075208 (2011).

3. A. Kostyuk, A.V. Korol, A.V. Solov'yov, W. Greiner, *Demodulation of a positron beam in a bent crystal channel*, Nucl. Instrum. Meth. B 269, 1482-1492 (2011).

4. A. Kostyuk, A.V. Korol, A.V. Solov'yov, W. Greiner, *Monte Carlo simulations of electron channelling a bent (110) channel in silicon*, arXiv:1104.3890.

MBN Explorer

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

[1] Frankfurt Institute for Advanced Studies, [2] UIUC, Urbana, USA

We have developed a multi-purpose computer code MBN Explorer. The package allows to model molecular systems of varied level of complexity. In particular, MBN Explorer is suited to compute system's energy, to optimize structures, as well as to consider the molecular and random walk dynamics. MBN Explorer allows to use a broad variety of interatomic potentials, to model different molecular systems, such as atomic clusters, fullerenes, nanotubes, proteins, composite systems, nanofractals, etc. A distinct feature of the program, which makes it significantly different from the already existing codes, is its universality and applicability to the description of a broad range of problems and molecular systems. Most of the existing codes are developed for particular classes of molecular systems, and do not permit multiscale approach, while MBN Explorer goes beyond these drawbacks. On demand, MBN Explorer allows to group particles in the system into rigid fragments, thereby significantly reducing the number of degrees of freedom. Despite the universality, the computational efficiency of MBN Explorer is comparable (and in some cases even higher) than the computational efficiency of other software packages, making MBN Explorer a possible alternative to the available codes.

MBN Explorer features:

- Universality
- Tunable force fields
- Flexible molecular systems
- Multi-scale approach
- Computational efficiency
- File format compatibility
- Object-oriented design

Figure 1. MBN Explorer is a universal program for multi-scale simulation of complex molecular structure and dynamics.

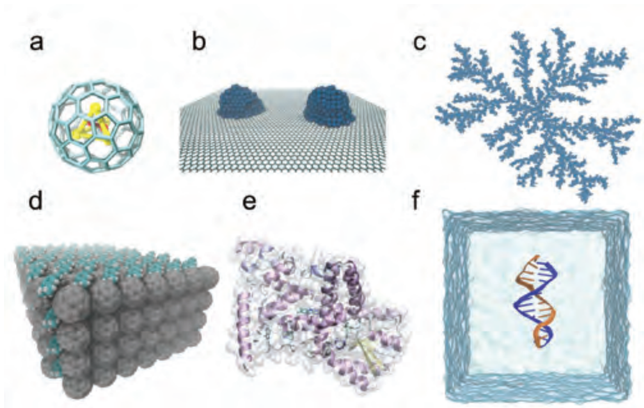


Figure 2. Variety of molecular systems which can be simulated using MBN Explorer: (a) encapsulated clusters, (b) deposited nanoparticles, (c) nanofractals, (d) composite nanowires, (e) proteins, (f) biomolecules, e.g., DNA, in solution. Structure and properties of any of these objects or any of their combinations can be studied using MBN Explorer.

Related reference in 2011:

1. I.A. Solov'yov, P.N. Nikolaev, A.V. Yakubovich, I. Volkovetz, V.V. Dick, A.V. Solov'yov, 'MBN Explorer User's Guide', Frankfurt Institute for Advanced Studies, pp. 1-188 (2011) (unpublished)

Monte-Carlo code for channeling dynamics and radiation

Collaborators: A.Kostyuk[1], A.V. Korol[1], A.V. Solov'yov[1], Walter Greiner[1], H. Backe[2], W. Lauth[2]

[1] Frankfurt Institute for Advanced Studies, [2] Johannes Gutenberg-Universität Mainz, Germany

The FORTRAN 95 code has been used for a comprehensive numerical study of the channeling process of ultrarelativistic particles as well as of the properties of radiation formed in a crystalline undulator [1]. Currently the algorithm is being further developed and refined for the Monte-Carlo simulation of the dynamics of relativistic particle channeling in straight and periodically bent crystals. The algorithm accounts for a number of phenomena: the action of the interplanar and centrifugal potentials combined with the stochastic force due to the random scattering from lattice electrons and nuclei, the transition between axial and planar channeling, the rechanneling effect as well as the influence of the temperature on the channeling process. The algorithm is combined with another one that allows to calculate spectral-angular distribution of the electromagnetic radiation produced by a relativistic charged particle in its motion along the simulated trajectory.

Presently, the code is able to simulate planar channeling of relativistic electrons and positrons in straight and bent crystals. Examples of the simulated electron trajectories in a periodically bent crystal are shown in the figure. A number of parameters can be varied: the energy of the projectile, the type and size of the crystal and its orientation relative to the beam direction. The analysis routine allows to estimate the dechanneling length and analyse the probability distributions of the channeling and dechanneled particles [2,3]. Spectral and angular distribution of the emitted photons can be calculated.

Recently, the code has been modified and supplemented with Linux shell scripts to allow for parallel running of the calculations on hundreds of processor cores within a Linux cluster.

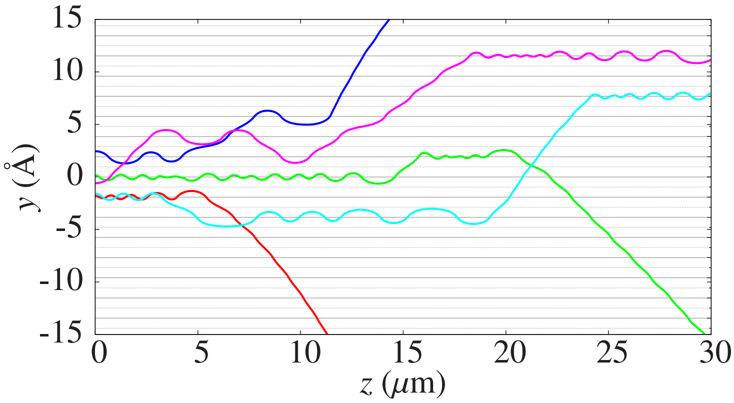


Figure 1: Examples of the simulated trajectories of electrons in an oriented crystal.

Related publications in 2011:

1. A. Kostyuk, A. Korol, A. Solov'yov, W. Greiner, *Planar channeling of 855 MeV Electrons in Silicon: Monte-Carlo simulations*, J. Phys. B: At. Mol. Opt. Phys. 44, 075208 (2011).

2. A. Kostyuk, A.V. Korol, A.V. Solov'yov, Walter Greiner, *Planar channelling of electrons: Numerical analysis and theory*, Nuovo Cimento C 34, 167–174 (2011).

3. A. Kostyuk, A.V. Korol, A.V. Solov'yov, W. Greiner, *Monte Carlo Simulations of electron channelling in bent (110) channel in Silicon*, The preprint see at http://arxiv.org/abs/1104.3890 (2011).

Development of computer tools for graphical processors

Collaborators: A.V. Yakubovich[1], V. Dick[1], A.V. Solov'yov[1], S. Schramm[1]

[1] Frankfurt Institute for Advanced Studies

Short description:
The aim of extension of MBN Explorer code for GPU-based calculations is to exploit the advantages of a novel superiorly fast computational devices – special graphical cards available at the novel supercomputer center LOEWE-CSC.

Main results:
All-atom molecular dynamic simulations is widely used computational approach to study the behavior of various complex molecular systems such as biomolecules, atomic clusters, carbon nanostructures and others at an atomistic level of detail. The capabilities of such simulations are limited by available computer resources. State of-the-art graphics processing units (GPUs) can perform over 500 billion arithmetic operations per second, a tremendous computational resource that can now be utilized for general purpose computing as a result of recent advances in GPU hardware and software architecture. In simple molecular dynamic calculations the GPU-accelerated implementations are observed to run 10 to 100 times faster than equivalent CPU implementations.

We have extended the software package MBN Explorer that has been developed at our group for almost a decade in order to make use of GPU facilities. Now MBN Explorer is capable of performing calculations on graphical processors. The "GPU-branch" of MBN Explorer includes a specific force fields for modeling the carbon-based materials, metal clusters and carbon-metal systems, treating composite alloys of transition metals.

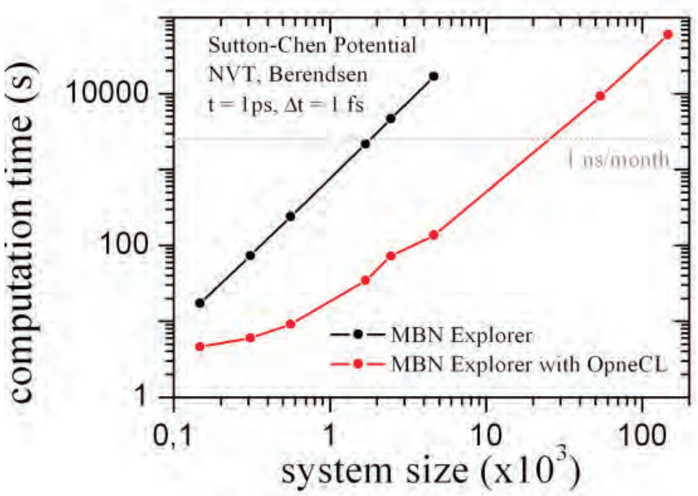


Figure 1. Performance of the OpenCL version of MBN Explorer as compared to the conventional CPU version of the code. For systems consisting of more that 1 thousand of particles the computational advantage of the OpenCL version can be more than 100 times.

Programs for many-body descriptions of clusters and fullerenes

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

[1] Frankfurt Institute for Advanced Studies, [2] St. Petersburg State Polytechnic University, Russia

• The package of codes has been developed for numerical description of spherically symmetric endohedral systems A@C_{60}. Ground and excited states are calculates within the jellium model approach using the Hartree-Fock and the local density approximations.
The codes allow one to compute:
(a) electronic wave functions of the ground state, single-electron energy and total energy of the system treating self-consistently all electrons of the encapsulated atom and 240 valence electrons of the fullerene;
(b) discrete and continuum wave functions, energy spectrum of discrete excitations and the scattering phaseshifts;
(c) cross section of photoabsorption and angular distribution of photoelectrons within the random phase approximation with exchange which accounts for the many-electron correlations.

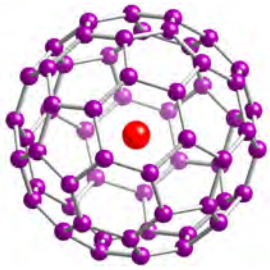


Figure 1: Endohedral compound Ar@C_{60}. The HF ground and excited states were calculated by self-consistent treatment of all 258 electrons [1].

• A new code has been developed to relate parameters of the fulllerene's ground state obtained within the jellium model with these from a quantum-chemical calculation (performed by Gaussian 09 package). The code allows one to extract electron density distribution and electrostatic potential of a fullerene from the Gaussian 09 output file as well as to perform spherical averaging of these parameters. With the help of the code, a new type of a pseudopotential has been constructed to improve the electron density distribution of fullerenes within the spherical jellium model.

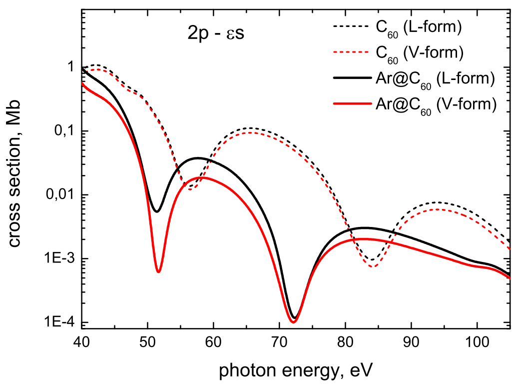


Figure 2: Partial 2p $\rightarrow$ εs photoionization cross section in C_{60} and Ar@C_{60} calculated within the HF + RPAE scheme [2].

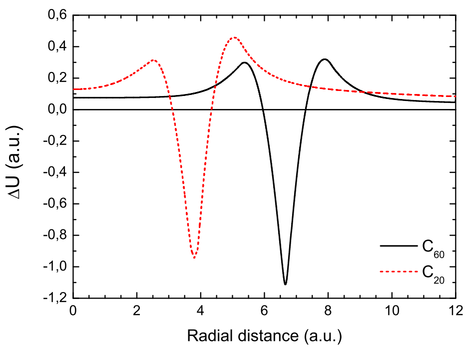


Figure 3: Pseudopotential ΔU constructed as a difference between total electrostatic potential obtained from the quantum-chemical calculation and the one within the jellium model.

Related publications in 2011:

1. A.V. Verkhovtsev, R.G. Polozkov, V.K. Ivanov, A.V. Korol, A.V. Solov'yov, *Self-Consistent Hartree-Fock approach to electronic structure of endohedral Fullerenes*, p. 311, Book of Abstracts of International Conference 'Advanced Carbon Nanostructures (ACN 2011)' (St. Petersburg, Russia, July 4-8, 2011).

2. R.G. Polozkov, A.V. Verkhovtsev, V.K. Ivanov, A.V. Korol, A.V. Solov'yov, *Oscillation phenomenon in photoionization cross section of Ar@C_{60}*, p. 287, Book of Abstracts of International Conference 'Advanced Carbon Nanostructures (ACN 2011)' (St. Petersburg, Russia, July 4-8, 2011).

