FIAS Frankfurt Institute for Advanced Studies

Physics

Computer Science

Neuro-science

Life Science + Chemistry

FIAS

FIAS Scientific Report 2010

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Preface

In the year 2010 the Frankfurt Institute for Advanced Studies has successfully continued to follow its agenda to pursue theoretical research in the natural sciences. As stipulated in its charter, FIAS closely collaborates with extramural research institutions, like the Max Planck Institute for Brain Research in Frankfurt and the GSI Helmholtz Center for Heavy Ion Research, Darmstadt and with research groups at the science departments of Goethe University. The institute also engages in the training of young researchers and the education of doctoral students. This Annual Report documents how these goals have been pursued in the year 2010. Notable events in the scientific life of the Institute will be presented, e.g., teaching activities in the framework of the Frankfurt International Graduate School for Science (FIGSS), colloquium schedules, conferences organized by FIAS, and a full bibliography of publications by authors affiliated with FIAS. The main part of the Report consists of short one-page summaries describing the scientific progress reached in individual research projects in the year 2010.

As far as funding is concerned, FIAS has been able to attract further grants for research projects. In the field of neuroscience the Hertie Foundation has decided to grant an additional amount of 440.000 EUR over three years. FIAS will also benefit from the new LOEWE project NeFF (Neuronale Koordination Forschungs-schwerpunkt Frankfurt). The year 2010 has also seen the beginning of operations of the NanoBiC initiative ("Nano, Bio, Chemistry and Computing") financed by the Beilstein Institute, with FIAS participation. Also in 2010 the European Union has initiated the European Concerted Research Action "Nano-scale insights in ion beam cancer therapy" (Nano-IBCT) in which FIAS plays a leading role. In the field of nuclear and high-energy physics the cooperation with the GSI Helmholtz Center for Heavy Ion Research, with the Helmholtz International Center for FAIR (HIC for FAIR), and with the Extreme Matter Institute (EMMI) provides for a stable framework of collaboration and funding. Several new Fellows and Junior Fellows in this field have started their work at FIAS in the year 2010.

The standing of FIAS in the scientific community is demonstrated by the fact that many of its scientists have received attractive offers from other institutions. After the former Fellows Christian Holm and Robert Berger had been appointed to professorships at the universities of Stuttgart and Darmstadt, respectively, in the year 2010 it was FIAS Fellow Michael Meyer-Hermann's turn. He assumed a professorship at the Technical University of Braunschweig and simultaneously became head of the Department of Systems Immunology at the Helmholtz Center for Infection Research. Furthermore, his collaborator, Junior Fellow Marc Thilo Figge, was offered a professorship at the Leibniz Institute for Natural Product Research and Infection Biology associated to the University of Jena.

These appointments impressively bear witness to the quality of researchers and research at FIAS, but they also exacerbate a structural imbalance which had been recognized already earlier. While the disciplines of physics and neuroscience thrive at FIAS, receiving substantial funding and prevailing in terms of personnel and number of publications, the fields of biological and chemical sciences are not as well represented, particularly now, after many of the group leaders have left the institute. It is an ongoing concern of the leadership of FIAS to maintain a sufficiently broad diversity of research and an interdisciplinary spirit. Under discussion are both the establishment of new junior research groups and the appointment of senior scientists to leading positions. This can be realized together with Goethe University by making joint appointments to professorships at the Department of Biochemistry, Chemistry and Pharmacy and/or the Department of Life Science. FIAS is in the fortunate position that the member and former president of its Board of Trustees, Dr. Helmut Maucher, has pledged a substantial amount to finance such a new endowed professorship. Intense efforts are under way to put this into practice and thus to allow FIAS to continue with its ambitious plans of fostering top-level interdisciplinary research.

Research highlights 2010

Physics

The main focus of the nuclear and high-energy group at FIAS is concentrated on the investigation of elementary matter under extreme conditions of temperature, pressure, and density. This involves analytical studies and intensive numerical simulations of the properties of QCD-matter and of high-energy nuclear collisions. Progress has been achieved by the development of a conceptually novel model for the description of the Quark-Gluon Plasma (QGP) including dynamical hadronisation, i.e., the Parton-Hadron String Dynamics (PHSD) transport approach (E. Bratkovskaya and collaborators). This is a fully microscopic covariant transport model based on the dynamical quasiparticle model for partons (DQPM) and adapted to recent lattice-QCD results. PHSD has been applied to nuclear collisions from 20 to 160 A·GeV and it was found that even central collisions show a substantial 'corona' of non-partonic, i.e., hadronic or string-like matter. Details of strangeness and antibaryon production as well as dilepton production have been worked out, the latter allowing for the investigation of electromagnetic properties of the strongly interaction QGP.

Another project deals with the production of multi-hypernuclei in peripheral heavy-ion collisions (I. Mishustin, M. Bleicher). In a new mechanism Λ hyperons are produced in secondary reactions and captured by spectators, allowing the formation of multi-strange cold nuclear matter. A hybrid approach for the description of such processes has been developed, building on the Quark Gluon String Model (QGSM) or on Ultrarelativistic Quantum Molecular Dynamics (UrQMD). The production of double and even triple Λ-hypernuclei is predicted.

Dense baryonic matter also was explored using a chiral model for mesons and baryons (C. Sasaki) which consistently describes the ground state and the phase diagram of nuclear matter. A unified description of hadrons and quarks was developed (S. Schramm) which allows to study the QCD phase transition towards deconfinement and the restoration of chiral symmetry as well as the properties of groundstate nuclear matter and neutron stars in a single model.

A lattice study of net-baryon number fluctuations in 2+1 flavor QCD has been performed (Ch. Schmidt) using extensive GPU-based numerical calculations. Along the freeze-out curve, fluctuations were found to agree with recent measurements at RHIC and with the resonance gas model for energies below 20 AGeV.

In nuclear-structure physics, extreme neutron-rich nuclei at and outside the neutron drip line were investigated using Hartree-Fock-Bogolyubov studies (W. Greiner, S. Schramm). These nuclei can be produced with pulsed neutron beams. Furthermore, he question of long-living superheavy elements was studied. A novel production mechanism using low-yield nuclear explosions was proposed in which up to 60 neutrons may be absorbed by heavy nuclei.

Neuroscience

Research in the field of neuroscience at FIAS spans a wide range of topics, e.g. computational neuroscience, the modeling of information processing in the brain, the study of plasticity in cortical networks related to various types of learning and habituation, and fundamental and applied vision research, which is the main subject of the Bernstein Focus Neurotechnology.

As an example, in a study published in the Journal of Machine Learning Research (J. Lücke) a novel strategy for unsupervised learning to recognize visual images or acoustic data was developed. Using state-of-the-art probabilistic approaches a meta-algorithm (Expectation Truncation) for generative modeling was devised that reduces the calculational complexity from exponential to approximately linear scaling, thus making the problem solvable in practice. The algorithm takes the form of a variational Bayesian approach.

A study by G. Pipa et al. has investigated the flow of information between different parts of the brain. This is important because a large part of the brain's activity is internally generated and, hence, quantifying stimulus-response relationships alone does not fully describe brain dynamics. In the study the transfer entropy (TE) has been identified as a measure of effective connectivity based on information theory. TE does not require a model of the interaction and is inherently non-linear. The method has been applied to test for effective

connectivity using electrophysiological data based on simulations and magnetoencephalography (MEG) recordings in a simple motor task.

The role of cortical gamma oscillations has been studied by T. Burwick who concentrated on finding their possible functional relevance by using appropriate dynamical system models of the oscillatory processes. Based on recent experimental work it was shown that the oscillatory state may realize a form of selective inhibition – resulting in the recognition processes – that could not be achieved without including the temporal structure as it arises with the gamma oscillations.

In collaboration with the Department of Developmental Psychology at Goethe University the group of J. Triesch has developed a new method to study the cognitive abilities of infants. An eye-tracker is used to analyze the direction of gaze of the infant and the outcome is used to influence the scenes shown on a computer display. In this way 6-month old children obtain the ability to manipulate their environment and learn to anticipate the outcomes of their actions. This opens the possibility to address a wide variety of classic questions including habituation, joint attention, and object conception in a new way.

Meso-Bio-Nano-Science

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

Recently the group has increasingly focused its attention on the molecular-level assessment of radiation biodamage, in particular in connection with the method of heavy-ion tumour therapy. In 2010 the MBN group initiated the European COST Action 'Nano-scale insights into ion beam cancer therapy'. A. Solov'yov was elected to chair the Management Committee of the Action.

The MBN group has suggested a multi-scale approach to the scenario of irradiation of biological targets with ions aiming to understand the physics of radiation biodamage. This was used to calculate probability of DNA damage as a result of the irradiation with energetic ions, up to several hundreds of MeV/u. The approach covers different time and spatial scales, defined by different physical processes such as the ion stopping, the propagation of secondary electrons and radicals, the interactions of secondaries with the DNA and proteins, thermo-mechanical effects etc. The probabilities of single and double strand breaks were calculated.

In 2010 important advances of the molecular level assessments of radiation damage were made. The energy distributions of secondary electrons produced by energetic carbon ions incident on liquid water in the energy range used in hadron therapy were calculated and parametrizations for the differential cross sections of ionization were developed. Calculations of the complex DNA damage and the effects of thermal spikes on biomolecules in the context of the multiscale approach were worked out, allowing to quantify the occurrence of complex clustered damage to DNA. Furthermore, the shock wave produced by an energetic ion in liquid water was investigated. The pressure in the overheated water increases by several orders of magnitude and drives a cylindrical shock wave on the nanometer scale, possibly providing an important mechanism for causing DNA damage.

Another achievement of the MBN group ist the development of a radiation source based on the principle of a crystalline undulator. The newest scheme for a hard-X-ray and gamma laser is based on the combination of a conventional undulator with an undulator utilizing a periodically bent crystal. A patent for the new source of coherent radiation has been submitted.

Biology

The systems immunology group at FIAS (M. Figge, M. Meyer-Hermann, now at Braunschweig) in 2010 has reached a major new insight concerning the relation between adaptive and innate immunity.

In germinal centers where the affinity maturation of antibodies takes place, antigen-activated B cells undergo proliferation, somatic hypermutation, and selection with regard to the antibody affinity. Follicular dendritic cells (FDCs) are key players in driving these events of adaptive immunity via direct interaction with germinal

center B cells. A series of in vivo experiments provided evidence that FDCs express and upregulate Toll-like-receptor (TLR) 4 in situ during germinal center reactions, confirm that FDC maturation is driven by TLR4, and associated the role of FDC-expressed TLR4 with quantitative and qualitative affects of germinal center biology. In an iterative process of in vivo experiments and in silico modeling it could be demonstrated that TLR4 signaling significantly modulates FDC activation and is required for a proper functioning of the germinal center reaction. This places the common host pattern recognition receptor TLR4 of innate immunity at the heart of adaptive humoral immunity. Thus, innate and adaptive immunity are shown to be closely interwoven.

Computer Science

Computer science has strong tries to all other FIAS research areas. In physics and life sciences all flavors of high-performance computing are needed for the analysis of experimental data and for carrying out theoretical modeling. This is perfectly illustrated by the needs for computing power in high-energy physics, e.g. by the experiments carried out at CERN-LHC. FIAS scientists are involved in the ALICE experiment at LHC which measures up to a thousand collision events per second, each requiring the reconstruction of several thousand particle tracks. An essential part of the ALICE data analysis is the High Level Trigger (HLT) which was conceived and constructed by the group of FIAS Fellow V. Lindenstruth. The planned experiments at the future accelerator facility FAIR will put even higher demands on computing power.
The year 2010 has seen a major development at Frankfurt concerning high-performance computing. The LOEWE-CSC supercomputer, inaugurated in November 2010, combines cost efficiency with energy efficiency and environmental compatibility. It is ranked 22th place in the list of the world's fastest computers and 8th place in the list of most energy efficient computers. It is the fastest computer operated by a European university and needs only about one third of the investment costs and operational costs compared to machines of similar performance. Achieving maximum utilization of available computer capacities requires the collaboration of computer scientists and scientists from other disciplines. Therefore "SimLabs" for the development of modern algorithms have been set up, focusing, inter alia, on neuroscience, physics event reconstruction, quantum chromodynamics etc.

1. Research Centers

Helmholtz International Center for FAIR (HIC for FAIR)

by Marcus Bleicher

In the year 2010 we have successfully established the Helmholtz-LOEWE research center Helmholtz International Center for FAIR (HIC for FAIR) at the Universities of Frankfurt, Darmstadt, Gießen and at the Frankfurt Institute for Advanced Studies together with the Helmholtz Association and the GSI Helmholtz Center for Heavy Ion Research. At FIAS, the activities are led by Profs. M. Bleicher and V. Lindenstruth as Scientific Council members. HIC for FAIR has built up and secured an internationally leading role of FIAS and the Hessian universities at the new and worldwide unique "Facility for Anti-Proton and Ion Research" (FAIR) close to the GSI Helmholtzzentrum für Schwerionenforschung in Darmstadt. FAIR has now entered the construction phase with the signing of the FAIR convention in Wiesbaden on October 4th, 2010.

HIC for FAIR explores new theoretical concepts and numerical methods and develops state-of-the-art accelerator and detector designs for FAIR. It plays a leading role in the construction of FAIR, and in the planning, analysis and interpretation of FAIR experiments with strong involvement of the local universities. The main strategic goal is to explore the multifaceted manifestations of Quantum Chromodynamics (QCD), modern accelerator physics and applied sciences by fully exploiting the research opportunities of FAIR. Of central importance is the creation and investigation of exotic forms and phases of elementary matter and of unknown particles in experiments with energetic protons, anti-protons, and heavy ions. A vigorous program in plasma physics and medical applications with light and heavy ions is also established.

As a "Think Tank", HIC for FAIR provides a comprehensive and widely visible forum for the international scientific community and for the next generation of young scientists. This is underlined by the highly visible guest scientist and conference program established by HIC for FAIR.

HIC for FAIR focuses and strengthens the expertise of the participating institutions, the Johann Wolfgang Goethe-Universität Frankfurt, the Technische Universität Darmstadt and the Justus-Liebig- Universität Gießen, and the Frankfurt Institute for Advanced Studies (FIAS). It utilizes and strengthens the excellent existing infrastructure and the new initiatives currently being set up (high-performance computing clusters).

The center has extended its scientific reach to all areas of the FAIR-project by including particular atomic physics, plasma physics and applied science activities at FAIR (APPA). The center has incorporated the Universities of Kassel, and Marburg as well as the Universities of Applied Sciences in Darmstadt and Gießen-Friedberg as new associated partners in Hesse for these activities.
HIC for FAIR provides high-level training of outstanding junior scientists and promotes their careers in a unique interdisciplinary environment among world experts in experimental and theoretical subatomic physics and computer science. Within the Helmholtz Graduate Schools HGS-HIRe and H-QM, more than 190 students are currently enrolled or have already graduated in a structured doctoral training program.

HIC for FAIR has successfully appointed 14 faculty members on the W3 and W2 level (6 at GU Frankfurt, 4 at TU Darmstadt, 2 at FIAS and 2 at JLU Gießen). 12 are currently in the appointment process. As a result of our active targeting initiative of female scientists HIC for FAIR is employing 2 female scientists in permanent positions, one female scientist as a FIAS-Research Fellow on a longer term basis, and one female

scientist as a Helmholtz Young Investigator (HYI).

To underline the strategic importance of HIC for FAIR, the Helmholtz Association has committed additional financial support of more than 48 million Euro over a period of 12 years via strategic bilateral partnerships, and 15 million Euro by establishing 7 permanent professorships at the partner institutions. It is envisaged that HIC for FAIR will continue with sustained financial support from the Helmholtz Association.

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 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 and has particularly close ties. The Scientific Director of EMMI, Prof. Peter Braun-Munzinger, is also a Senior Fellow of FIAS. The four EMMI Fellow positions (leaders of EMMI Fellow Groups) are now all filled. The EMMI Fellows are also Fellows at FIAS. In 2010, more than 350 scientist contributed to the activities in EMMI, among them more than 150 doctoral students and more than 100 postdocs. The structural graduate education of doctoral students within EMMI is organized in close collaboration with the sourrounding graduate schools, for example with the Helmholtz Graduate School for Hadron and Ion Research (HGS-HIRe) and the Heidelberg Graduate School of Fundamental Physics (HGSFP). Two Memoranda of Understanding aiming at close scientific collaboration have been signed in 2010 with the Polish Academy of Arts and Sciences in Krakow, and with the Helmholtz-Institut Jena.

In 2010, EMMI members have published more than 300 papers in refereed journals, and more than 100 contributions to conference proceedings. EMMI runs an active workshop program. 12 EMMI workshops with strong international participation were organized in 2010, many of them focussing on interdisciplinary aspects. In addition, EMMI runs a visiting professor program that allows its partner institutions to invite renowned expert for extended periods. These and further EMMI activities are listed at `www.gsi.de/emmi`

Neuroscience Collaborations

1. Bernstein-Focus Neurotechnology Frankfurt

Collaborators:

Jörg Bornschein, Pramod Chandrashekhariah, Zhenwen Dai, Marc Henniges, Alexander Heusel, Michael Hoffer, Rudra Hota, Jenia Jitsev, Manu Punnen John, Christian Keck, Markus Knodel, Daniel Krieg, Jörg Lücke, Daniela Pamplona, Gervasio Puertas, Wang Quan, Constantin Rothkopf, Jacquelyn Shelton, Abdul Saboor Sheikh, Jochen Triesch, Christoph von der Malsburg, Thomas Weisswange, Junmei Zhu

This project (which is coordinated by C. v.d. Malsburg, with the assistance of J. Triesch and R. Mester (Goethe-University) has the aim of building a computer-based vision system. There are 15 sub-projects, comprising participants at FIAS, Goethe-University, Honda Research Labs Europe (Offenbach), Max-Planck-Institute for Brian Research, and Technical University Darmstadt. To realize the project, a number of fundamental difficulties have to be solved, among them the scaling-up of previous model systems to realistic size, the absorption of great masses of visual structure from natural environments as well as its storage and quick recovery, sub-system integration and massively parallel computer implementation. So far, the project has built up a full complement of co-workers as far as was possible before filling the three professorship positions (see below), has acquired computing and data collection hardware, has achieved a number of supporting problem solutions and has constructed a "seed system", a simple version of a vision engine. Besides specific vision goals (recognition and reconstruction of visual input) the project aims at establishing a model of brain function and at serving as pilot application for a novel kind of information technology based on self-organization, learning and massively parallel computation. The project will finance and fill three professor positions, two (W3, W1) at Goethe-Uni, one (W2) at FIAS. All three positions are ready to be filled in 2011.