Two-photon absorption of few-electron heavy ions

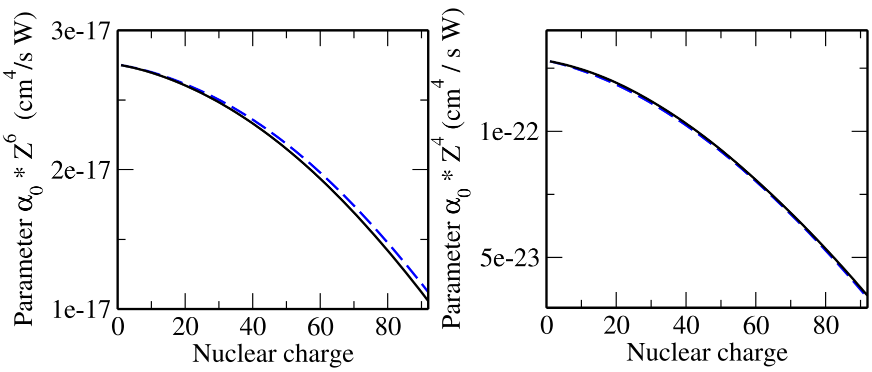
Collaborators: S. Fritzsche[1,2], P. Indelicato[3], J. P. Santos[4], P. Amaro[4], A. Surzhykov[2,5]

[1] Frankfurt Institute for Advanced Studies [2] GSI, Darmstadt [3] Laboratoire Kastler Brossel, Paris, France [4] Universidade Nova de Lisboa, Portugal [5] Physikalisches Institut Heidelberg, Germany

The recent progress in developing coherent light sources have opened new avenues for studying two- and multi-photon transitions in ions, atoms and molecules. For example, the $ns \to n's$ and $ns \to n'd$ two-photon excitation of atomic hydrogen and deuterium has been explored in great during recent years and and helped determine the *fundamental* constants with unprecendented accuracy. Less attention, however, has been paid until now to *induced* two-photon absorption processes in multiple and high-Z atoms and ions, though they are exptected to provide new insights into relativistic, many-body and QED phenomena in strong electromagnetic fields and, hence, may serve as a valuable alternative to x-ray absorption (XAS) spectroscopy and related techniques. Moreover, induced two-photon excitations have been proposed as a promising tool for studying parity-violating interactions in high-Z ions.

To explore and better understand the two-photon absorption in strong fields, we have recently worked out a (unified) relativistic formalism that enables one to describe the (spatial and polarization) properties of light in a consistent manner. Using second-order perturbation theory and Dirac's relativistic equation, expressions were derived for the two-photon excitation cross sections and rates, including the important many-electron effects as well as all (higher) multipoles in the expansion of the electron-photon interaction. While our derived expressions are general and independent of the particular shell structure of the ion, detailed computations have been carried out for the two-photon absorption of hydrogen-, helium-, and beryllium-like ions, and they are compared with the available theoretical and experimental data. Figure 1, for example, displays the (reduced) cross section $\alpha_0 = \sigma_{2\gamma}/g(\omega)G^{(2)}$ for the $1s \to 2s$ and $1s \to 2p_{1/2}$ absorption of hydrogen-like ions. Here, $G^{(2)}$ is the two-photon statistical factor and $g(\omega)$ is the line-shape function. As seen from the figure, the relativistic contraction of the wave functions toward the nucleus as well as the nondipole effects in the electron-photon interaction lead to a faster decrease of the cross sections than predicted by the non-relativistic $\alpha_0(1s \to 2s) \sim Z^6$ and $\alpha_0(1s \to 2p) \sim Z^4$ scalings.

In conclusion, our studies demonstrate the importance of relativistic and higher-multipole effects upon the two-photon absorption rates. Reliable theoretical rates are however required to plan and prepare future experiments on the parity violation in high-Z ions as they will be performed at the future Facility for Antiproton and Ion Research (FAIR) in Darmstadt.



The parameter α_0 for the two-photon $1s \to 2s$ (left panel) and $1s \to 2p_{1/2}$ (right panel) absorption of hydrogen-like ions.

Related publications in 2011:

1) A. Surzhykov, P. Indelicato, P. Amaro, J.P. Santos and S. Fritzsche, *Two-photon absorption of few-electron heavy ions*, Phys. Rev. A84 (2011) 022511.
2) F. Fratini, M.C. Tichy, T. Jahrsetz, A. Buchleitner, S. Fritzsche and A. Surzhykov, *Quantum correlations in the two-photon decay of few-electron ions*, Phys. Rev. A83 (2011) 032506.

Are ^{12}C radiation effects in liver tissue time-dependent?

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

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

This interdisciplinary project analyzes the effects of ^{12}C irradiation on normal and neoplastic liver tissue in order to evaluate whether this treatment offers new perspectives for the treatment of liver neoplasms such as hepatocellular carcinoma which have a poor prognosis in man, cannot be treated satisfactorily today and thus ask for the development of novel therapeutic strategies. Investigations are performed with organotypic slice cultures (OSC) of normal liver and hepatocellular carcinoma obtained from transgenic mice.

OSC comprise virtually all cell types present in the normal liver (hepatocytes, Kupffer cells, endothelial cells, fibroblasts) as well as the extracellular matrix and sustain the three-dimensional organ architecture. OSC are thus a more suitable model than monotypic cell lines to study the reaction to heavy-ion radiation. Moreover, OSC of liver maintain their physiological circadian rhythm in culture as experiments with transgenic Per2luc-mice have shown.

To evaluate whether the effects of the irradiation depend on the timepoint when it was applied, transgenic mice suffering from inducible hepatocellular carcinomas were killed at two different timepoints of a 12L:12D light-dark cycle (ZT06 and ZT18); liver OSC were prepared, cultured for 24 h and thereafter irradiated at two different timepoints: in the middle of the subjective day and of the subjective night, respectively. Each OSC comprised normal liver and tumor so that the normal and neoplastic tissues were exposed to the same experimental condition. The slices were irradiated with an extended Bragg peak typical for patient treatment at doses ranging from 2Gy to 10Gy. Samples were fixed 1h and 24hrs post-irradiation with 4% paraformaldehyde and subsequently cryosectioned. Cryosections were then subjected to double or triple immunofluorescence analysis. The irradiation effects were analyzed by markers for proliferation, apoptosis, and DNA damage.

Preliminary results indicate that there may be significant differences concerning the fixation timepoint and – as to be expected – tissue type. However, qualitatively no time-dependency could be established.

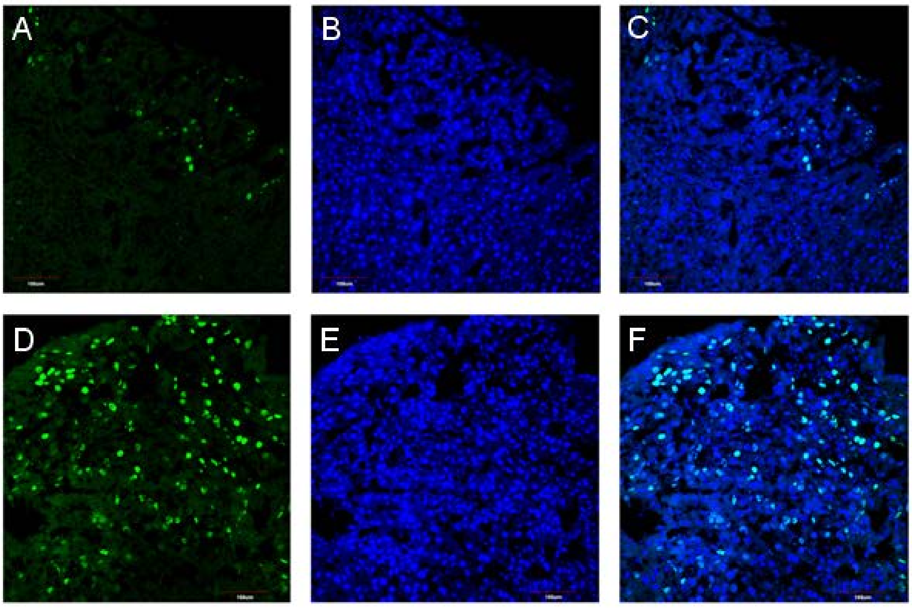


Figure: Immunofluorescent images of a healthy (A – C, ZT06, 5Gy, 24h) and pathological (D – F, ZT06, 5Gy, 1h) liver OSC stained for proliferation (Ki67 – green) and counterstained for cell nuclei (Hoechst – blue).

Exclusively NOESY-based automated NMR assignment and structure determination of proteins

Collaborators: Teppei Ikeya[1,2,3], Jun-Goo Jee[3], Yoshiki Shigemitsu[3], Junpei Hamatsu[3], Masaki Mishima[3], Yutaka Ito[3], Masatsune Kainosho[3,4], Peter Güntert[1,2,3]

[1] Institute of Biophysical Chemistry and Center for Biomolecular Magnetic Resonance, Goethe University Frankfurt am Main, [2] Frankfurt Institute for Advanced Studies [3] Graduate School of Science, Tokyo Metropolitan University, Japan [4] Graduate School of Science, Nagoya University, Japan

A fully automated method was developed for determining NMR solution structures of proteins using exclusively NOESY spectra as input, obviating the need to measure any spectra only for obtaining resonance assignments but devoid of structural information. Applied to two small proteins, the approach yielded structures that coincided closely with conventionally determined structures. Our results show that NOESY spectra alone can yield sufficiently accurate chemical shift assignments to obtain high-quality solution structures of proteins. This constitutes a significant conceptual advance by concentrating the whole NMR measurement effort on the spectrum type that provides the structural data. In practice, it enables faster structure determination. The NOESY-only chemical shift assignments are still less reliable than those of the conventional approach, but improving the NOESY spectra and assignment algorithms may in the future close the gap and make the approach applicable to larger proteins. We have given a proof of principle that NMR structures can be solved exclusively from NOESY spectra. To our knowledge, this had never been achieved so far, and is thus of interest even though the NOESY-only approach remains at present less robust than the conventional one and recording additional through-bond spectra for the backbone and side-chain chemical shift assignment would not be unfeasible.

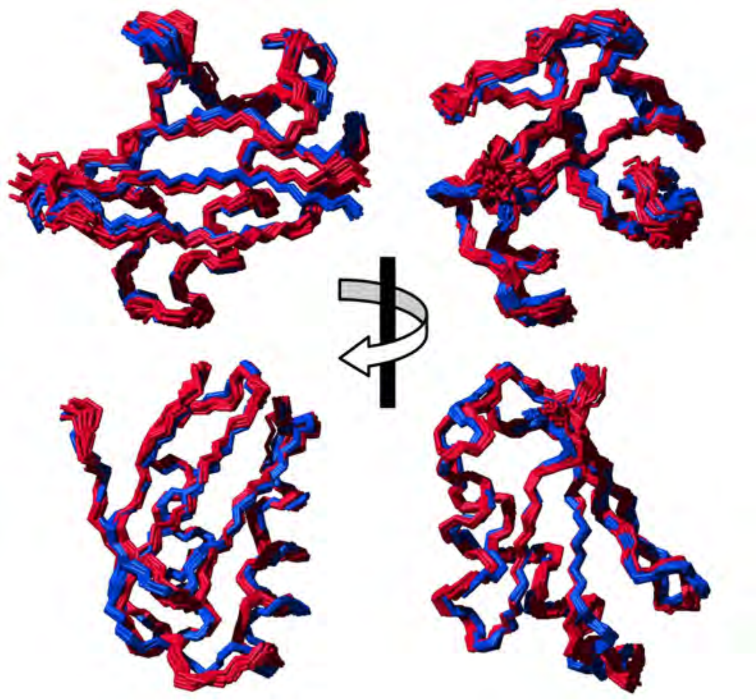


Figure: Structures of ubiquitin (top) and TTHA1718 (bottom) obtained using exclusively NOESY spectra for chemical shift assignment and structure calculation (blue) superimposed on the conventionally determined NMR solution structures (red).

Related publications in 2011:

1) Ikeya, T., Jee. J. G., Shigemitsu, Y., Hamatsu, J., Mishima, M., Ito, Y., Kainosho, M., Güntert, P. *Exclusively NOESY-based automated NMR assignment and structure determination of proteins*, J. Biomol. NMR. 50, 137-146 (2011)

Objective identification of residue ranges for the superposition of protein structures

Collaborators: Donata K. Kirchner[1,2] and Peter Güntert[1,2]

[1] Institute of Biophysical Chemistry and Center for Biomolecular Magnetic Resonance, Goethe University Frankfurt am Main, [2] Frankfurt Institute for Advanced Studies

The automation of objectively selecting amino acid residue ranges for structure superpositions is important for meaningful and consistent protein structure analyses. So far there is no widely-used standard for choosing these residue ranges for experimentally determined protein structures, where the manual selection of residue ranges or the use of suboptimal criteria remain commonplace. We present an automated and objective method for finding amino acid residue ranges for the superposition and analysis of protein structures, in particular for structure bundles resulting from NMR structure calculations. The method is implemented in an algorithm, CYRANGE, that yields, without protein-specific parameter adjustment, appropriate residue ranges in most commonly occurring situations, including low-precision structure bundles, multi-domain proteins, symmetric multimers, and protein complexes. Residue ranges are chosen to comprise as many residues of a protein domain that increasing their number would lead to a steep rise in the RMSD value. Residue ranges are determined by first clustering residues into domains based on the distance variance matrix, and then refining for each domain the initial choice of residues by excluding residues one by one until the relative decrease of the RMSD value becomes insignificant. A penalty for the opening of gaps favours contiguous residue ranges in order to obtain a result that is as simple as possible, but not simpler. Results are given for a set of 37 proteins and compared with those of commonly used protein structure validation packages. We also provide residue ranges for 6351 NMR structures in the Protein Data Bank. The CYRANGE method is capable of automatically determining residue ranges for the superposition of protein structure bundles for a large variety of protein structures. The method correctly identifies ordered regions. Global structure superpositions based on the CYRANGE residue ranges allow a clear presentation of the structure, and unnecessary small gaps within the selected ranges are absent. In the majority of cases, the residue ranges from CYRANGE contain fewer gaps and cover considerably larger parts of the sequence than those from other methods without significantly increasing the RMSD values. CYRANGE thus provides an objective and automatic method for standardizing the choice of residue ranges for the superposition of protein structures.