Related publications in 2010:

1) M.M. Hayhoe and C.A. Rothkopf, *Eye movements in natural behaviour*, in: Encyclopedia of Cognitive Science. Editor: Lynn Nadel, Wiley (2010)

2) M.M. Hayhoe. and C.A. Rothkopf, *Vision in the natural world*, in: Wiley Interdisciplinary Reviews: Cognitive Science, Wiley (2010)

3) M. Henniges, G. Puertas, J. Bornschein, and J. Lücke, *Binary Sparse Coding*, Proc. LVA/ICA 2010, LNCS 6365, 450-457

4) J. Jitsev and C. von der Malsburg, *Off-line memory reprocessing following on-line unsupervised learning strongly improves recognition performance in a hierarchical visual memory*, Proc. International Joint Conference on Neural Networks (IJCNN), Special Session on Organci Computing, IEEE World Congress on Computational Intelligence (WCCI). Barcelona, Spain, July 2010.

5) C. Keck and J. Lücke, *Learning of Lateral Connections for Representational Invariant Recognition*, Proc. ICANN 2010, LNVS 6354, 21-30

6) J. Lücke and J. Eggert, *Expectation Truncation and the Benefits of Preselection in Training Generative Models*, Journal of Machine Learning Research 11:2855-2900, 2010

7) W.A. Phillips and C. von der Malsburg, *Dynamic coordination in Brain and Mind*, Dynamic Coordination in the brain: From neurons to Mind. Edited by C. von der Malsburg, W.A. Philips and W. Singer. Strüngmann Forum Report Vol. 5, Cambridge, MA: MIT Press, 2010

8) G. Puertas, J. Bornschein, and J. Lücke, *The Maximal Causes of Natural Scenes are Edge Filters*, Advances in Neural Information Processing Systems 23, 1939-1947, 2010

9) U. Ramacher and C. von der Malsburg (Eds.), *On the Construction of Artificial Brains*, Springer-Verlag Berlin Heidelberg 2010

10) C. Rothkopf and D. Ballard, *Credit assignment in multiple goal embodied visuomotor behavior*, Frontiers in Psychology, Special Topic: 'Embodied and grounded cognition', (2010)

11) C. Rothkopf, T. Weisswange, and J. Triesch, *Computational modeling of multisensory object perception*, in: Multisensory Object Perception in the Primate Brain, Naumer, MJ. And J. Kaiser (Ed.). Springer New York 2010

12) J. Triesch, C.A. Rothkopf, and T. Weisswange, *Coordination in Sensory Integration*, Dynamic Coordination in the brain: From neurons to Mind. Edited by C. von der Malsburg, W.A. Philips and W. Singer. Strüngmann Forum Report Vol. 5, Cambridge, MA: MIT Press, 2010

13) Y. Sato, J. Jitsev, T. Burwick, and C. von der Malsburg, *Dynamic Link Models for Global Decision Making with Binding-by-Synchrony*, in: IEEE World Congress on Nature and Biologically Inspired Computing (NaBiC), 201-208, Kitakyushu, Japan, 2010, doi: 10.1109/NABIC.2010.5716291, URL: http://ieeexplore.ieee.org/xpls/abs_all.jsp?arnumber=5716291

14) Y. Sato, J. Jitsev, and C. von der Malsburg, *Visual object detection by specifying the scale and rotation transformations*, in Proceedings of the 17th international conference on Neural information processing: models and applications - Volume Part II (ICONIP'10), Kok Wai Wong, B. Sumudu U. Mendis, and Abdesselam Bouzerdoum (Eds.), Vol. Part II. Springer-Verlag, Berlin, Heidelberg, 616-624

15) C. von der Malsburg, *Coordination: What is it and why do we need it?*, Dynamic Coordination in the brain: From neurons to Mind. Edited by C. von der Malsburg, W.A. Philips and W. Singer. Strüngmann Forum Report Vol. 5, Cambridge, MA: MIT Press, 2010

16) J. Zhu, *A multi-factor winner-take-all dynamics*, Neural Compuation. 2010. Accepted

Talks and Poster Presentations

1) O. Aladini, C.A. Rothkopf, and J. Triesch, *Grasping image statistics*, Poster presentation at Computational and Systems Neuroscience 2010 (COSYNE), Salt Lake City, USA, February 2010

2) C. Savin and J. Triesch, *Structural plasticity improves stimulus encoding in a working memory model*, Poster presentation at Computational and Systems Neuroscience 2010 (COSYNE), Salt Lake City, USA, February 2010.

3) P. Schrater and C.A. Rothkopf, *Discounting as task termination, and its implications*, Poster presentation at Computational and Systems Neuroscience 2010 (COSYNE), Salt Lake City, USA, February 2010.

4) T. Weisswange, C.A. Rothkopf, T. Rodemann, and J. Triesch, *Model averaging as a developmental outcome of reinforcement learning*, Poster presentation at Computational and Systems Neuroscience 2010 (COSYNE), Salt Lake City, USA, February 2010.

5) Q. Wang and J. Triesch, *A Model of the Familiarity-to-Novelty-Shift in Infant Habituation*, Poster presentation at XVIIth Biennial International Conference on Infant Studies Baltimore, Maryland, USA, March 2010.

6) B. Sullivan, C.A. Rothkopf, M.M. Hayhoe, and D. Ballard, *Modeling gaze priorities in driving*, Poster presentation at 10th annual meeting of the Vision Science Society, Naples, Florida, USA, May 7-12 2010.

7) C.A. Rothkopf, *Visumotor behavior in naturalistic virtual environments: from receptive fields to value functions*, Talk at Gordon Conference on Sensory Coding and the Natural Environment, Bates College, Lewiston, ME, USA, July 25-30 2010.

8) J. Bornschein, M. Henniges, G. Puertas, J. Eggert, and J. Lücke, *Binary Hidden Variables and Sparse Sensory Coding*, Poster presentation at Bernstein Conference on Computational Neuroscience (BCCN) 2010, Berlin Institute of Technology, Berlin, 27.09.2010.

9) Z. Dai and J. Lücke, *A Probabilistic Generative Approach To Invariant Visual Inference and Learning*, Poster presentation at Bernstein Conference on Computational Neuroscience (BCCN) 2010, Berlin Institute of Technology, Berlin, 27.09.2010

10) J. Jitsev and C. von der Malsburg, *Self-generated off-line reprocessing in a recurrent hierarchical memory network and its functional consequences*, Poster presentation at Bernstein Conference on Computational Neuroscience (BCCN) 2010, Berlin Institute of Technology, Berlin, 27.09.2010

11) D. Krieg, A. Perianez, and J. Triesch, *An objective function for STDP: increasing the separability in self-organized recurrent neural networks*, Oral presentation at Bernstein Conference on Computational Neuroscience (BCCN) 2010, Berlin Institute of Technology, Berlin, 27.09.2010.

12) H. Toutounji, C.A. Rothkopf, and J. Triesch, *Learning hierarchical controllers through reinforcement learning*, Poster presentation at Bernstein Conference on Computational Neuroscience (BCCN) 2010, Berlin Institute of Technology, Berlin, 27.09.2010.

13) J. Zhu, U. Bergmann, and C. von der Malsburg, *Self-organization of steerable topographic mappings as basis for translation invariance*, Talk or poster presentation at International Conference on Artificial Neural Networks (ICANN 2010), Part II, LNCS 6353, Thessaloniki, Greece, September 2010.

14) J. Bornschein, Z. Dai, and J. Lücke, *Approximate EM Learning on Large Computer Clusters*, Talk or presentation at NIPS workshop: Learing on Cores, Clusters and Clouds, Vancouver, Canada, December 06-11, 2010.

15) J.A. Shelton, M.B. Blaschko, A. Gretton, J. Müller, E. Fischer, and A. Bartels, *Similarities in Resting State and Feature-driven Activity: Non-parametric Evaluation of Human fMRI*, Extended Abstract at NIPS workshop: Learing and Planing from Batch Time Series Data, Vancouver, Canada, December 06-11, 2010.

16) J.A. Shelton, M.B. Blaschko, and A. Bartels, *Augmentation of fMRI Data Analysis using Resting State Activity and Semi-supervised Canonical Correlation Analysis*, Poster presentation at Women in Machine Learning Workshop (WiML 2010), Vancouver, Canada, December 06-11, 2010.

17) Zhu, J., *Self-organization of two interacting winner-take-all systems*, Talk at International Joint Conference on Neural Networks (IJCNN 2010), Barcelona, Spain, June 2010.

2. Project "SECO"

FP7-2008-216593
Co-PI C. v.d. Malsburg
Period 01.03.2008-28.02.2012
Amount subproject FIAS: Euro 425.306

Collaborators: Urs Bergmann, Christoph von der Malsburg, Junmei Zhu, Alexander Schmid, Tomas Fernandes

This project is funded under the European program "Bio-ICT convergence". The project's full title is "Self-Constructing Computing Systems". The aim of the integrated project is to model the ontogenetic growth of neural circuits under genetic control. The FIAS subproject has two aims. The first is to model the pre-natal and post-natal self-organization of the specific circuit patterns that have been used as the basis of the FIAS invariant object recognition system developed in the DAISY project. The essential aims of this part of the project have been achieved in simple form within the reporting year. The second aim is the development of methodology for the semi-numerical analysis of sets of differential equations describing self-organizing systems, applied especially to network self-organization. Some applications to ontogenesis and to visual function have been published.