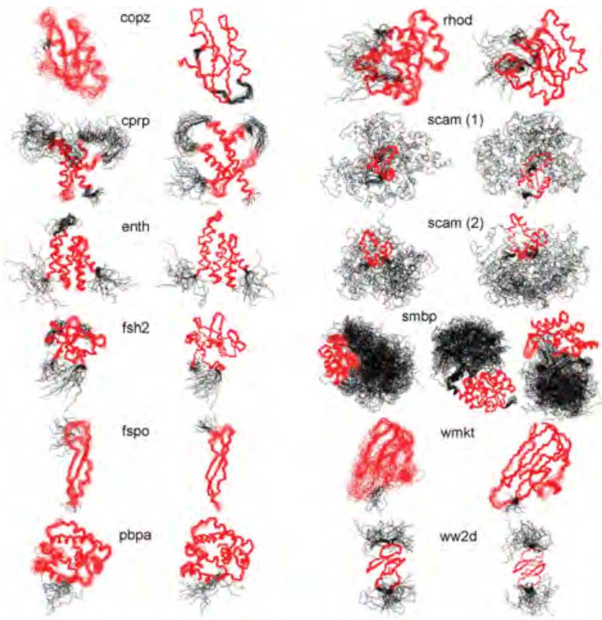


Figure: Structure bundles of 11 proteins for which low-precision (left) and high-precision (right) NMR structures are available superimposed for minimal backbone RMSD of the CYRANGE-determined residue ranges, indicated in red. Other residues are in black. Separate superpositions are shown for each domain.

Related publications in 2011:

1) Kirchner, D. K. and Güntert, P. *Objective identification of residue ranges for the superposition of protein structures*, BMC Bioinformatics 12, 170 (2011)

Solution NMR structure of proteorhodopsin

Collaborators: Sina Reckel[1], Daniel Gottstein[1,2], Jochen Stehle[3], Frank Löhr[1], Mirka-Kristin Verhoefen[4], Mitsuhiro Takeda[5], Robert Silvers[4], Masatsune Kainosho[5], Clemens Glaubitz[1], Josef Wachtveitl[4], Frank Bernhard[1], Harald Schwalbe[3], Peter Güntert[1,2], Volker Dötsch[1]

[1] Institute of Biophysical Chemistry and Center for Biomolecular Magnetic Resonance, Goethe University Frankfurt am Main, [2] Frankfurt Institute for Advanced Studies, [3] Institute for Organic Chemistry and Chemical Biology and Center for Biomolecular Magnetic Resonance, Goethe University Frankfurt am Main, [4] Institute of Physical and Theoretical Chemistry, Goethe University Frankfurt am Main, [5] Structural Biology Research Center, Nagoya University, Japan

Green-absorbing proteorhodopsin (PR), a light-driven proton pump, shows a strong dependence of its function on the pH. The primary proton acceptor D97 has an unusually high pKa value around 7.5 and its protonation state affects the absorption characteristics of the retinal cofactor. Furthermore, the direction of proton pumping switches in response to pH between an outward directed transport at alkaline pH and an inward directed transport at acidic pH. The potential function of this pH-dependency including the changing vectoriality is, however, still debated and a possible regulatory activity cannot be excluded. For a further insight into the structure-function relationship, we have solved the solution NMR structure of detergent-solubilized PR at acidic pH. NOE data was obtained with the help of stereo-array isotope labeling (SAIL) as well as selective labeling and complemented with a large number of distance restraints derived from paramagnetic relaxation enhancement (PRE). Additionally, restraints from residual dipolar couplings served to improve the structural accuracy of this seven-helix-bundle. The three-dimensional structure of PR reveals differences from its homologues such as the absence of the extended β-sheet in the B-C loop and enables insight into the mechanisms of color-tuning and proton transport.

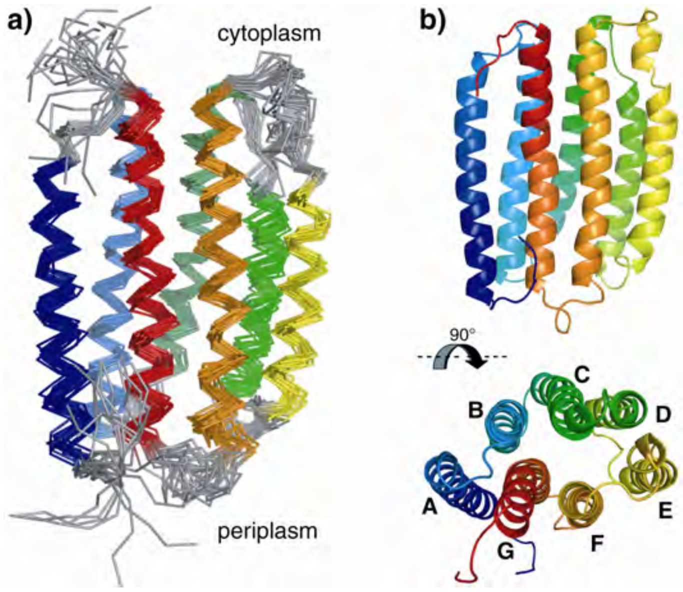


Figure: Structure of Proteorhodopsin. a) Bundle of the 20 conformers with lowest CYANA target function obtained from structure calculation. Helices are color-coded from helix A in dark blue to helix G in red. b) Cartoon representation of the conformer with the lowest CYANA target function seen from the side and from the top. In the lower panel helices are additionally labeled A-G.

Related publications in 2011:

1) Reckel, S., Gottstein, D., Stehle, J., Löhr, F., Verhoefen, M. K., Takeda, M., Silvers, R., Kainosho, M., Glaubitz, C., Wachtveitl, J., Bernhard, F., Schwalbe, H., Güntert, P., Dötsch, V. *Solution NMR structure of proteorhodopsin*. Angew. Chem. Int. Ed. 50, 11942–11946 (2011)

Structural basis for the dual RNA-recognition modes of human Tra2-β RRM

Collaborators: Kengo Tsuda[1], Tatsuhiko Someya[1], Kanako Kuwasako[1], Mari Takahashi[1], Fahu He[1], Satoru Unzai[1], Makoto Inoue[1], Takushi Harada[1], Satoru Watanabe[1], Takaho Terada[1], Naohiro Kobayashi[1], Mikako Shirouzu[1], Takanori Kigawa[1], Akiko Tanaka[1], Sumio Sugano[2], Peter Güntert[3,4,5], Shigeyuki Yokoyama[1,2], Yutaka Muto[1]

[1]RIKEN Systems and Structural Biology Center, Yokohama, Japan, [2] The University of Tokyo, Japan, [3] Institute of Biophysical Chemistry and Center for Biomolecular Magnetic Resonance, Goethe University Frankfurt am Main, [4] Frankfurt Institute for Advanced Studies, [5] Graduate School of Science, Tokyo Metropolitan University, Japan

Human Transformer2-β (hTra2-β) is an important member of the serine/arginine-rich protein family, and contains one RNA recognition motif (RRM). It controls the alternative splicing of several pre-mRNAs, including those of the calcitonin/calcitonin gene-related peptide (CGRP), the Survival Motor Neuron 1 (SMN1) protein, and the tau protein. Accordingly, the RRM of hTra2-β specifically binds to two types of RNA sequences (the CAA and $(GAA)_2$ sequences). We determined the solution structure of the hTra2-β RRM (spanning residues Asn110-Thr201), which has a canonical RRM fold, but an unusual alignment of the aromatic amino acids on the β-sheet surface. We then solved the complex structure of the hTra2-β RRM with the $(GAA)_2$ sequence, and found that the AGAA tetra-nucleotide was specifically recognized through hydrogen-bond formation with several amino acids on the N- and C-terminal extensions, as well as stacking interactions mediated by the unusually aligned aromatic rings on the β-sheet surface. Further NMR experiments revealed that the hTra2-β RRM recognizes the CAA sequence when it is integrated in the stem-loop structure. This study indicates that the hTra2-β RRM recognizes two types of RNA sequences in different RNA binding modes.

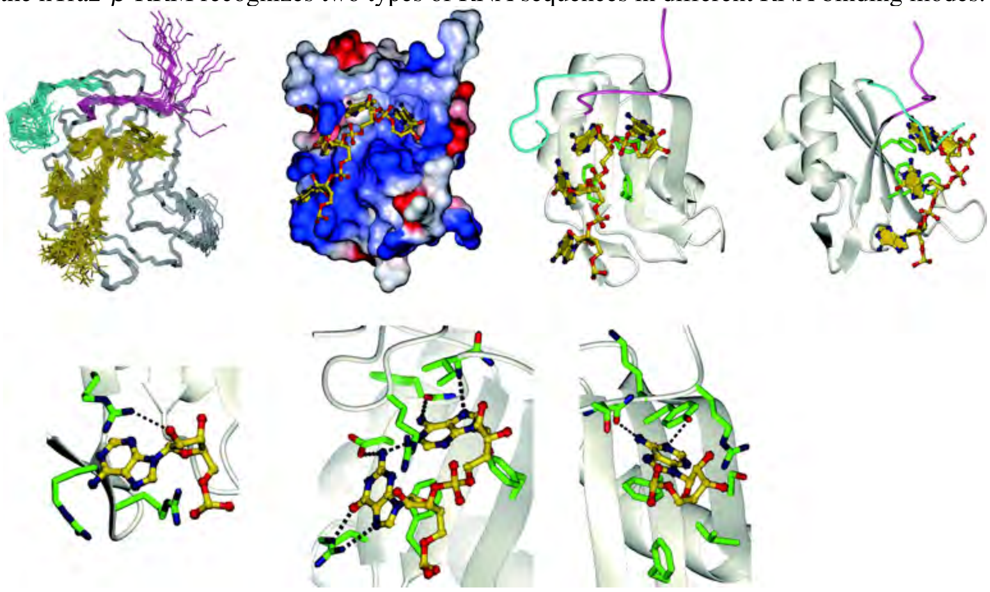
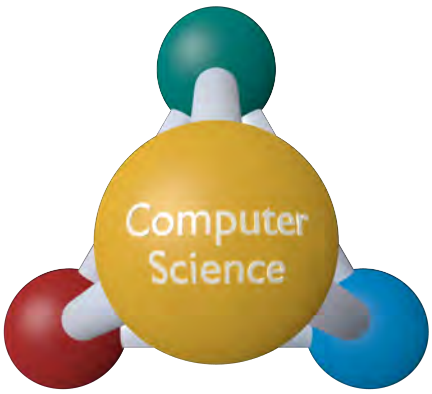


Figure: Solution structure of the hTra2-β RRM-[5'-(GAAGAA)-3'] complex. (A) Backbone traces of the 20 conformers of the hTra2-β RRM complex. The protein structures are shown in the same orientation as that of the free form of the hTra2-β RRM in Figure 2. Within the RNA molecules, the well-structured AGAA sequence (corresponding to A3-A6) is shown in gold. (B) Electrostatic potential surface of the hTra2-β RRM-[5'-(GAAGAA)-3'] complex. The atoms of the RNA molecule are shown in red (oxygen), blue (nitrogen) and gold (other heavy atoms). (C) Ribbon representation of the hTra2-β RRM-[5'-(GAAGAA)-3'] complex. The atoms of the RNA molecule are shown as in (B). (D) Close-up views of the RNA recognition by the hTra2-β RRM. On the ribbon representation of the backbone of protein, the side chains for the RNA recognition in the hTra2-β RRM and the RNA molecule are colored green for carbons in the protein, red for oxygens, and blue for nitrogens. The RNA molecule is shown as in (B). The hydrogen bonds were calculated by MOLMOL, and are represented by black dashed lines.

Related publications in 2011:

1) Tsuda, K., Someya, T., Kuwasako, K., Takahashi, M., Fahu, H., Inoue, M., Harada, T., Watanabe, S., Terada, T., Kobayashi, N., Shirouzu, M., Kigawa, T., Tanaka, A., Sugano, S., Güntert, P., Yokoyama, S., Muto, Y. *Structural basis for the dual RNA-recognition modes of human Tra2-β RRM*, Nucl. Acids Res. 39, 1538-1553 (2011)

4.4 Scientific Computing, Information Technology



The ALICE High Level Trigger

Collaborators: T. Kollegger[1], T. Alt[1], S. Gorbunov[1], S. Kalcher[1], M. Kretz[1], M. Langhammer[1], V. Lindenstruth[1], D. Ram[1], D. Rohr[1], O. Smørholm[1], T. Steinbeck[1]

[1] Frankfurt Institute for Advanced Studies

ALICE is one of the four main experiments at the Large Hadron Collider (LHC) at the European Center for Particle Physics CERN, Geneva. Its main goal is to study the properties of the hot and dense medium created in collisions of heavy ions. In the autumn of 2011, LHC was operating with lead (Pb) ions and achieved luminosities an order of magnitude higher than in previous years, with up to 6kHz of Pb+Pb collisions. This new record interaction rates posed a challenge for the read-out of the detector. Each Pb+Pb collision creates up to 80MB of total data volume from the various sub-detectors of ALICE, with the Time Projection Chamber (TPC) by far the largest (∼60MB). This data rate by far exceeds the performance of the detector read-out systems, so events of interest have to be selected, the task of the trigger system. Another bottleneck is the mass-storage system, whose sustained bandwidth is significantly lower than the maximum detector read-out bandwidth.

The ALICE High Level Trigger (HLT) was designed to close the gap between the maximum detector read-out bandwidth and the storage bandwidth. Being the first point in ALICE where the data from all sub-detectors is available, the HLT reconstructs the full event, i.e. the trajectories of the several thousand particles emitted from the collission and passing through the detector system. Figure 1 shows a visualization of a fully reconstructed event.

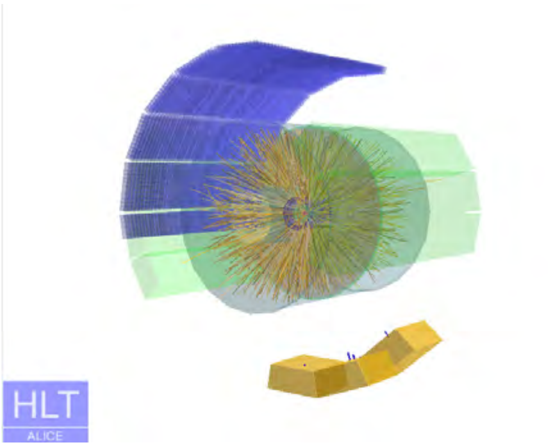


Figure 1: A central Pb+Pb event as reconstructed by the ALICE High Level Trigger.

After sucessful operation in 2009 and 2010, the HLT was upgraded in 2011 to deal with the higher data rates. The particle track reconstruction in the HLT uses graphic cards (GPUs) in addition to the CPUs, the number of nodes with GPUs was doubled to a total of 64. The output bandwidth of the system was increased by a factor 4, now reaching more than 3GB/s. With these upgrades, the HLT was able to deal with the maximum possible detector read-out rates of more than 20 GB/s.

A special emphasis in 2011 was the improvment of the physics reconstruction performance. For this the first processing step of the TPC reconstruction, the identification of charge clusters deposited by charged particles traversing the TPC gas, has been optimized. After optimization of the FPGA based HLT cluster finder algorithm and its parameters, detailed studies showed only negligibale differences in the final track reconstruction parameters compared to using the, by far slower, offline cluster finder.

Having demonstrated this excellent physics performance, ALICE decided to discard the TPC raw data, relying for the particle reconstruction soley on the HLT cluster finder output. Together with data format optimizations, entropy-reducing transformations of the cluster data and subsequent lossless Huffman-compression, the HLT reduced the 20 GB/s input rate to 4 GB/s storage rate, enabling the recording of all events which could be handeld by the detector read-out system and thus maximizing the physics reach of ALICE.

ALICE HLT TPC Tracking on GPU

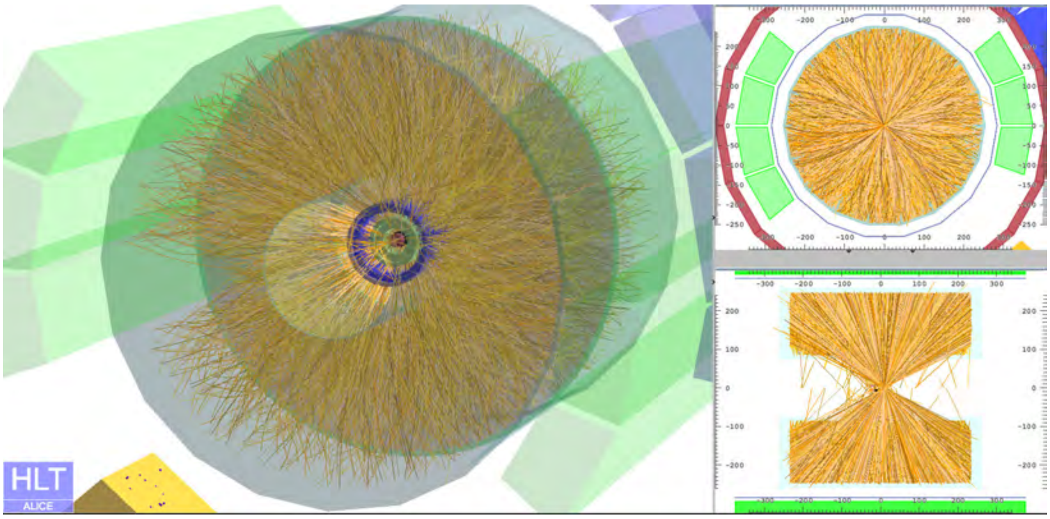
Collaborators: D. Rohr[1], S. Gorbunov[1], V. Lindenstruth[1]

[1] Frankfurt Institute for Advanced Studies

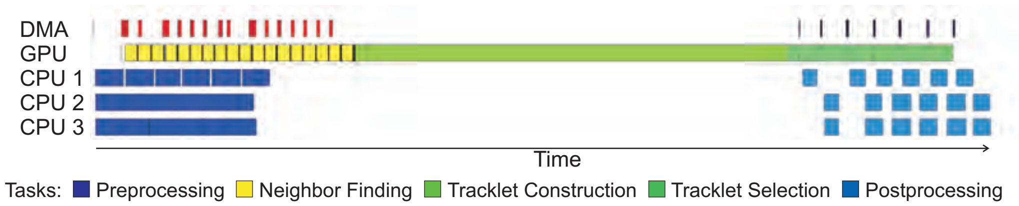
ALICE is one of the major four experiments of the Large Hadron Collider at CERN in Geneva, which today is the most powerful particle accelerator. The ALICE High Level Trigger is capable of a full real-time event reconstruction based on the raw data obtained from the detector. In this process, reconstruction of particle trajectories (tracking) is the most compute intensive task – especially for heavy ion collisions with the detector being filled with several thousands of particles. Since many particles can be tracked in parallel, GPUs can be employed to accelerate the tracking.

The ALICE HLT tracker combines the cellular automaton principle with the Kalman filter for the track fit. From the beginning it was designed with parallelism in mind and a GPU enabled version of the tracker has been created [I]. Both CPU and GPU tracker essentially share the same common source code for the tracker, which is encapsulated by two specialized wrappers for both hardware architectures. GPU and CPU tracker have been proven to produce identical results. Marginal differences arise only from different rounding due to non-associative floating-point arithmetic but there are no influences of concurrency on the tracking result.

The ALICE GPU tracker was operated during the heavy ion phases in November 2010 and November 2011. The below figure shows a screenshot of the ALICE online event display during the first physics run with active GPU tracker.



One particular challenge of the implementation is to ensure continuous GPU utilization. The ALICE GPU tracker accomplishes this with a pipeline, which overlaps pre- and postprocessing on CPU and tracking on GPU of multiple sectors of the detector. Since a single CPU core cannot keep step with the GPU, the pipeline is multithreaded. The below figure visualizes the parallel processing of several subtasks of tracking for different sectors of the detector.



Related publications in 2011:

1) S. Gorbunov, D. Rohr, et al. *ALICE HLT high speed tracking on GPU*, IEEE Transactions on Nuclear Science 58 (2011) 1845

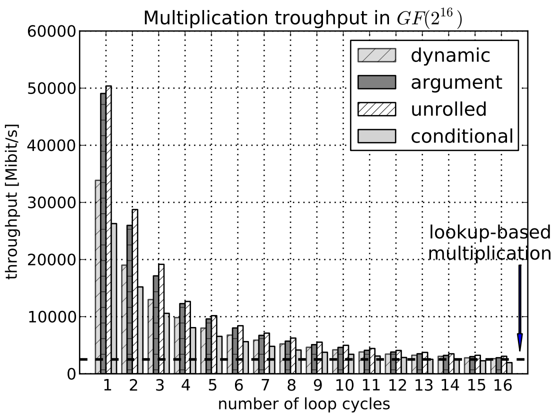
Arithmetic over Galois fields on modern processor architectures

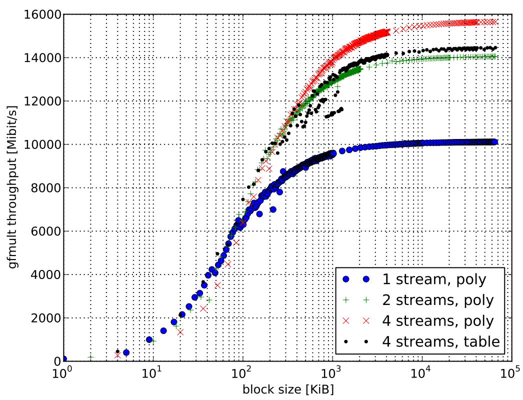
Collaborators: S. Kalcher[1], V. Lindenstruth[1]

[1] Frankfurt Institute for Advanced Studies

Galois fields (also called finite fields) play an essential role in the areas of cryptography and coding theory. They are the foundation of various error- and erasure-correcting codes and therefore central to the design of reliable storage systems. The efficiency and performance of these systems depend considerably on the implementation of Galois field arithmetic, in particular on the implementation of the multiplication. In current software implementations multiplication is typically performed by using pre-calculated lookup tables for the logarithm and its inverse or even for the full multiplication result. However, today the memory subsystem has become one of the main bottlenecks in commodity systems and relying on large in-memory data structures accessed from inner loop code can severely impact the overall performance and deteriorate scalability. In this study, we implemented a variant of Galois field multiplication on modern processor architectures without using lookup tables. Instead we trade computation for memory references and perform full polynomial multiplication with modular reduction using the generator polynomial of the Galois field. The basis for the vectorized polynomial multiplication is the well known Russian peasant multiplication algorithm (also known as Egyptian multiplication). Integer multiplication can be performed by only using integer doubling, halving, and addition. The classical multiplication tables for numbers from one to ten are not required. Since only XOR, AND and shift operations are used, the algorithm can be vectorized with the integer part of the Streaming SIMD Extensions (SSE). The presented implementation uses SSE compiler API extensions, the so called intrinsics. The core multiplication code uses only integer SIMD instructions available in SSE version 2, but some instructions from SSE version 3 and 4 (shuffle, min/max, extract) can be beneficial for reducing the number of loop cycles. In addition to the SIMD instruction extensions of commodity processors, the algorithm is well suited for execution on graphics processing units (GPUs), which have evolved rapidly in recent years as general purpose co-processors.

The figures show the results of the vectorized (left) and GPU (right) implementation of the polynomial multiplication algorithm in $GF(2^{16})$, each compared to the table-based approach.





Left: Multiplication throughput for the vectorized implementation depending on the actual number of required loop cycles. *Right:* Multiplication throughput of the GPU implementation for different numbers of overlapping execution streams.

Related publications in 2011:

1) Sebastian Kalcher, Volker Lindenstruth, *Accelerating Galois field arithmetic for Reed-Solomon erasure codes in storage applications*, pp.290-298, 2011 IEEE International Conference on Cluster Computing, 2011

Vc: Development of a C++ library for explicit, portable, and intuitive SIMD programming

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

[1] Frankfurt Institute for Advanced Studies

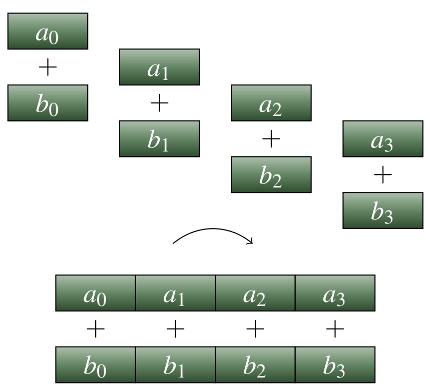
Modern CPU architectures include support for vector (SIMD) instructions, which enable operations on **M**ultiple **D**ata with a **S**ingle **I**nstruction. On the widely used x86 CPUs there have been several releases of vector extensions, ranging from MMX and SSE up to SSE4 and AVX. With the latest extension (AVX), there are 8 single-precision floating-point values (or 4 double-precision values) per vector register. The computational instructions can thus execute up to eight (four) times more operations, leading to a significant speed-up of the data-parallel computations in an application.

The use of these vector instructions is not directly possible with standard C/C++. This is why compilers try to auto-vectorize. But as it would be prohibitively expensive to vectorize perfectly, compilers resort to simplified rules for vector transformation. Often the results are extra work to enable auto-vectorization and frail performance.

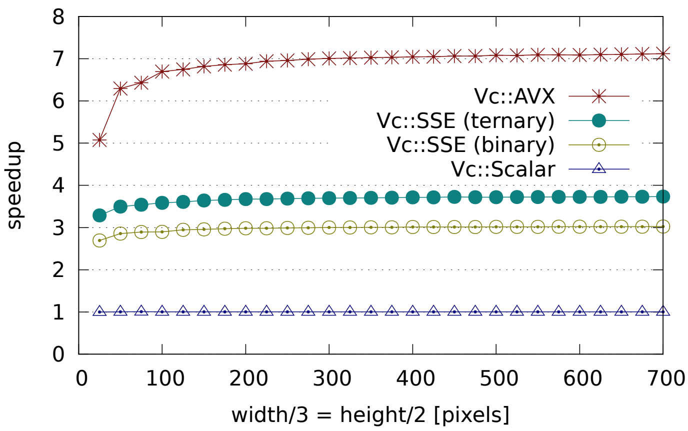
Vc was developed to solve this issue by providing a C++ library that allows to explicitly write intuitive, portable, and fast vector code. The Vc library includes several implementations, which can be used to optimize for a given target system without loss of portability. As the use of Vc does not require any changes in the toolchain it has a relatively low entry-barrier for most projects.

Recently support for the new AVX instructions, which required the development of a new Vc backend, was added. Furthermore, the library received more documentation, features, and API consistency.

It is planned to show applicability of Vc in large projects, many of which are often memory-bound instead of compute-bound. This will help to document best-practices and enhance Vc where needed. Ultimately, the aim is for Vc to become a reliable and standard building-block for C++ programs.



SIMD allows to transform four (or two/eight/sixteen/...) separate computational instructions into a single instruction.



The plot shows the relative speed of a Mandelbrot picture calculation of the different Vc implementations on an Intel Core i5-2500 (Sandy-Bridge). The Mandelbrot implementation using Vc requires no code changes or `#ifdefs` to optimize for the different SIMD extensions.