Related publications in 2010:

1) Urs Bergmann and C. von der Malsburg, *A Bilinear Model for Consistent Topographic Representations*, International Conference on Artificial Neural Networks (ICANN), 2010.

2) Junmei Zhu, Urs Bergmann and C. von der Malsburg, *Self-Organization of Steerable Topographic Mappings as Basis for Translation Invariance*, International Conference on Artificial Neural Networks (ICANN), 2010.

3) Urs Bergmann and C. von der Malsburg, *Self-Organization of Topographic Bilinear Networks for Invariant Recognition*, Neural Computation. In second review, 2011.

4) Junmei Zhu, *Self-organization of two interacting winner-take-all systems*, In Proceedings *International Joint Conference on Neural Networks (IJCNN)*, 2010.

3. Project "PLICON": Plasticity and Learning in Cortical Networks

Collaborators: Dana Ballard[3], Guido Marco Cicchini[2], Arthur Franz[1], Mary Hayhoe[3] Manu Punnen John[1], Prashant Joshi[1], Africa P[1], Constantin Rothkopf[1], Cristina Savin[1], Lisa Scocchia[1], Paul Schrater[4] Brian Sullivan[3], Jochen Triesch[1], Thomas Weisswange[1]

[1] FIAS, [2] University of Florence, and Institute of Neuroscience, National Research Council, Italy, [3] University of Texas Austin, [4] University of Minnesota

The brain is a very plastic organ. A plethora of plasticity mechanisms are constantly adapting its structure and optimize its function, allowing us to learn and adapt to changing environments. Many of these individual plasticity mechanisms have been carefully characterized in experimental studies and their properties have been described theoretically. However, there is little understanding of how the various mechanisms are interacting in the brain and what emergent properties result from these interactions at the network level. This project

studied such interactions through computer simulations and theoretical analysis. For example, an important recent finding is our demonstration that the combination of so-called spike-timing-dependent plasticity with intrinsic plasticity of neuron excitability can allow a network of spiking neurons to perform ICA-like learning, which is a standard theoretical model of how the brain learns sensory representations. In a second related line of research, we tried to better understand the cognitive development of human infants, by making computer models of their learning processes, as they grasp concepts like object permanence, i.e. the understanding that objects that become occluded continue to exist.

Related publications in 2010:

1) M.M. Hayhoe and C.A. Rothkopf *Eye movements in natural behaviour*, in: Encyclopedia of Cognitive Science. Editor: Lynn Nadel, Wiley (2010).

2) M.M. Hayhoe and C.A. Rothkopf *Vision in the natural world*, in: Wiley Interdisciplinary Reviews: Cognitive Science, Wiley (2010).

3) C. Rothkopf and D. Ballard, *Credit assignment in multiple goal embodied visuomotor behavior*, Frontiers in Psychology, Special Topic: 'Embodied and grounded cognition', (2010).

4) C. Rothkopf, T. Weisswange, and J. Triesch, *Computational modeling of multisensory object perception*, in: Multisensory Object Perception in the Primate Brain, Naumer, MJ. And J. Kaiser (Ed.). Springer New York 2010.

5) C. Savin P. Joshi, and J. Triesch, *Independent Component Analysis in Spiking Neurons*, PLoS Comput. Biol 6(4): e1000757 (2010), doi:10.1371/journal.pcbi.1000757

6) J. Triesch, C.A. Rothkopf, and T. Weisswange, *Coordination in Sensory Integration*, Dynamic Coordination in the brain: From neurons to Mind. Edited by C. von der Malsburg, W.A. Philips and W. Singer. Strüngmann Forum Report Vol. 5, Cambridge, MA: MIT Press, 2010.

Talks and Poster Presentations

1) C.A. Rothkopf, *Visumotor behavior in naturalistic virtual environments: from receptive fields to value functions*, Talk at Gordon Conference on Sensory Coding and the Natural Environment, Bates College, Lewiston, ME, USA, July 25-30 2010.

2) C. Savin and J. Triesch, *Structural plasticity improves stimulus encoding in a working memory model*, Poster presentation at Computational and Systems Neuroscience 2010 (COSYNE), Salt Lake City, USA, February 2010

3) P. Schrater and C.A. Rothkopf, *Discounting as task termination, and ist implications*, Poster presentation at Computational and Systems Neuroscience 2010 (COSYNE), Salt Lake City, USA, February 2010.

4) L. Scocchia, G.M. Cicchini and J. Triesch, *What's up? Orientation discrimination while holding orientations in memory*, Poster presentation at 33th European Conference on Visual Perception (ECVP) Abstract Supplement, Lausanne, Switzerland, August 2010.

5) B. Sullivan, C.A. Rothkopf, M.M. Hayhoe, and D. Ballard, *Modeling gaze priorities in driving*, Poster presentation at 10th annual meeting of the Vision Science Society, Naples, Florida, USA, May 7-12 2010.

4. Project "IM-CLeVeR": Intrinsically Motivated Cumulative Learning Versatile Robots

Collaborators: C. Dimitrakakis[1], L. Lonini[1], C. A. Rothkopf[1], J. Triesch[1], R. Pramod[1]

[1] Frankfurt Institute for Advanced Studies

IM-CLeVeR is an integrated project (IP) funded by the European Union and involves partners from multiple European countries. The overall goal of the project is to better understand:

– The development of intrinsic motivation mechanisms for driving exploration and autonomous development.

– Cumulative learning of multiple skills, through the efficient building of new skills by reusing or refining old skills.

IM-CLeVeR brings together Neuroscientists, Psychologists, Roboticists, and machine learning experts to tackle these problems. There are diverse research efforts around these core areas, including exploration and exploitation trade-offs, optimal planning, efficient representations, novelty detection and hierarchical world models, to name but a few.

At FIAS, the research focuses in the following main areas:

1. *Applied vision research.* Using a mobile robot head, efficient algorithms for perceptual abstraction, object recognition, tracking and autonomous learning are investigated. This effort also lays the groundwork for models developed in other parts of the research to be implemented in the robot itself.

2. *Hierarchical models for reinforcement learning, estimation and control.* Complex inference and planning problems can be more easily managed in a hierarchical framework. A number of statistical techniques are investigated for efficient and accurate learning and planning.

3. *Links between utility theory and apprenticeship learning.* Apprenticeship learning is a potentially important learning mode. The objective is not only to imitate what a demonstrator is doing, but to furthermore infer what he is doing and improve upon it.

4. *Links between models and animal learning.* Investigate whether models exhibit emergent behaviour reminiscent of animal learning, then design experiments to test this hypothesis.

5. *Near-optimal Bayesian planning.* Since Bayesian planning is intractable, investigate efficient approximate algorithms that do as well as possible given a computational budget.

6. *Utility theory models for curiosity.* Characterise the value of information in an abstract classes of tasks, thus obtaining a well-defined measure of curiosity. Derive approximate, but nearly optimal, "curiosity-based" algorithms based on this measure.

Related publications in 2010:

1) A. Alessi, L. Zollo, L. Lonini, R. De Falco, E. Guglielmelli, *Incremental learning control of the DLR-HIT-Hand II during interaction tasks*, Engineering in Medicine and Biology Society (EMBC), 2010 Annual International Conference of the IEEE. pp.3194–3197.

2) C. Dimitrakakis, *Bayesian variable order Markov models*, In Proceedings of the 13th International Conference on Artificial Intelligence and Statistics (AISTATS), volume 9 of JMLR: W.CP, Chia Laguna Resort, Sardinia, Italy, 2010

3) C. Dimitrakakis, *Complexity of stochastic branch and bound methods for belief tree search in Bayesian reinforcement learning*, in International conference on Agents and Artificial intelligence (ICAART 2010), pages 259-254.

4) C. Dimitrakakis, *Context model inference for large or partially observable MDPs*, in ICML Workshop on reinforcement learning and search in very large spaces.

5) C. Dimitrakakis, *Context models on sequences of covers*, arXiv:1005.2263, submitted to AAAI 2011.

6) C. Dimitrakakis, *Efficient Methods for Near-Optimal Sequential Decision Making Under Uncertainty*, in Robert Babuska and Frans Groen, editors, Interactive Collaborative Information Systems, SCI 81, pages 125-153, Springer, 2010

7) L. Lonini, C. Dimitrakakis, C. Rothkopf, J. Triesch (2010) *Generalization and Interference in Human Motor Control* in "Cumulative Learning and Intrinsic Motivations in Organisms and Robots", IM-CLeVeR book chapter (submitted)

8) C. A. Rothkopf, D. H. Ballard, *Credit assignment in multiple goal embodied visuomotor behavior*, Frontiers in Psychology, Special Topic: 'Embodied and grounded cognition', 2010

9) C. A. Rothkopf, T. H. Weisswange, J. Triesch, *Computational modeling of multisensory object perception*, in 'Multisensory Object Perception in the Primate Brain', Editors: M. J. Naumer & J. Kaiser, New York: Springer, 2010

10) C. A. Rothkopf, C. Dimitrakakis, *Preference elicitation and inverse reinforcement learning*, submitted to AAAI-2011.

11) C. Savin, P. Joshi, J. Triesch, *Independent component analysis in spiking neurons*, PLOS Computational Biology,6(4), 2010 :e1000757. doi:10.1371/journal.pcbi.1000757.

12) C. Savin, J. Triesch, *Structural plasticity improves stimulus encoding in a working memory model*, Conference Abstract: Computational and Systems Neuroscience 2010. doi: 10.3389/conf.fnins.2010.03.00231.

5. Project "NeFF"

In the context of the newly established LOEWE project NeFF (Neuronale Koordination Forschungsschwerpunkt Frankfurt) funded by the state of Hesse, FIAS has won research funding to investigate the emergence of coordinated patterns of neural activity. From 2011–2013 we will develop neural-network models to explain how different forms of neuronal plasticity mechanisms can shape the network dynamics to produce coherent activity patterns that are functionally meaningful. The project starts in January 2011. It provides funding for one postdoctoral position.

2. Graduate Schools

Helmholtz Graduate School for Hadron and Ion Research

and

Helmholtz Research School for Quark Matter Studies

by Henner Büsching and Gerhard Burau

The Helmholtz Graduate School for Hadron and Ion Research (HGS-HIRe for FAIR), established in October 2008 as a joint endeavor of GSI and the universities at Darmstadt, Frankfurt, Giessen, Heidelberg and Mainz together with FIAS looks back on a successful second year of operation. It provides a common platform for structured doctoral education in the scientific fields of hadron and ion research. By the end of 2010, more than 200 doctoral students from more than 30 nations are participating in the program of HGS-HIRe - an increase of roughly 25% compared to the previous year. 20% of the participants are female students. 17 participants graduated in 2010.

The integration of the Helmholtz Research School for Quark Matter Studies (H-QM) in HGS-HIRe to specially support a selected group of outstanding students working in the field of theoretical and experimental heavy-ion physics has been progressed. H-QM is a joint project of Goethe University Frankfurt and FIAS together with GSI. In 2010 a third H-QM group of 8 students have started the three-year educational program. Both, H-QM and HGS-HIRe are supported by the Initiative and Networking Fund of the Helmholtz Association.

In 2010 the ambitious education program of HGS-HIRe continued with a series of lectures, colloquia, lecture weeks and soft skill seminars. In summary five lecture weeks, two power weeks and six softskill seminars on various topics have been organized in 2010. As public outreach the exhibition "Die Weltmaschine" on the start of the CERN-LHC with more than 5000 visitors and 100 school classes has been organized at Frankfurt university by HGS-HIRe in fall 2010.

To facilitate career planning after the PhD, HGS-HIRe introduced a new series of events, "HGS-HIRe Perspectives": Invited speakers from applied science or industry who graduated in natural science meet with HGS-HIRe participants and discuss current career opportunities. Since spring 2010 HGS-HIRe organizes the HGS-HIRe Summer Student Program at GSI to attract undergraduate students to the scientific fields of the school. In October 2010 the HGS-HIRe signature event, the HGS-HIRe Graduate Days was held in Hanau-Steinheim: For two days everybody involved with HGS-HIRe came together to get an exciting view of the science the participants and members of the school are working on.

Other pillars of the program were strengthened in 2010: The HGS-HIRe Scientific Travel Program for participants with the optional inclusion of long-term stays at institutes abroad and individual PhD committees which meet every six months to discuss the current status and future plans of the PhD project.

In addition to the programmatic activities, HGS-HIRe provides and centrally organizes – strongly supported by FIAS – the very successful PhD scholarship programs of GSI (Graduate Program for Hadron and Ion Research - GP-HIR), HIC for FAIR and EMMI.

FIGSS

The Frankfurt International Graduate School for Science

by Jochen Triesch

Enrolment in the Frankfurt International Graduate School for Science (FIGSS) has further risen in the year 2010; the number of FIGSS students now stands at 56. About 43% of the students are of non-German nationality and about 20% are female. As in the years before, the majority of students work in neuroscience (23) and physics (22), in addition there are 7 students in biochemistry/chemistry and 4 students in computer science. A total of 11 FIGSS students have received their PhDs in the year 2010.

Presently the rules and procedures of FIGSS are being updated and developed further. In particular, provisions for PhD committees are being made which meet regularly and monitor the progress of the individual students. Furthermore, details of the cooperation with the 'Goethe Graduate Academy' (GRADE) are being worked out. The newly established GRADE is meant to form the joint platform for doctoral education at Goethe University.

All PhD students associated with FIAS have one advisor at the Institute and one at a department of Goethe University. The duration of PhD studies normally amounts to three years. While research work for the thesis is of central importance, the students are expected to actively participate in the seminars and colloquia at FIAS and also to attend lecture courses.

In the FIGSS Seminar, being held on Mondays at noon in the form of a lunch seminar with free pizza, FIGSS students report on the status of their PhD work. Care is taken that the talks are prepared in such a way that they are understandable to an interdisciplinary auditorium. In 2010 we have improved the format of the FIGSS Seminar. In order to maximize the quality of presentations we have introduced a feedback form that listeners fill out for every presentation. The presentations are also videotaped to give speakers valuable feedback about their presentation style. Finally, we have established a best presentation prize that is awarded to the best presentation of the semester according to the scores on the feedback forms. These changes were generally well received by the participants.

Courses offered at FIGSS

Summer Semester 2010

E. Bratkovskaya, I. Mishustin	Dynamical models for relativistic heavy-ion collisions, 2h
T. Burwick	Synchronization in oscillatory networks, 2h
E. Engel	Quantum many-particle theory, 2+1h
W. Greiner	Quantum electrodynamics, 2h
P. Joshi	Computational neuroscience, 2+1h
J. Lücke	Probabilistic unsupervised learning, 2h
H. Lüdde	Nonlinear dynamics and complex systems, 2+1h
S. Schramm	Quantum theory on the lattice, 3h
D. Schuch	Nonlinearities and dissipation in classical and quantum physics
A. Solov'yov	Theoretical and computational methods in Meso-Bio-Nano-Science, 2h

Winter Semester 2010/11

T. Burwick	Visual System - Neural Structure, Dynamics, and Function, 1h
W. Greiner	Quantum Electrodynamics II, 2h
C. Gros	Complex Adaptive Dynamical Systems, 3h
I. Mishustin	Physics of Strongly Interacting Matter 2h
P. Nicolini	Quantum fields in curved space, AdS/CFT correspondence, 3h
P. Romatschke	Hydrodynamics and Transport Theory, 2+2h
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
J. Triesch	Methods for the study of complex systems 2+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

Ph.D. degrees received by FIAS/FIGSS students in the year 2010

1	Andreea Lazar	5.04.2010	Self-organization of recurrent neural networks with plasticity
2	Mauricio Martinez Guerrero	30.04.2010	Phenomenological aspects of an anisotropic Quark-Gluon Plasma
3	Michael Hauer	17.06.2010	Statistical fluctuations and correlations in hadronic equilibrium systems
4	Adilah Hussien	16.07.2010	Phase transitions in carbon-based nanoclusters as seen via molecular dynamics simulations
5	Stephanie G. Lo	28.07.2010	Dynamical screening of an endohedral atom
6	Nan Su	16.08.2010	A gauge-invariant reorganization of thermal gauge theory
7	Alexander Yakubovich	29.09.2010	Theory of phase transitions in polypeptides and proteins
8	Graziela Grise	6.10.2010	Simulating the cell internal structure using Delaunay triangulation
9	Arthur Franz	29.10.2010	Neural network models of cognitive development in infancy
10	Jenia Jitsev	5.11.2010	On the self-organization of a hierarchical memory for compositional object representation in the visual cortex
11	Jacquelyn Noronha-Hostler	8.12.2010	Properties of hadronic matter near the phase transition

3. FIAS Scientific Life

Seminars and Colloquia at FIAS in the year 2010

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

7.01.2010 **Prof. Dr. Alexandre Pouget,** University of Rochester, Rochester, NY
Probabilistic population coding

14.01.2010 **Prof. Dr. Herbert Jäger***, School of Engineering and Science, Jacobs University, Bremen
Observable operator models - Introduction and current research

21.01.2010 **Prof. Dr. Frauke Zipp***, Klinik für Neurologie, Johannes Gutenberg-Universität Mainz
Molecular imaging in neurological diseases

4.02.2010 **Prof. Dr. Xavier Viñas,** Physics Faculty, University of Barcelona
Finite-nucleus description based on microscopic Brueckner-Hartree-Fock calculations

22.02.2010 **Prof. Dr. Peter O. Hess,** Instituto de Ciencias Nucleares, UNAM, Mexico
Pseudo-complex general relativity

26.02.2010 **Dr. Dennis Dietrich,** University of Southern Denmark, Odense
What if there were no Higgs at the LHC?

15.04.2010 **Dr. Michael Spratling,** Division of Engineering, King's College, London
Unifying predictive coding and biased competition into a model of viisual attention and V1 response properties

29.04.2010 **Prof. Dr. Ernst Bamberg,** Max Planck Institute of Biophysics, Frankfurt
Optogenetics – the successful story of a rhodopsin-like protein

6.05.2010 **Prof. Dr. Nigel Mason,** The Open University, London
Molecular synthesis in space – The cradle of life?