Related publication in 2011:

M. Kretz, V. Lindenstruth, *Vc: A C++ library for explicit vectorization*, Software: Practice and Experience (2011), doi: 10.1002/spe.1149

High Performance GPU-based DGEMM and Linpack

Collaborators: D. Rohr[1], M. Bach[1], M. Kretz[1], V. Lindenstruth[1]

[1] Frankfurt Institute for Advanced Studies

Linpack is a popular benchmark for supercomputers and builds the basis of the half-yearly Top500 list. It iteratively solves a dense system of linear equations. Each iteration consists of panel factorization, panel broadcast, LASWP, U-matrix broadcast and trailing matrix update [1]. The trailing matrix update is performed via a matrix multiplication (DGEMM) and is the most compute intensive step. It is a well known fact that GPUs excel at matrix multiplication. For these reasons, a heterogeneous Linpack has been implemented for the LOEWE-CSC cluster, which performs the update step on the GPU and all other tasks on the processor.

Since only one process per node can use the GPU efficiently, instead of one MPI process per CPU core only one process pre node is used, which uses the GPU and is multi-threaded itself. Therefore, all other tasks during Linpack have been parallelized. The employed multi-threaded BLAS libraries were to support reservation of CPU cores for GPU pre- and postprocessing. A binary patch to the AMD driver reduces the page fault rate.

The DGEMM of the update step is split in many multiplications of submatrices called tiles, which are small enough to fit in GPU memory. Processing of these tiles is arranged in a pipeline which ensures continuous GPU utilization and allows for concurrent GPU and CPU processing as well as DMA transfer. In addition, a dynamic buffering ensures that no tile is ever retransferred. For not wasting GPU cycles during non-DGEMM Linpack-tasks, the implementation allows for executing factorization and broadcast for the next iteration in parallel to the DGEMM of the current iteration and pipelines the LASWP task. Linpack performance has been demonstrated to scale linearly up to several hundreds of nodes [1].

Usually, the per-node performance of multi-node Linpack runs is limited by the slowest nodes. For clusters with nodes of different performance levels, e.g. the LOEWE-CSC has CPU-only and GPU-enabled compute notes, the new Linpack allows for an unequal distribution of the workload among the systems. Measurements show that the implementation is actually able to achieve almost the accumulated performance of all participating nodes with less than 3% granularity loss.

Multiple GPUs can be used in parallel with e.g. two GPUs showing a speedup of about factor 1.98. Up to four GPUs in one system have been tested reaching 2 TFlop/s of Linpack performance. With three GPUs an efficiency of about 1200 GFlop/J was demonstrated, corresponding to a second place in the Green500 list at the time the experiment was conducted [2]. The DGEMM kernel on the GPU achieves about 90% of the theoretical peak performance on both the Cypress and Cayman series of AMD GPUs. 75% of the accumulated theoretical CPU and GPU performance are available in Linpack. The LOEWE-CSC ranked place 22 in the November 2010 Top500 list demonstrating the highest efficiency of all listed GPU clusters with respect to theoretical peak performance.

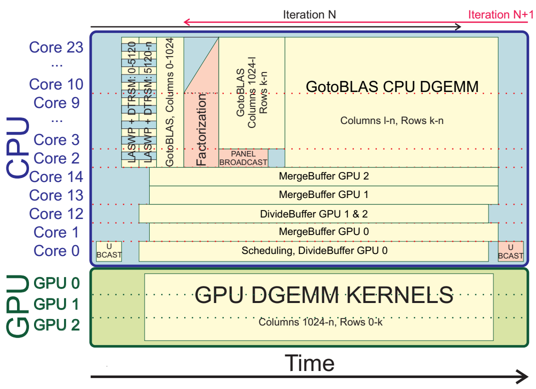


Figure 1: Concurrent execution of all HPL tasks on CPU cores and GPUs

The current implementation for the CAL-framework is momentarily being improved to support OpenCL and CUDA and the new AMD Graphics Core Next GPU.

Related publications in 2011:

1) M. Bach, M. Kretz, V. Lindenstruth, D. Rohr *Optimized HPL for AMD GPU and multi-core CPU usage*, Computer Science - Research and Development 26, 153 (2011)

2) D. Rohr, M. Bach, M. Kretz, V. Lindenstruth *Multi-GPU DGEMM and HPL on highly energy efficient clusters*, IEEE Micro, Special Issue: CPU, GPU, and Hybrid Computing

Lattice QCD on GPUs

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

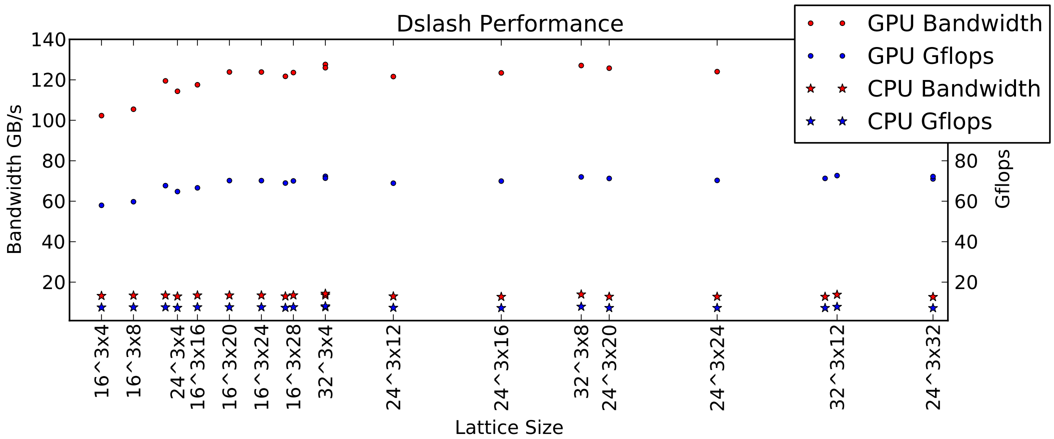
[1] Frankfurt Institute for Advanced Studies, [2] Institut für Theoretische Physik, Goethe-Universität Frankfurt am Main

Quantum Chromodynamics (QCD) is the known theory of the strong force and part of the Standard Model of particle physics. Its phase diagram is a problem of particular interest and is investigated in current, state-of-the-art collider experiments at CERN and, in the near future, at FAIR. Lattice QCD provides a first principle access to this problem.

Lattice simulations require an enormous amount of computing power. They sample the phase space using Hybrid Monte Carlo techniques, requiring the fermion matrix to be inverted many times. The inversion of this sparse quadratic matrix, typically of size $10^8 \times 10^8$, is the most time consuming part of the algorithm. To get physical results simulations need to be carried out at different lattice spacings and extrapolated to the continuum limit.

Sparse matrix inversion is completely dominated by the memory bandwidth available in the system. Today Graphics Processing Units (GPUs) provide significantly more bandwidth than CPUs, making them a promising platform for QCD codes. However, so far GPU-enabled Lattice QCD codes have always been focused on the proprietary NVIDIA CUDA programming interface, locking the usability of the code to hardware of this one vendor.

We aim at building a versatile Lattice QCD solution that can achieve optimum performance on a wide variety of modern hardware architectures. Therefore we base our solution on OpenCL, an open programming standard for parallel programming supported by all major hardware vendors. We focus on remaining with a single source source code, ensuring maintainability and easier verification of code correctness, while achieving maximum performance over a wide range of system configurations.



Dslash Performance on one AMD HD5870 and two Operon 6172 in LOEWE-CSC for a variety of lattice sizes

Our first focus for performance optimization was the LOEWE-CSC supercomputer, implementing AMD GPUs. We have carefully analyzed the characteristics of the memory controller of AMD GPUs. Using that knowledge we were able to achieve more than 70 double precision Gflops in the Dslash calculation, the main part of the fermion matrix, while still being able to run the same code parallelized on CPU only system. This is competitive with NVIDIA-only solutions, however, in addition, the methods for memory controller analysis and the OpenCL based code that can be parametrized to match different memory controllers enable high performance on a wider range of hardware.

Related publications in 2011:

M. Bach, O. Philipsen, C. Pinke, C. Schäfer, L. Zeidlewicz, *LatticeQCD using OpenCL*, Proceedings of the XXIX International Symposium on Lattice Field Theory - Lattice 2011.

How stable are transport model results to changes of resonance parameters? A UrQMD model study

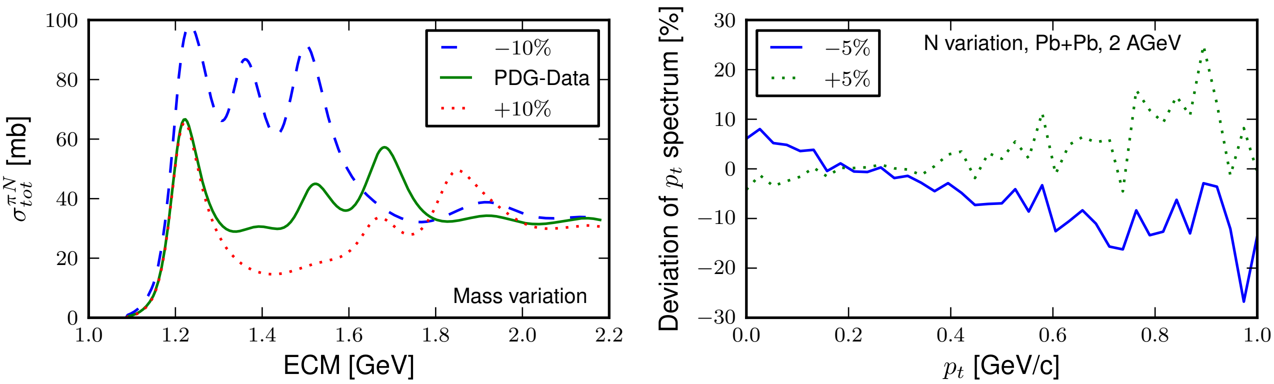
Collaborators: J. Gerhard[1,2], B. Bäuchle[1,3], V. Lindenstruth[1,2], M. Bleicher[1,3]

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

Transport models like the Ultra-relativistic Quantum Molecular Dynamics model (UrQMD) rely as an Input heavily on measured quantities like hadron masses, the hadron decay widths, individual branching ratios, and cross sections. Unfortunately these parameters are often not known exactly, as one can see from an inspection of the Particle Data Group (PDG) tables. In the light of the current experiments with the LHC at CERN and the upcoming high precision experiments of FAIR at GSI, it is of crucial interest to validate the transport models.

In this interdisciplinary study between computer science and theoretical physics, we have applied meta programming techniques to the UrQMD model in order to do cope with the combinatoric difficulties of a multidimensional parameter scan. We employed the Frankfurt LOEWE-CSC to carry out the systematic analysis on hadron masses and decay withs in order to check the stability of UrQMD. We addressed the question by simulating nucleus-nucleus interactions in an energy regime from 2 AGeV to 30 AGeV, while varying the parameters within the error estimates of the PDG (or $\pm 10\%$).

Although we have restricted our research to the UrQMD model in this study, the results should (at least qualitatively) also be transferable to other transport simulations based on similar physics assumptions, like the Parton-Hadron-String Dynamics or the Multi-Phase-Transport model.



Left: When varying the masses of all nucleons simultaneously one can observe a strong shift of the cross sections.
Right: Also the p_t-spectra of outgoing pions is affected by a simultaneous shift of the nucleon masses.

Related publications:

1) J. Gerhard, B. Bäuchle, V. Lindenstruth, M. Bleicher, *How stable are transport model results to changes of resonance parameters? A UrQMD model study*, submitted to Phys. Rev. C.
2) Klaus Aehlig, Helge Dietert, Thomas Fischbacher, Jochen Gerhard, *Casimir forces via worldline numerics: Method improvements and potential engineering applications*, arXiv:1110.5936v1.

Complete and Clustered Synchronization in Complex Networks

Collaborators: S. Becker[1], M. Schäfer[1], M. Greiner[2], S. Schramm[1]

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

We consider the dynamics of a complex network, consisting of N nodes and L links. The dynamics are given in the following way: Each node is assigned a (for simplicity scalar) variable $x_i \in [-1,1]$, which evolves in time according to

$$x_i^{t+1} = (1-\varepsilon) f(x_i^t) + \varepsilon \sum_{j=0}^{N} A_{ij} g(x_j^t),$$

where f and g are bounded functions and A_{ij} is the adjacency matrix of the network (including suitable normalization).

More specifically, we are interested in almost bipartite networks in the sense that in addition to the bipartite structure of links between two groups of nodes in a graph, there exist a few extra links within these two groups. We call the links between the two clusters "inter-cluster links" and the links within a cluster "intra-cluster links". We look at the collective dynamics, i.e. the synchronization behavior of such systems. It has been noted in numerical studies that the presence of additional intra-cluster links may lead to enhanced synchronization, an analytical treatment of the problem is, however, still missing.

To investigate the synchronization behavior, we have analytically reformulated the problem in terms of a perturbed master stability approach. Due to the presence of the non-bipartite links, this does not decouple into a set of two-dimensional parametric equations, but remains N dimensional, however, since the coupling within the two clusters is small, we hope that we may be able to treat the synchronization perturbatively.

As a complementary approach, we simulated bipartite networks numerically. On this route, we have succeeded to reproduce an important result on network synchronization, namely the effect that a small coupling ε leads to synchronization among connected nodes, while a large coupling causes those nodes to synchronize that are not connected, i.e. the two bipartite groups.

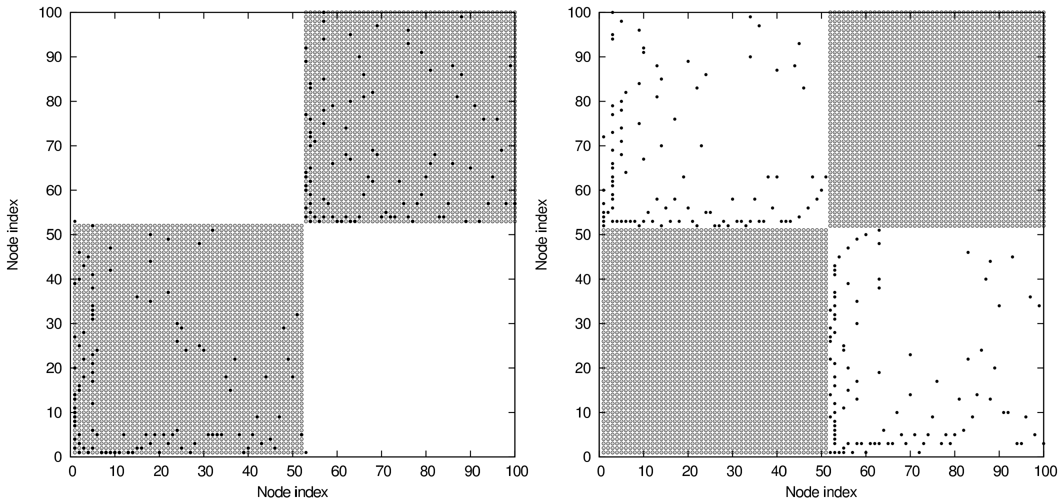


Figure: Node-node plot of links and synchronization. In both figures, open circles indicate that the two nodes are synchronized, full circles represent links. *Left:* For small coupling ($\varepsilon = 0.16$), we observe synchronization among connected nodes (dominated by intra-cluster links). *Right:* Large coupling ($\varepsilon = 0.80$) leads to synchronization among the two bipartite groups (dominated by inter-cluster links).

5. Talks and Publications

Conference and Seminar Talks by FIAS Members 2011

Jaan Aru

– Association of Communication Trainers of Estonia, Tartu, 20 August 2011: *The sizzle of the brain cells*
– Institute of Public Law and Institute of Psychology of the University of Tartu, Estonia, 29 November 2011: *Building consciousness: the basic circuitry*,

Alexander Botvina

– 2nd International Workshop on Accelerator Radiation Induced Activation ARIA2011, Ma'ale Hachamisha, Judean Hills, Israel, 15-19 May 2011, *Production of isotopes as signature of reaction mechanisms*
– International Workshop "Strange hadronic matter", ECT*, Trento, Italy, 26-30 September 26- 30 2011, *Production of hypernuclei in reactions induced by relativistic light- and heavy-ions*
– International conference on nuclear fragmentation NUFRA2011, Kemer, Turkey, 2-9 October 2-9 2011, *Production of spectator hypermatter in relativistic light- and heavy-ion collisions*

Elena Bratkovskaya

– International Conference on Primordial QCD Matter in LHC Era, Cairo, Egypt, 4-8 December 2011, *Dynamics of QGP in relativistic heavy-ion collisions*
– International Conference on Exciting Physics, Makutsi, South Africa, 13-20 November 2011, *The QGP phase in relativistic heavy-ion collisions*
– 18th CBM Collaboration Meeting, Beijing, China, 29 September 2011, *Signatures of the QGP in Relativistic Heavy-Ion Collisions*
– International Conference Strangeness in Quark Matter (SQM11), Cracow, Poland, 18-24 September 2011, *What strange particle observables tell us about the expansion of the plasma*
– 26th Winter Workshop on Nuclear Dynamics, Winter Park, Colorado, USA, 6-13 February 2011, *Properties of the partonic phase at RHIC within PHSD*

Walter Greiner

– Preconference School, Habana, Cuba, 3-5 February 2011, *Extension of the Periodic System: Superneutronic, Superheavy, Superstrange Elements*
– XIII Workshop on Nuclear Physics and VII International Symposium on Nuclear and Related Techniques (WONP-NURT), Habana, Cuba, 7-11 February 2011, *There are no Black Holes. Pseudo-Complex General Relativity Review and some Predictions*
– Nuclear Physics in Astrophysics V, Eilat, Israel, 3-8 April 2011, *Extension of the Periodic Table: Superheavy, Superneutronic, Strange Elements and Antinuclei*
– First Caribbean Symposium on Nuclear and Astroparticle Physics (STARS 2011), Habana, Cuba, 1-4 May 2011, *Extension of the Periodic System: Superneutronic, Superheavy, Superstrange Elements*
– Fifth International Symposium on Atomic Cluster Collisions (ISACC), Berlin, Germany, 20-25 July 2011, *Clusters of Matter, Antimatter and Strange Matter*
– 4th International Conference on the Chemistry and Physics of the Transactinide Elements (TAN2011), Sochi, Russia, 5-7 September 2011, *Nuclear Clusters: Superheavy, Neutron Rich, of Matter, Antimatter, Strange Matter*
– International Conference on Exotic Atoms and Related Topics (EXA2011), Vienna, Austria, 5-9 September 2011, *Fundamental Problems in Physics*

– “Highlights in Heavy-Ion Physics”, A Symposium in Honour of Nikola Cindro, Split, Croatia, 22-24 September, *There are no black holes - Pseudo-Complex General Relativity. From Einstein to Zweistein*
– Stuttgart/Hospitalhof, 25. October 2011, *Gott hinter den Naturgesetzen: War es ein Gott, der diese Zeilen schrieb?*
– Physikalischer Verein, Frankfurt, 26. October 2011, *Von Einstein zu Zweistein - Allgemeine Relativitätstheorie im Pseudokomplexen*,
– International Conference on Exciting Physics, Makutsi, South Africa, 13-20 November 2011, *Opening lecture*

Peter Güntert

– Recent Advances in High-Resolution NMR Workshop, Hyderabad, India, 12-17 December 2011, *3D structure calculations from NMR data: Theory and application*,
– Bio-NMR Joint Research Activities Meeting, Berlin, Germany, 10-11 November 2011:, *CYANA for solid-state NMR*
– Institute of Molecular Biology and Biophysics, ETH Zürich, Switzerland, 9 November 2011, *Automated NMR structure determination with CYANA*
– Physikalische Chemie Kolloquium, Laboratorium für Physikalische Chemie, ETH Zürich, Switzerland, 8 November 2011, *Whatcan computation do for NMR with proteins?*
– Bio-NMR Joint Research Activities Meeting, Frankfurt am Main, Germany, 25 August 2011, *CYANA for solid-state NMR*
– Foresight Meeting sponsored by Bio-NMR: NMR Structure Determination of Membrane Proteins, Bad Homburg, 19-20 August 2011, *Membrane protein structure calculation with CYANA*
– EMBO Practical Course on Structure Determination of Biological Macromolecules by Solution NMR, München, Germany, 29 July - 5 August 2011, *NMR structure calculation*
– Advanced course: Protein NMR Structure Calculation and Validation, Vilnius, Lithuania, 17-19 May 2011, *Automated NOE assignment and structure calculation*
– Advanced course: Protein NMR Structure Calculation and Validation, Vilnius, Lithuania, 17-19 May 2011, *CYANA*
– BIOGUNE, Bilbao, Spain, 11 March 2011, *Automated NMR protein structure determination*
– Novartis, Basel, Switzerland, 12 January 2011, *Automated NMR structure analysis of proteins and protein-ligand complexes*

Xu-Guang Huang

– Seminar given in Institut de Ciències de l’Espai (ICE), Barcelona, Spain, 22 November 2011, *Anisotropic viscosities of strange quark matter and neutron star phenomenology*
– Seminar given at Tsinghua University, Beijing, China, 24 July 2011, *Ferromagnetism in repulsive fermi gases and fermion ladder resummation*
– 9th conference on QCD Phase Transition and RHIC physics, Hangzhou, China, 18-21 July 2011, *Viscous relaxation times in relativistic hydrodynamics*
– ‘Summer working month in CCNU, Wuhan, China, 10-17 July 2011, *Ferromagnetism in repulsive fermi gases and fermion ladder resummation*
– Seminare E6, Bielefeld, Germany, 16 June 2011, *Ferromagnetism in repulsive fermi gases and fermion ladder resummation*

V. K. Ivanov

– Fifth International Symposium ”Atomic Cluster Collisions ISACC 2011”, Berlin, Germany, 20-25 July 2011, *Photoionization Process with Negative Ions of Atomic Clusters*,

Vladimir Konchakovski

- 7th Workshop on Particle Correlations and Femtoscopy (WPCF2011), Tokyo, Japan, 20-24 September 2011, *Evolution of electro-magnetic field in relativistic heavy-ion collisions from the HSD transport approach*
- Workshop of the European Network TORIC, Heraklion, Crete, Greece, 5-9 September 2011, *Chiral Magnetic Effect and Evolution of Electromagnetic Field in relativistic heavy-ion collisions*

Andrey Korol

- Fifth International Symposium "Atomic Cluster Collisions ISACC 2011", Berlin, Germany, 20-25 July, 2011, *Auger Processes in Endohedral Atoms: the Role of Non-Central Position of the Atom*,

Andrey Kostyuk

- Fifth International Symposium "Atomic Cluster Collisions ISACC 2011", Berlin, Germany, 20-25 July, 2011, *Crystalline Undulator and Crystalline Undulator Based Gamma Laser: Current Status and Perspectives*

Volker Lindenstruth

- Woche der Informatik, Goethe-Universität Frankfurt, 7 April 2011 *Wie baut man einen Supercomputer?*
- Future Thinking-Event "Grenzenlos – RZ-Technologien im Wandel", Technik-Museum Sinsheim, 7 April 2011, *Das FAIR Tier-0 3D Green-IT Rechenzentrum*
- HEPiX Spring Meeting, GSI Darmstadt, 2-6 May 2011, *FAIR 3D Tier-0 Green-IT Cube*
- VZM Workshop, Bonn, 18. May 2011, *Neue Green-IT Standards*
- German-Russian Science Year Kick-off event, Moscow, 24. May 2011, *FAIR Computing Strategies and the FAIR Green-IT Cube*
- International Supercomputing Conference ISC2011, Hamburg, 19-23 June 2011, *Energy Efficiency or Net Zero Carbon by 2020?*
- VRZM Workshop, Hamburg, 22 June 2011, *Das FAIR Tier-0 3D Green-IT Rechenzentrum*
- Night of Science, Goethe-University, Frankfurt, 22. June 2011, *Grüne schnelle Computer in Frankfurt*
- The 2011 Saudi International Conference on Information Technology, Riyadh, 18-19 Sept. 2011, *Energy efficient scalable Green Computing*
- Datacenter Dynamics, Messe Frankfurt, 5 Oct. 2011, *Green Cube - Das 3diemensionale Rechenzentrum*
- Wissenschaft für Alle, GSI Helmholtzzentrum für Schwerionenforschung, Darmstadt, 19 Oct. 2011, *Supercomputer für die Forschungsanlage FAIR*
- Infraserv, LOEWE-CSC ECO visit, Frankfurt, 6. Dec. 2011, *LOEWE-CSC and its data center*
- FIAS Forum, Frankfurt, 8 Dec. 2011, *Musikkodierung heute und vor 300 Jahren*

Jörg Lücke

- International Bernstein Symposium on Bayesian Inference: From Spikes to Behaviour, Tübingen, Germany, 9-10 December 2011, *Non-Linear Components in Sensory Data and the Requirement for Bayesian Inference*
- Talk at the Department of Software Engineering and Theoretical Computer Science, TU Berlin, Nov. 2011, *Representational Learning of Non-linear and Occlusive Data Components*
- Talk at the Department of Computer Science, University of Magdeburg, Germany, Nov. 2011, *Efficient Extraction of Non-linear and Occlusive Data Components*

– Talk at the Institute for Adaptive and Neural Computation, University of Edinburgh, UK, Nov. 2011, *Representational Learning of Sensory Data Components*

Olena Lynnik

– 26th Winter Workshop on Nuclear Dynamics, Winter Park, Colorado, USA, 6-13 February 2011, *Dilepton production at SPS and RHIC energies within the PHSD off-shell transport approach*
– XLIX International Winter Meeting on Nuclear Physics, Bormio, Italy, 24-28 January, 2011, *Dilepton production at SPS and RHIC energies*

Igor Mishustin

– NanoBIC Winter School, Arnoldshain, Germany, 2 March 2011, *MC simulations of ion-beam cancer therapy on macro and micro scales*,
– XXVIII Max Born Symposium 2011 "Three Days on Quarkyonic Island", Wroclaw, Poland, 19-21 May 2011, *Hydrodynamic evolution of fluctuations in hot quark matter*
– Seminar on Electronic Structure and Quantum Chemistry, Technische Universität Darmstadt, 29 June 2011,*Nuclear fragmentation reactions in basic research and medical applications*
– International conference on nuclear fragmentation NUFRA2011, Kemer, Turkey, 2-9 October 2011, *Nuclear fragmentation reactions from research to applications*,

Rodrigo Picanço Negreiros

– DPG Frühjahrstagung, Münster, 21- 25 March 2011, *Composition, structure, and thermal evolution of magnetized and rotating compact stars*, group report
– First Caribbean Symposium on Nuclear and Astroparticle Physics (STARS 2011), Habana, Cuba, 1-4 May 2011, *Cooling of spinning-down and young neutron stars*
– 2nd International Symposium on Strong Electromagnetic Fields and Neutron Stars (SMFNS2011), Varadero, Cuba, 5-7 May 2011
– From Nuclei to White Dwarfs and Neutron Stars, Les Houches, France, 3-8 April 2011, *Cooling of young neutron stars*