27.05.2010 **Dr. Peter Dittrich,** Institute for Computer Science, Friedrich-Schiller-University Jena
Organic structural sciences: From chemical organizations to semiotic molecular systems

10.06.2010 **Prof. Dr. Kim Sneppen,** Niels Bohr Institute, Copenhagen
Lessons from phage biology

17.06.2010 **PD Dr. Nikolai Bagdassarov,** Institute for Geosciences, Goethe University, Frankfurt
Earth's dynamics: earthquakes, volcanism, plate tectonics

24.06.2010 **Prof. Dr. Achilleas Frangakis,** Institute for Biophysics, Goethe-University, Frankfurt
Cryo-electron tomography: The computational aspect

1.07.2010 **Prof. Dr. Mark Strikman,** Penn State University, University Park, PA
Nucleon close encounters

8.07.2010   **Prof. Dr. Gilles Laurent,** Max-Planck-Institute for Brain Research, Frankfurt
Learning and oscillations in an olfactory network

15.07.2010   **Prof. Dr. Paul Kienle,** Cluster of Excellence "Origin and Structure of the Universe",
Technical University of Munich
Time-modulation of two-body weak decays with massive neutrinos

24.08.2010   **Prof. Dr. Konrad Körding,** Northwestern University, Chicago, IL
How advances in neural recording will affect future data analysis techniques

16.09.2010   **Prof. Dr. Andreas Dreuw,** Institute of Physical and Theoretical Chemistry, Goethe
University, Frankfurt
*Excited electronic states of large molecular systems: a challenge to quantum
Chemistry*

30.09.2010   **Prof. Dr. Chhanda Samanta,** Saha Institute of Nuclear Physics, Kolkata and Virginia
Comonwealth University, Richmond, Virginia
Strangeness: A new dimension in nuclear physics

4.11.2010   **Dr. Jörg Lücke,** Frankfurt Institute for Advanced Studies
Probabilistic models of unsupervised learning in man and machine

18.11.2010   **Prof. Dr. Albert Newen,** Institut für Philosophie, Ruhr-Universität Bochum
Understanding oneself and understanding others

25.11.2010   **Prof. Dr. Joachim Ullrich,** Max-Planck-Institut für Kernphysik, Heidelberg
Free Electron Lasers: Ultra-brilliant light for science

2.12.2010   **Prof. Dr. Erin Schuman,** Max Planck Institute for Brain Research, Frankfurt
Local control of neuronal synaptic function

9.12.2010   **Prof. Dr. Herbert Zimmermann,** Institute of Cell Biology and Neuroscience, Goethe
University, Frankfurt
Neurogenesis in the adult mammalian brain: Signalling via nucleotides

16.12.2010   **Prof. Dr. Berndt Müller,** Dept. of Physics, Duke University, Durham NC
Physics with two time dimensions

FIGSS Seminar

18.01.2010   **Jenia Jitsev**
*Unsupervised learning of object identity and category in a hierarchical visual memory
running in on- and off-line modes*

25.01.2010   **Arthur Franz**
*A unified computational model of the development of object unity, object permanence,
and occlusion perception in infancy*

8.02.2010   **Harald Kempf**
Spatio-temporal cell dynamics in tumour spheroid irradiation

3.05.2010   **Dr. Jörg Lücke**
Computational intelligence and unsupervised learning

17.05.2010 **Alexander Heusel**
Piecewise linear interface reconstruction as a method to reconstruct smooth geometries from volumetric data

31.05.2010 **Katharina Schmitz**
Graph theory analysis of local functional networks in cat visual cortex

7.06.2010 **Luis Felipe Ruiz**
Study of stability parameters in super-heavy elements using the two center shell model

21.06.2010 **Daniel Krieg**
Internal representations and self-organization in recurrent neural networks

28.06.2010 **Mareike Müller**
Effects of X-ray and heavy ion radiation on tissue slice cultures made of liver and pancreas

5.07.2010 **Dr. Dominik Heyers,** Department of "Neurosensorik", University of Oldenburg
Neuroanatomy of avian magnetoreception

12.07.2010 **Marc Henniges**
Learning and object recognition in generative models of occlusion

19.07.2010 **Daniela Pamplona**
Space variant duckies recognition

8.11.2010 **Bin Wu**
Looking inside neutron stars: Microscopic calculations confront observations

15.11.2010 **Tim Schuster**
Hadron ratio fluctuations in heavy ion collisions

22.11.2010 **Veronika Dick**
Mechanisms of fractal formation and fragmentation on a surface

29.11.2010 **Xu-guang Huang**
Neutron star, r-mode, and magnetized quark matter

6.12.2010 **Rodrigo Negreiros**
Quark matter in compact objects

13.12.2010 **Joonsuk Huh**
Probability density functions of harmonic transitions

20.12.2010 **Sohrab Saeb**
Development of coordinated eye and head movements in primates

Conferences and meetings (co)organized by FIAS in the year 2010

▷ **Mini-Workshop** *"Photon emission in crystalline undulators"*, Frankfurt, February 25, 2010

▷ **42. Heidelberger Bildverarbeitungsforum,** *" Lernende Bildverarbeitung - Neuroinformatische und statistische Ansätze"*, Frankfurt, March 10, 2010
`www.bv-forum.de/rb/bvf42.html`

▷ **Ernst Strüngmann Forum,** *"Disease Eradication in the Context of Global Health in the 21st Century "*, Frankfurt, August 29 – Sept. 3, 2010
`www.esforum.de/forums/esf07_disease_eradication.html`

▷ **Ernst Strüngmann Forum,** *"Animal Thinking - Contemporary Issues in Comparative Cognition"*, Frankfurt, September 26 – October 1, 2010
`www.esforum.de/forums/esf08_animal_thinking.html`

▷ **DySoN 2010, International Conference** *"Dynamics of Systems on the Nanoscale"*, Rome, November 16-19, 2010
`fias.uni-frankfurt.de/dyson2010/`

▷ **Symposion on** *"Advances in Nuclear Physics in Our Time "*, Goa, India, November 28 - December 2, 2010
`http://www.saha.ac.in/cs/capp.sinp/`

Talks at the FIAS Forum in the year 2010

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.

14.01.2010 **Prof. Dr. Reinhard Stock,** FIAS Adjunct Fellow, Goethe Universität
Die Entstehung der Materie im Urknall

24.02.2010 **Dr. Michael Meyer-Hermann,** ALTANA-Fellow am FIAS
Unser Immunsystem: Wie funktioniert es – wie schützt sich der Körper?

15.04.2010 **Prof. Dr. Jochen Triesch,** Johanna-Quandt-Forschungsprofessor am FIAS
Können wir unseren Augen trauen? Was uns Wahrnehmungsfehler über das Gehirn verraten.

20.05.2010 **Prof. Dr. Volker Lindenstruth,** FIAS und Institut für Informatik, Goethe-Universität
Green IT - das Frankfurter Konzept: Neue Möglichkeiten, effizient und umweltfreundlich mit Hochleistungs-Computern umzugehen

1.07.2010 **Prof. Dr. Dirk Rischke,** Institut für Theoretische Physik und FIAS
Von kalten Atomen zu Neutronensternen

26.02.2010 **Prof. Dr. Walter Greiner,** FIAS Senior Fellow
Es gibt keine schwarzen Löcher – Von Einstein zu Zweistein

4. Research Reports

4.1 Nuclear Physics, Particle Physics, Astrophysics

Heavy-Ion Physics and Nuclear Astrophysics Group
Group Leader: Prof. Dr. Igor Mishustin, FIAS Senior Fellow

Main research fields: Physics of strongly interacting matter (equation of state, QCD motivated effective models, hadron resonance gas); Heavy-Ion collisions at intermediate and high energies (statistical, kinetic and fluid-dynamical models, non-equilibrium phase transitions); Nuclear astrophysics (structure and dynamics of compact stars, nuclear composition and EOS of stellar matter); Medical and technical applications (modeling heavy-ion and proton beam energy deposition in extended media, radiation damage of biomolecules, physics of ADS systems).

Group members: Dr. Chichiro Sasaki (junior fellow), Dr. Giorgio Torrieri (postdoc), Dr. (Hab.) Leonid Satarov (long-term visitor), Dr. Igor Pshenichnov (long-term visitor), Dr. Alexander Botvina (long-term visitor).

PhD students: Johan Bjerrum-Bohr, Claudio Ebel, Daniel Yueker, Alessandro Brillante.

Short-term visitors: Prof. Laszlo Csernai (Bergen University), Prof. Konstantin Gudima (Moldavian Academy of Sciences), Dr. Nihal Buyukcizmeci (Selchuk University, Turkey), Andrey Merdeev (Kurchatov Institute, Moscow). Lucas N. Burigo (Univesidade Federal do Rio Grande do Sul, Porto Alegre, Brazil).

Collaborators a) inside FIAS: Prof. W. Greiner, Prof. M. Bleicher, Prof. S. Schramm, Prof. A. Solov'yov, Dr. R. Negreiros, J. Steinheimer; b) in ITP, Goethe University: Dr. T. Koide, G. Denicol; c) at GSI (Darmstadt): Prof. W. Trautmann, Prof. M. Durante, Dr. D. Schardt; d) at Niels Bohr Institute (Copenhagen): Prof. J. Bondorf, Prof. Jens Joergen Gaardhoje, Dr. Th. Dossing; e) elsewhere: Dr. (Hab) Yu. Ivanov (Kurchatov Institute, Moscow), Prof. V. Zagrebaev (JINR, Dubna), Dr. A. Larionov (Giessen University), Prof. J. Schaffner-Bielich (Heidelberg University), Prof. D. Bandyopadhyay and Prof. Sh. Samanta (Saha Institute of Nuclear Physics, Calcutta), Prof. J. Kapusta (University of Minnesota), Prof. J. Pochodzalla (Mainz University), Prof. L. Bravina (Oslo University), Prof. Riza Ogul (Selcuk University, Turkei).

Invited seminar and conference talks in 2010

1. A.B. Larionov, I.N. Mishustin, L.M. Satarov, and W. Greiner, Dynamical compression of the ^{16}O nucleus by a moving antiproton, talk given at the meeting of the German Physical Society (DPG), Bonn, March 16, 2010.

2. Igor Mishustin, Nuclear fragmentation reactions in basic research and medical applications, DISCOVERY colloquium at Niels Bohr Institute, Copenhagen, March 24, 2010;

3. Igor Mishustin, Hydrodynamic modeling of relativistic heavy-ion collisions, ALICE group seminar, Niels Bohr Institute, Copenhagen, March 23, 2010;

4. A.S. Botvina, Multifragmentation of nuclei and stellar matter in supernova explosions, seminar of Physics Department, Liege University, June 4, 2010;

5. Igor Mishustin, Optimization of neutron flux and energy deposition in spallation targets, ADS Working group meeting, Juelich Forschung Zentrum, September 23, 2010;

6. I.N. Mishustin, A.V. Merdeev, L.M. Satarov, Hydrodynamic modeling of deconfinement phase transition in nuclear collisions, International Workshop "Critical Point and Onset of Deconfinement" CPOD 2010 (Dubna, Russia, August 22-27, 2010), arXiv:1012.4364 [hep-ph];

7. Giorgio Torrieri, Igor Mishustin, How large is "large N_c" for Nuclear matter?, the same conference as in 5), arXiv:1102.2310 [hep-ph];

8. Igor Mishustin, Non-equilibrium phase transitions in relativistic heavy-ion collisions, the same conference as in 5);

9. A.S.Botvina, Production of hyper-nuclei in reactions induced by relativistic hadrons and heavy-ions, joint SPHERE (Strange Particles in Hadronic Environment Research in Europe) and JSPS Meeting 2010 (Prague, Czech Republic, September 4-6, 2010);

10. Igor Mishustin, Production of hypernuclei in relativistic heavy-ion collisions, International Workshop "Strangeness in nuclei" (ECT* Trento, Italy, October 3-7, 2010);

11. Igor Mishustin, Monte Carlo simulations of ion-beam cancer therapy: from nuclear fragmentation to micro-dosimetry, International Conference "Dynamics of Systems on the Nanoscale" DySoN 2010 (NRC, Rome, Italy, November 16-19, 2010);

12. Igor Mishustin, Production of heavy and superheavy nuclei in explosive processes, International Symposium "Advances in Nuclear Physics in Our Time" (Goa, India, November 28 - December 2, 2010).

Papers published and submitted in 2010

1. Igor Pshenichnov, Alexander Botvina, Igor Mishustin, Walter Greiner, Nuclear fragmentation reactions in extended media studied with Geant4 toolkit, Nucl. Instr. Meth. B 268, 604-615 (2010); arXiv:0911.2017v1 [physics.med-ph].

2. A.B. Larionov, I.N. Mishustin, L.M. Satarov and W. Greiner, Possibility of cold nuclear compression in antiproton-nucleus collisions, Phys. Rev. C 82, 024602(15) (2010); arXiv:0912.1794 [nucl-th].

3. Igor N. Mishustin, Claudio Ebel and Walter Greiner, Strong electric fields induced on a sharp stellar boundary, J. Phys. G: Nucl. Part. Phys. 37, 075201 (2010); arXiv:1002.2541v1 [astro-ph.SR].

4. I. Mishustin, I. Pshenichnov, and W. Greiner, Modeling heavy-ion energy deposition in extended media, Eur. Phys. J. D 60, 109-114 (2010).

5. A.S. Botvina, I.N. Mishustin, Statistical approach for supernova matter, Nucl. Phys. A 843, 98-132 (2010); arXiv:0811.2593 [nucl-th].

6. Chihiro Sasaki and Igor Mishustin, Thermodynamics of dense hadronic matter in a parity doublet model, Phys. Rev. C 82, 035204 (2010); arXiv:1005.4811 [hep-ph].

7. Giorgio Torrieri and Igor Mishustin, The nuclear liquid-gas phase transition at large N_c in the Van der Waals approximation, Phys. Rev. C 82, 055202(10) (2010); arXiv:1006.2471 [nucl-th].

8. R. Ogul, A.S. Botvina, U. Atav, N. Buyukcizmeci, I.N. Mishustin et al., Isospin dependent multifragmentation of relativistic projectiles, to be published in Phys. Rev. C; arXiv:1006.3723 [nucl-ex].

9. Alexander Botvina, Igor Mishustin, Valery Zagrebaev and Walter Greiner, Possibility of synthesizing superheavy elements in nuclear explosions, Int. J. Mod. Phys. 19, 2063-2075 (2010); arXiv:1006.4738 [nucl-th].

10. Rodrigo Picanco Negreiros, Igor N. Mishustin, Stefan Schramm, Fridolin Weber, Properties of Bare Strange Stars Associated with Surface Electric Fields, Phys. Rev. D 82, 103010(6) (2010); arXiv:1008.0277 [astro-ph.HE].

11. Rana Nandi, Debades Bandyopadhyay, Igor N. Mishustin and Walter Greiner, Inner crusts of neutron stars in strongly quantising magnetic fields, submitted for publication in Astrophys. J.; arXiv:1012.5970 [astro-ph.HE].

12. I.A. Pshenichnov, E.V. Karpechev, A.B. Kurepin, I.N. Mishustin, Electromagnetic and hadronic interactions of ultrarelativistic nuclei, to be published in J. Atom. Nucl.

13. Sven Zschocke, Szabolcs Horvat, Igor N. Mishustin, Laszlo P. Csernai, Non-equilibrium hadronization and constituent quark number scaling, Phys. Rev. C (in press); arXiv:1102.2310 [hep-ph].

14. I.N. Mishustin, K.A. Lyakhov, Baryon stopping and partonic plasma production by strong chromofields in relativistic heavy-ion collisions, to be published in the volume of J. Atom. Nucl. dedicated to 100th Anniversary of Arcady Migdal.

Production of multi-hyper-nuclei in peripheral heavy-ion collisions

Collaborators: I.N. Mishustin[1], J. Steinheimer[1], M. Bleicher[1], A. Botvina[1,2], K. Gudima[3]

[1] Frankfurt Institute for Advanced Studies, [2] Institute for Nuclear Research, RAS, Moscow, [3] Institute of Applied Physics, Moldavian Academy of Sciences

We study a new mechanism of hyper-nuclei production in peripheral collisions of relativistic nuclei when hyperons are produced in secondary reactions and can be captured by spectators. In this way, a piece of relatively cold (multi-)strange nuclear matter can be formed in the laboratory under conditions similar to the interiors of neutron stars. In the following this excited strange matter will disintegrate into several ordinary and hyper-fragments. Experiments on production of hyper-nuclei in relativistic nucleus-nucleus collisions are now under-way at GSI (HypHI collaboration) and are also planed for FAIR. Within this project we have developed a hybrid approach for description of hyper-fragment production in such reactions. The first dynamical stage of the reaction is described by the Quark Gluon String Model (QGSM) or by Ultra-relativistic Quantum Molecular Dynamics (UrQMD), which have demonstrated previously a very good description of strange hadron production. We have applied a new criterion for the absorption of produced hyperons, e.g. Λ is captured when its kinetic energy is less than the hyperon potential generated by surrounding nucleons. The characteristics of the hyperonic spectator matter and probability of producing multi-strange systems were also investigated. For reliable predictions we need to generate about 10^6 events. The calculations are performed at the CSC using a vectorization algorithm. Our calculations show that double- and even triple-Λ-hypernuclei can be produced by the proposed mechanism. This project is a very good example of the close cooperation of different FIAS groups.
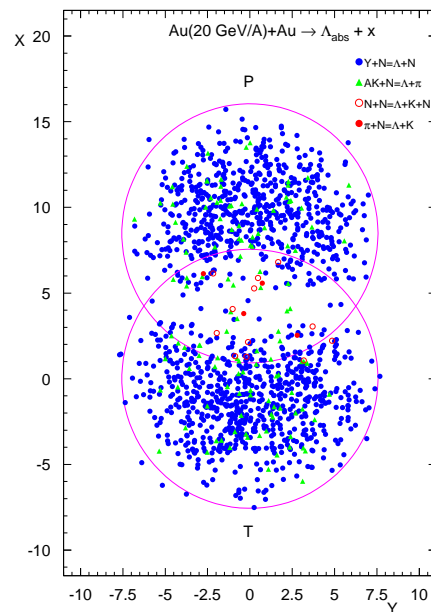
Projections of the Λ-hyperon absorption points on the X-Y plane perpendicular to the beam axis. The counters of the projectile (P) and target (T) nuclei are shown by the circles. The various processes leading to the hyperon production are shown by different symbols. One can clearly see the accumulation of the absorbed Λ's in the spectator parts of the colliding nuclei. Presented results correspond to 10000 events.