Piero Nicolini

– Workshop on new trends in the physics of the quantum vacuum: from condensed matter, to gravitation and cosmology, European Centre for Theoretical Studies in Nuclear Physics and Related Areas (ECT), Trento, Italy, 27 June - 1 July 2011, *Mini black holes at the LHC*
– Black holes in TeV gravity and holography – Steklov Mathematical Institute of the Russian Academy of Sciences, Moscow, Russia, 2011 *Quantum gravity improved black holes at the LHC*
– Seminar talk at The University of Sheffield, UK, March 2011 *Quantum black holes: the effect of a minimal length*
– Seminar talk at Johannes Gutenberg Universität, Mainz, Germany, May 2011, *Quantum black holes: the effect of a minimal length*
– Seminar talk at CERN, Geneva, Switzerland, August 2011, *Quantum gravity improved black holes*
– Seminar talk at Durham University, UK, October 2011, *Evaporation of quantum gravity improved black holes*

V. Ozvenchuk

– Workshop of the European Network TORIC, Heraklion, Crete, Greece, 5-9 September 2011, *Dynamical equilibration of strongly interacting "infinite" parton matter*
– Critical point and onset of deconfinment (CPOD-2011), Wuhan, China, 7-11 November 2011, *Dynamical equilibration of strongly interacting "infinite" parton matter*

Igor Pshenichnov

- International NanoBIC-Workshop on Structure Formation on the Nanometer Scale by Focused Energy Application, Rauischholzhausen, Germany 9-11 October 2011, *Monte Carlo simulations of ion-beam cancer therapy at macro- and microscopic scales*
- Dual year Russia-Spain conference on Particle Physics, Nuclear Physics and Astroparticle Physics, Barcelona, Spain, 8-11 November 2011, *Heavy-ion physics applied to cancer therapy: between basic science and medicine*

Philip Rau

- DPG Frühjahrstagung, Fachverband Hadronen und Kerne, Münster, Germany, Mar. 21 - 25 March 2011, *Quark Hadron Matter in a Unified Approach*
- Critical point and onset of deconfinment (CPOD-2011), Wuhan, China, 7-11 November 2011, *Hadronic Resonances in a Chiral Hadronic Model for the QCD Equation of State*
- International School for High-Energy Nuclear Collisions 2011, Wuhan, China, 31 October - 5 November 2011, *Hadron Resonances in a Chiral Hadronic Model*

Constantin Rothkopf

- IMCLeVeR focused workshop in Capo Caccia, Italy, 28-30 April 2011, *Structural credit assignment in hierarchical reinforcement learning*
- 22nd European Conference on Machine Learning (ECML), Athens, Greece, 5-9 September 2011, *Preference elicitation and inverse reinforcement learning*
- Talk at the Hong Kong University for Science and Technology, 14 September 2011, *Visuomotor behavior in naturalistic task: from receptive fields to value functions*

Chihiro Sasaki

- XXVIII Max Born Symposium 2011 “Three Days on Quarkyonic Island”, Wroclaw, Poland, 19-21 May 2011, *Conformal Anomaly, Chiral Symmetry Breaking and Baryons in Hot and Dense Matter* (invited talk)
- 7th International Workshop on Critical Point and Onset of Deconfinement, Wuhan, China, 7-11 November 2011, *Suppression of the Repulsive Force in Nuclear Interactions near the Chiral Phase Transition*
- Seminar talk, TU Darmstadt, Darmstadt, Germany, 18 March 2011, *Problems and Challenges in Hadron Physics – Toward an Understanding of Fundamental Issues based on QCD*,
- Seminar talk, Hanyang University, Korea, 31 March 2011, *Role of the dilaton and the repulsive force in nuclear interactions near chiral symmetry restoration*

Stefan Schramm

- First Caribbean Symposium on Cosmology, Gravitation, Nuclear and Astroparticle Physics STARS2011, Havana, Cuba, 1-4 May 2011, *Dense Matter and Neutron Stars in Parity Doublet Models*
- 2nd International Symposium on Strong Electromagnetic Fields and Neutron Stars SMFNS2011, Varadero, Cuba, 5-7 May 2011, *Nuclear Matter and Neutron Stars in a Quark-Hadron Model*
- XXVIII Max Born Symposium “Three Days on Quarkyonic Island”, Wroclaw, Poland, 19-21 May 2011, *Hot and Dense Matter in Quark-Hadron Models*
- Intl. Conference on Strangeness in Quark Matter SQM2011, Krakow, Poland, 18-24 September 2011, *Hybrid Stars - Properties and Stability*
- International Conference on Exciting Physics, Makutsi, South Africa, 13-20 November 2011, *Structure and Cooling of Neutron and Hybrid Stars*

Wolf Singer

- Grand Challenges in Neural Computation II: Synthetic Cognition and Neuromimetic Processes, Center for Nonlinear Studies, Santa Fe, 21-24 Feb. 2011, *Dynamic coordination of functional networks in the cortex*
- COSYNE 11 Workshop at Computational and Systems Neuroscience, Snowbird, Utah, 28 Feb. - 1 March 2011, *The role of oscillatory phenomena in sensory processing*
- 9th Meeting of the German Neuroscience Society, Göttingen, 23-26 March 2011, *Die Suche nach dem neuronalen Code*
- BioVision – The World Life Sciences Forum, Lyon, 27-29 March 2011, *Dynamic coordination of distributed cortical processes*
- Nobel Symposium "Mind, Machines and Molecules", Stockholm, 25-28 May 2011, *Dynamic coordination of distributed processing in the brain*
- FENS-IBRO Summer School "Development and plasticity of cortical representation", Bertinoro, Italy, 5-10 June 2011, *Distributed representation in the cerebral cortex and the binding problem*
- Höllerer Lecture, TU Berlin, 16 June 2011, *Konflikte zwischen Intuition und neurobiologischer Evidenz*
- Kongress Neurobiologie der Psychotherapie – Perspektiven und systemtherapeutische Innovationen, Salzburg, Austria, 1-3 July 2011, *Schizophrenie – eine Störung der dynamischen Koordination kortikaler Funktionen*
- International Symposium "The Legacy of Sir John C. Eccles", Düsseldorf, 10-11 Sept. 2011, *Synchronized oscillations: A basic mechanism for dynamic coordination of cortical functions*
- XXII. Deutscher Kongress für Philosophie, Munich, 11-15 Sept. 2011, *Neuronale und bewusste Prozesse – Eine schwierige Beziehung*
- Forschungskonferenz Koevolution, FAME, Goethe-University Frankfurt am Main 14.-16. September 2011, *Mehr vom Gleichen macht den großen Unterschied*
- EMBL Heidelberg Forum, Heidelberg, 22. Sept. 2011, *Conflicts between intuition and neurobiological evidence*
- MPS-UT Joint Symposium Neuroscience, Tokyo, Japan, 28-29 Oct. 2011, *Dynamic coordination of functional networks in the cerebral cortex: mechanisms, development and psychiatric diseases*
- International Opening Symposium "Multi-Site Communication in the Brain", Hamburg, 2-3 Dec. 2011, *Dynamic coordination of distributed cortical processes*

Andrey Solov'yov

- First Nano-IBCT Conference "Radiation damage of biomolecular systems: Nano-scale insights into Ion Beam Cancer Therapy", Caen, France, 2-6 October 2011, *COST Action MP1002/ NANO-IBCT: Nanoscale Insights into Ion-Beam Cancer Therapy*
- First Nano-IBCT Conference "Radiation damage of biomolecular systems: Nano-scale insights into Ion Beam Cancer Therapy", Caen, France, 2-6 October 2011, *Multiscale Approach to Radiation Damage by Ions*
- FIAS-Extreme Matter Institute(EMMI) Day, Frankfurt, January 2011, *Multiscale Approach to the Physics of Ion Beam Cancer Therapy*
- International Symposium on Size Selected Clusters (S3C), Davos, Switzerland, 20-25 March 2011, *The Multiscale Physics of Nanostructures Design*,
- General Assembly of Virtual Institute of Nano Films Ancona, Italy, April 2011, *A Real Program for the Virtual Institute: a New Period of the VINF Development*

- COST MPNS 5th Annual Progress Conference (APC), Tartu, Estonia, September 2011, *Initial Steps on the Implementation of the COST Action Nano-IBCT*,
- Conference ”Electron Driven Processes at Molecular Level”, Prague, Czech Republic, 18-21 October 2011, *Molecular Level Assessment of Biodamage: Multiscale Approach*
- International Symposium on Exciting physics, Makutsi, South Africa, 13-18 November 2011, *Crystalline Undulator Based GAMMA-Laser: Current Status and Perspectives*
- *Assessment of Cluster Damage of DNA Irradiated with Ions*. A Talk at The Fifth International Symposium ”Atomic Cluster Collisions ISACC 2011” (20-25 July, 2011, Berlin, Germany).

Jan Steinheimer

- Critical point and onset of deconfinment (CPOD-2011), Wuhan, China, 7-11 November 2011, *The hadronic SU(3) parity doublet model for dense matter, its extension to quarks and the strange equation of state*
- International Conference Strangeness in Quark Matter (SQM11), Cracow, Poland, 18-24 September 2011, *From FAIR to RHIC, hyper clusters and the strange EoS*

Horst Stöcker

- Public evening talk, Deutsche Physikalische Gesellschaft, Berlin, 1 March 2011, *Kosmische Materie im Labor - FAIR*
- 1. Oberurseler Werte- und Wirtschaftskongress “Wissensbasierte Ökonomie”, Oberursel, 20 May 2011, *FAIR - Ein neuer Superbeschleuniger in Darmstadt*
- International Symposium on Subnuclear Physics: Past, Present and Future, Pontifical Academy of Sciences, Vatican, 30 Oct. - 2 Nov. 2011, *From Antideuterons to Antimatter-Clusters and Hyperclusters*,
- International Conference on Exciting Physics, Makutsi, South Africa, 13-20 November 2011, *The future of GSI and FAIR*
- Hessisches Transferforum, IHK Fankfurt, 5 Dec. 2011, *Das Projekt FAIR als Beispiel für einen gelungenen Transfer mit internationalem Erfolg*

Giorgio Torrieri

- RIKEN-BNL workshop on Initial State Fluctuations and Final-State Particle Correlations, BNL, New York, 2-4 February 2011: *Mach cones from fluctuations in initial conditions*
- XXVIII Max Born Symposium 2011 “Three Days on Quarkyonic Island”, Wroclaw, Poland, 19-21 May 2011: *The phase diagram in* T-μ-N_c *space*
- Strangeness in Quark Matter (SQM2011), Krakow, Poland, 18-24 September 2011: *Theoretical summary talk*
- Colloquium, Wayne State University, Detroit, 25 January 2011
- Colloquium, UNESP Instituto de Fisica Teorica, Sao Paulo, Brazil, 22 February 2011
- Theoretical Physics seminar, Brookhaven National Laboratory (BNL), Upton, NY, 30 June 2011
- Theoretical Physics seminar, Massachusetts Institute of Technology (MIT), Boston, Massachussetts, 31 October 2011
- Theoretical Physics seminar, City College of New York, NY, 11 November 2011

Alexander Yakubovich

- First Nano-IBCT Conference ”Radiation damage of biomolecular systems: Nano-scale insights into Ion Beam Cancer Therapy”, Caen, France, 2-6 October 2011, *Nucleosome Thermo-Mechanical Damage Caused by Ion Irradiation*.

– 5th Conference on Elementary Processes in Atomic Systems Belgrade, Serbia, 21-25 June 2011, *Thermo-Mechanical Impact on Biomolecules Induced by Heavy Ions*
– International Symposium on Exciting physics, Makutsi, South Africa, 13-18 November 2011, *Theory of Phase Transitions in Polypeptides and Proteins*
– Conference ”Electron Driven Processes at Molecular Level”, Prague, Czech Republic, 18-21 October 2011, *Electron Relaxation-Induced Thermo-Mechanical Effects in Biodamage: Molecular Dynamics Simulations*

FIAS conference abstracts and posters 2011

Computational and Systems Neuroscience (COSYNE2011)

24-27 Feb. 2010, Salt Lake City, Utah, USA

- J. Bornschein, M. Henniges, G. Puertas, J. Lücke, *Sparse codes of V1 simple cells and the emergence of globular receptive fields – a comparative study*
- C. Keck, C. Savin, J. Lücke, *Input normalization and synaptic scaling - two sides of the same coin?*
- Daniel Krieg, Jochen Triesch, *STDP explained? Connecting function and biophysics*, Poster I-52
- Daniela Pamplona, Jochen Triesch, Constantin A Rothkopf, *Predicting Ganglion Cells Variability*, Poster III-75
- Constantin A. Rothkopf, Paul Schrater, *Coupling perception and action using probabilistic control*, Poster II-13
- P. Schrater, C. A. Rothkopf, M. Siegel, C. Kallie, *Learning cue integration via control: I perceive because I control*, Poster II-48
- Quan Wang, Constantin A Rothkopf, Jochen Triesch, *Unifying procedural memory consolidation and structure learning in motor control*, Poster II-25

American Physical Society April Meeting

30 April - 3 May 2011, Anaheim, California

- Sean Gavin and George Moschelli, *Glasma and the Ridge at LHC*, http://meetings.aps.org/Meeting/APR11/Event/145722
- B. Betz, G. Torrieri, M. Gyulassy, *Higher Harmonic Jet Tomography as a Probe of Fluctuating Initial Condition Geometries in A+A*, Abstract ID: BAPS.2011.APR.E10.2

First Caribbean Symposium on Nuclear and Astroparticle Physics STARS2011

1-4 May 2011, La Habana, Cuba

- M. Sprenger, P. Nicolini and M. Bleicher, *Neutrino oscillations as a novel probe for a minimal length*

CompStar 2011 School and Workshop on Gravitational Waves and Electromagnetic Radiation from Compact Stars

3-12 May 2011, Catania, Italy

- Xu-Guang Huang, *Anisotropic bulk viscosities and r-mode of magnetized quark star*, poster

11th annual meeting of the Vision Science Society

6-11 May 2011, Naples, Florida, USA

- B. Sullivan, C. A. Rothkopf, M. Hayhoe, D. Ballard, *Task-dependent gaze priorities in driving*

2nd International Conference on Ultra-Relativistic Nucleus-Nucleus Collisions – Quark Matter 2011

23-28 May 2011, Annecy, France

- J. J. Bjerrum-Bohr, The dynamics of quark droplets, poster
- Xu-Guang Huang, *Viscous Relaxation Times in Causal Dissipative Relativistic Hydrodynamics*, poster
- V. Konchakovski, E.L. Bratkovskaya, W. Cassing, V.D. Toneev, V. Voronyuk, *Elliptic Flow from the Parton-Hadron-String-Dynamics*, poster
- O. Linnyk, E.L.Bratkovskaya, W.Cassing *Dilepton production in heavy-ion collisions within the parton hadron string dynamics (PHSD) transport approach*, poster

- V. A. Ozvenchuk, O. Linnyk, E.L. Bratkovskaya, M. Gorenstein, W. Cassing, *Dynamical equilibration of the infinite strongly interacting parton matter*, poster
- C. Sasaki, *Suppression of the repulsive force in nuclear interactions near the chiral phase transition*, poster
- M. Sprenger, P.Nicolini, M. Bleicher, *Neutrino oscillations as a novel probe for a minimal length*, poster
- G. Torrieri, poster

14 European Congress of Clinical Neurophysiology and 4 International Conference on Transcranial Magnetic and Direct Current Stimulation (ECCN 2011)

21-25 June 2011, Rome, Italy

- L. Lonini, L. Dipietro, L. Zollo, E. Guglielmelli, H. I. Krebs, *A computational model of the effects of training schedules in neurorehabilitation*, Clinical Neurophysiology 122 (2011) S177

International Conference ”Advanced Carbon Nanostructures (ACN 2011)

4-8 July 2011, St. Petersburg, Russia

- R.G. Polozkov, A.V. Verkhovtsev, V.K. Ivanov, A.V. Korol, A.V. Solov’yov, *Oscillation phenomenon in photoionization cross section of* $Ar@C_{60}$, Book of Abstracts, p. 287
- A.V. Verkhovtsev, R.G. Polozkov, V.K. Ivanov, A.V. Korol, A.V. Solov’yov, *Self-Consistent Hartree-Fock Approach to Electronic Structure of Endohedral Fullerenes*, Book of Abstracts, p. 311

International Conference on the Physics of Neutron Stars

11-15 July 2011, Saint Petersburg, Russia

- A. Brillante, I. Mishustin, J. Schaffner-Bielich, S. Schramm, *Gravitational collapse to third family compact stars*, Book of Abstracts p. 20

Fifth International Symposium on Atomic Cluster Collisions (ISACC)

20-25 July 2011, Berlin

- V. K. Ivanov, R. G. Polozkov, A. V. Verkhovtsev, A. V. Solov’yov, A. V. Korol, *Photoionization Process with Negative Ions of Atomic Clusters*, Book of Abstracts, p. 44
- A. V. Korol, A. V. Solov’yov, *Auger Processes in Endohedral Atoms: the Role of Non-Central Position of the Atom*, Book of Abstracts, p. 20
- A. Kostyuk, A. V. Korol, A. V. Solov’yov, Walter Greiner, *Crystalline Undulator and Crystalline Undulator Based Gamma Laser: Current Status and Perspectives*, Book of Abstracts, p. 48
- E. Surdutovich, A.V. Solov’yov, *Assessment of Cluster Damage of DNA Irradiated with Ions*, The Fifth International Symposium ”Atomic Cluster Collisions ISACC 2011” Book of Abstracts, p. 40
- M. Nakamura, A. Yakubovich, A.V. Solov’yov, *Stability of Multiply Charged Rare Gas Clusters*, Poster, Book of Abstracts, p. 68
- A.V. Verkhovtsev, R.G. Polozkov, V.K. Ivanov, A.V. Korol, A.V. Solov’yov, *Self-Consistent Description of Endohedral Fullerenes Electronic Structure within the Hartree-Fock and the Local Density Approximations*, Poster, Book of Abstracts, p. 76
- I.A. Solov’yov, A.V. Yakubovich, P.V. Nikolaev, Ilya Volkovetz, V.V. Dick, A.V. Solov’yov, *MBN-Explorer - a Flexible Program for Simulating Molecular and Nanostructured Materials*, Poster, Book of Abstracts, p. 93

Twentieth Annual Computational Neuroscience Meeting: CNS*2011

23-28 July 2011, Stockholm, Sweden

- Juhan Aru, Jaan Aru, Michael Wibral, Viola Priessemann, Wolf Singer, Raul Vicente, *Analyzing possible pitfalls of cross-frequency analysis*, BMC Neuroscience 12 (Suppl. 1) (2011) p. 303
- Stefanos E. Folias and Danko Nikolic and Jonathan E. Rubin, *Synchronization hubs may arise from strong rhythmic inhibition during gamma oscillations in primary visual cortex*, BMC Neuroscience 12 (Suppl. 1) (2011) p. 277

European Conference on Visual Perception ECVP2011

28 Aug. - 1 Sept. 2011, Toulouse, France

- Lisa Scocchia, Matteo Valsecchi, Karl R. Gegenfurtner, Jochen Triesch, *Working memory contents influence binocular rivalry*, Perception 40, ECVP Abstract Suppl., p. 84

SPARC 2011 School and Workshop

5-10 Sept. 2011, Moscow, Russia

- T. Kühl et al., *X-Ray Laser Spectroscopy*, Book of Abstracts p. 45
- S. Fritzsche, A. Surzhykov, Th. Stöhlker *Relativistic dynamics of electrons and ions in strong Coulomb fields*, Book of Abstracts p. 86
- Filippo Fratini et al., *Polarization correlations in the two-photon decay of helium-like heavy ions*, Book of Abstracts p. 96

IX International Symposium Radiation from Relativistic Electrons in Periodic Structures, RREPS-11

12-16 September 2011, Egham, UK

- A. Kostyuk, A. V. Korol, A. V. Solov'yov, W. Greiner, *From Crystalline Undulator to Gamma Laser* Structures

Third International Workshop on Compound-Nuclear Reactions and Related Topics (CNR*11)

19-23 September 2011, Prague, Czech Republic

- Y. Malyshkin, I. Pshenichnov, I. Mishustin, W. Greiner, *Modeling spallation reactions in tungsten and uranium targets with the Geant4 toolkit*, poster

The First Nano-IBCT Conference "Radiation damage of biomolecular systems: Nano-scale insights into Ion Beam Cancer Therapy"

2-6 October 2011, Caen, France

- A.V. Solov'yov, *COST Action MP1002/ NANO-IBCT: Nanoscale Insights into Ion-Beam Cancer Therapy*, Book of Abstracts, p. 19
- A.V. Solov'yov, E. Surdutovich, A.V. Yakubovich, *Multiscale Approach to Radiation Damage by Ions*, Book of Abstracts, p. 36
- E. Surdutovich, A.V. Solov'yov, *Calculation of Clustered Damage of DNA Irradiated with Ions*
- A.V. Yakubovich, E. Surdutovich, A.V. Solov'yov, *Nucleosome Thermo-Mechanical Damage Caused by Ion Irradiation*, Book of Abstracts, p. 24

Bernstein Conference Computational Neuroscience BCCN2011

4-6 October 2011, Freiburg, Germany

Abstracts published in "Frontiers in Compuational Neuroscience"

- J. Bornschein, A. S. Sheikh, J. A. Shelton, J. Lücke, *The Maximal Causes of Binary Data*, Poster
- G. Exarchakis, M. Henniges, J. Lücke, *Discrete Symmetric Priors for Sparse Coding*, Poster
- Daniel Krieg, Jochen Triesch, *How metabolic constraints shape neuronal adaptation: A unifying objective function for synaptic plasticity*, Poster

- Daniela Pamplona, Jochen Triesch, Constantin A. Rothkopf, *Edge and image statistics across the visual field*, Poster
- Philip Sterne, Jochen Triesch, *Principled homeostatic mechanisms from mutual information maximization*, Poster
- Quan Wang, Constantin A. Rothkopf, Jochen Triesch, *Unifying procedural memory consolidation and structure learning in a recurrent network model of motor control*, Poster

Neuroscience 2011

12-16 November 2011, Washington, DC, USA

- W. Feng, R. Vicente, W. Singer, D. Nikolić, *Gamma synchronization and spike timing dependent plasticity in the cortex*, Poster 451.09
- F. Roux, H. Mohr, M. Wibral, W. Singer, P. J. Uhlhaas, *Development of neural oscillations and visuo-spatial working memory during adolescence*, Poster 93.10
- S. Sritharan, C. E. Han, A. Rotarska-Jagiela, W. Singer, R. Deichmann, K. Maurer, M. Kaiser, P. J. Uhlhaas, *Increased long-range connectivity in schizophrenia: A graph theoretical analysis of DTI data*, Poster 566.19
- P. Wang, B. Lima, W. Singer, N. Neuenschwander, D. Nikolić, *Beta/gamma oscillations increase neural complexity*, Poster 483.16

International Symposium on Exciting Physics

13-18 November 2011, Makutsi, South Africa

- E. Bratkovskaya, *The QGP phase in relativistic heavy-ion collisons*, Book of Abstracts p. 8
- R.A. Gherghescu, W. Greiner, D.N. Poenaru, *Pairing interaction in binary systems*, Book of Abstracts p. 11
- P.O. Hess, W. Greiner, G. Caspar, Th. Schnenbach, *Black holes or gray stars? That's the question: Pseudo-complex General Relativity*, Book of Abstracts p. 15
- A. Karpov, V. Zagrebaev, W. Greiner, *Decay properties and stability of heaviest elements*, Book of Abstracts p. 20
- A. Kostyuk, A.V. Korol, A.V. Solov'yov, W. Greiner, *Crystalline undulator based Gamma-laser: Current status and perspectives*, Book of Abstracts p. 35
- D.N. Poenaru, R.A. Gherghescu, W. Greiner, *Unexpected strong decay mode of superheavy nuclei*, Book of Abstracts p. 26
- J. Reinhardt, W. Greiner, *Supercritical QED and time-delayed heavy ion collisons*, Book of Abstracts p. 28
- S. Schramm, *Structure and cooling of neutron and hybrid stars*, Book of Abstracts p. 32
- I. Solov'yov, W. Greiner, K. Schulten, *Magnetoreception mechanisms in birds – Towards the discovery of the sixth sense*, Book of Abstracts p. 37
- R. Stock *Antinuclei produced in relativistic nucleus collisions: Results and expectations*, Book of Abstracts p. 39
- A.V. Yakubovich, *Theory of Phase Transitions in Polypeptides and Proteins*. Book of Abstracts p. 45

Advances in Neural Information Processing Systems 24 (NIPS 2011)

12-15 Dec. 2011, Granada, Spain

- J. A. Shelton and J. Bornschein and A.-S. Sheikh and P. Berkes and J. Lücke, *Select and Sample – A Model of Efficient Neural Inference and Learning*, Abstract W008

FIAS Publications 2011

In the following all publications from the year 2011 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. Journal publications

[1] K. Aamodt and others (ALICE collaboration), "Centrality Dependence of the Charged-Particle Multiplicity Density at Midrapidity in Pb-Pb Collisions at $\sqrt{s_{NN}}$=2.76 TeV," *Phys. Rev. Lett.* **106** (2011) 032301, `arXiv:1012.1657 [nucl-ex]`.

[2] K. Aamodt and others (ALICE collaboration), "Higher Harmonic Anisotropic Flow Measurements of Charged Particles in Pb-Pb Collisions at $\sqrt{s_{NN}}$=2.76 TeV," *Phys. Rev. Lett.* **107** (2011) 032301, `arXiv:1105.3865 [nucl-ex]`.

[3] K. Aamodt and others (ALICE collaboration), "Two-pion Bose-Einstein correlations in central Pb-Pb collisions at $\sqrt{s_{NN}} = 2.76$ TeV," *Phys. Lett. B* **696** (2011) 328–337, `arXiv:1012.4035 [nucl-ex]`.

[4] K. Aamodt and others (ALICE collaboration), "Femtoscopy of pp collisions at $\sqrt{s}$ = 0.9 and 7 TeV at the LHC with two-pion Bose-Einstein correlations," *Phys. Rev.* **84** (2011) 112004, `arXiv:1101.3665 [hep-ex]`.

[5] K. Aamodt and others (ALICE collaboration), "Production of pions, kaons and protons in pp collisions at $\sqrt{s} = 900$ GeV with ALICE at the LHC," *Eur. Phys. J.* **71** (2011) 1655, `arXiv:1101.4110 [hep-ex]`.

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[11] H. Agakishiev and others (STAR collaboration), "Observation of the antimatter helium-4 nucleus," *Nature* **475** (2011) 353–356, `arXiv:1103.3312 [nucl-ex]`.

[12] 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* (2011) . Online first.

[13] J. O. Andersen, L. E. Leganger, M. Strickland, and N. Su, "NNLO hard-thermal-loop thermodynamics for QCD," *Phys. Lett. B* **696** (2011) 468–472, `arXiv:1009.4644 [hep-ph]`.

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[15] J. O. Andersen, L. E. Leganger, M. Strickland, and N. Su, "The QCD trace anomaly," *Phys. Rev.* **D84** (2011) 087703, `arXiv:1106.0514 [hep-ph]`.

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C. Patents

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