Related publications and talks in 2010:

1. A.S. Botvina, K.K. Gudima, J. Steinheimer, M. Bleicher and I.N. Mishustin, *Production of spectator hypermatter in relativistic heavy-ion collisions*, paper in preparation;

2. Igor Mishustin, *Production of hypernuclei in relativistic heavy-ion collisions*, invited talk at the International Workshop "Strangeness in Nuclei" (ECT*, Trento, November 3-7, 2010).

Non-equilibrium hadronization and constituent quark number scaling

Collaborators: I.N. Mishustin[1], L. Csernai[1,2], S. Zschocke[3], S. Horvát[2]

[1] Frankfurt Institute for Advanced Studies, [2] University of Bergen, Norway, [3] Technical University Dresden,

Following our earlier works (see, e.g. L.P. Csernai, I.N. Mishustin, Phys. Rev. Lett. 74, 5005 (1995), I.N. Mishustin, Phys. Rev. Lett. 82, 4779 (1999)) we study a non-equilibrium hadronization scenario with rapid dynamical transition from the state of ideal and chirally symmetric Quark Gluon Plasma, to the final state of non-interacting hadrons. In this transition a Bag model of constituent quarks is considered, where the quarks gain constituent quark mass while the background Bag-field breaks up and vanishes. The constituent quarks then recombine into simplified hadron states, while chemical, thermal and flow equilibria break down one after the other. In this scenario the resulting temperatures and flow velocities of baryons and mesons are different. Using a simplified few source model of the elliptic flow, we are able to reproduce the constituent quark number scaling, with some additional assumptions on the details of the non-equilibrium processes.
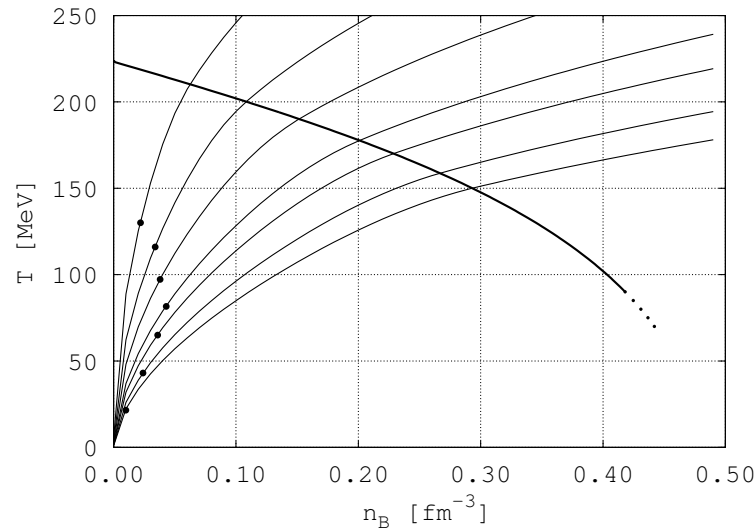
A series of curves of adiabatic expansion (thin solid lines) of the gas of quarks and anti-quarks acquiring the constituent mass. The dots on the adiabatic expansion curves indicate where the rapid freeze-out and hadronization happens. These points are determined based on the condition that the energy of the system, including the background field, divided by the estimated number of hadrons reaches 1.2 GeV per hadron. The initial conditions for the non-equilibrium expansion are defined on the thick solid line calculated assuming that the quark masses are equal to the current quark mass, $M_f = m_f$.

**Related publications and talks in 2010:**

1. Sven Zschocke, Szabolcs Horvát, Igor N. Mishustin, Laszlo Csernai, *Non-equilibrium hadronization and constituent quark number scaling*, Phys. Rev. C (in press); arXiv:1102.2310 [hep-ph];

2. L.P. Csernai et al., *How collective flow observables indicate the QGP fluid?*, invited talk at the International Symposium "Advances of Nuclear Physics in Our Time", Goa, India, Nov. 28 - Dec. 2, 2010), to be published in Proceedings.

Baryon stopping and partonic plasma creation by strong chromofields

Collaborators: I.N. Mishustin[1], K.A. Lyakhov[1]

[1] Frankfurt Institute for Advanced Studies

It is expected that strong chromofields can be generated at early stages of ultrarelativistic nuclear collisions (Color Glass Condensate). In this paper we demonstrate that these fields may explain not only creation of the quark-gluon plasma but also collective deceleration of net baryons. At ultrarelativistic energies two colliding nuclei can be represented by two thin sheets interpenetrating each other at t=0. Due to the soft gluon interactions, after the collision these sheets acquire stochastic color charges. To simplify the treatment we subdivide the sheets on smaller elements (slabs) of area $\mathscr{A} = \frac{\pi}{Q_s^2}$, where Q_s is so-called saturation scale for high-density QCD. Then we solve classical equations of motion for pairs of baryonic slabs under the action of a time-dependent chromofield generated by their color charges. In this scenario the partonic plasma is produced as result of the chromofield decay via the Schwinger mechanism. We have studied sensitivity of the slab trajectories and their final rapidities to the initial strength and decay time of the chromofield, as well as to the back reaction of the produced plasma. By proper choice of the initial chromofield energy density we can reproduce significant baryon stopping observed for Au+Au collisions at RHIC, i.e. an average rapidity loss $< \delta y >$ of about 2 units. Using a Bjorken-like hydrodynamical model with the particle production source, we also study the evolution of partonic plasma created by the chromofield decay. Because of the delayed formation and expansion of plasma its maximum energy density is significantly lower than the initial energy density of the chromofield. It is shown that the fluctuations of the chromofield due to the stochastic distribution of color charges help to populate the midrapidity region in the net-baryon distribution. To fit the midrapidity data we need the chromofields with initial energy densities in the range of 30 to 60 GeV/fm^3. We have found a nearly linear dependence of the mean baryon rapidity loss as a function of the beam rapidity (see the figure). Predicted values of $< \delta y >$ for Pb+Pb collisions at LHC energies are within the range 3÷4.5.
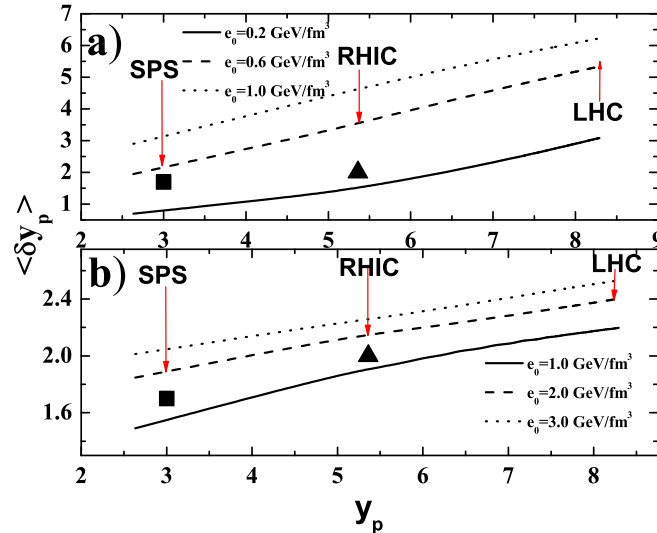
Projectile slab rapidity loss as a function of initial beam rapidity calculated for the power-law of chromofield decay. Results are shown for the collision of two equal slabs with $N_p = N_t = 5.8$, representing a central Au+Au collision. Different curves correspond to different values of parameter ε_0 displayed in the figures. Upper and lower panels represent the calculations without and with the back reaction of produced plasma, respectively. Symbols show the values of mean rapidity loss measured at SPS and RHIC energies.

Related publications in 2010:

I.N. Mishustin, K.A. Lyakhov, *Baryon stopping and partonic plasma production by strong chromofields in relativistic heavy-ion collisions*, to be published in the volume of J. Atom. Nucl. dedicated to 100th Anniversary of Arcady Migdal.

Hydrodynamic modeling of deconfinement phase transition in heavy-ion collisions at NICA–FAIR energies

Collaborators: I. N. Mishustin[1,2], A. V. Merdeev[1,2], L. M. Satarov[1,2]

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

Three–dimensional ideal hydrodynamics is applied to simulate Au+Au and Pb+Pb collisions at bombarding energies $E_{lab} = 1 - 160$ AGeV. For comparison, two equations of state are used in the calculations: 1) EOS-HG which is purely hadronic and includes all resonances up to 2 GeV, and 2) EOS-PT with contains additionally a phase transition from the hadron gas to the Quark-Gluon plasma. The initial state is represented by two cold Lorentz–boosted nuclei. The numerical code is based on the flux–corrected transport algorithm SHASTA. Dynamical trajectories of matter produced in central Au+Au collisions at different E_{lab} are shown in the figure below. As one can see, in comparison with a purely hadronic scenario, the phase transition leads to stronger compression and longer life-times of compressed states. Formation of the mixed phase is possible already at bombarding energies above approximately 3 AGeV. It is interesting to note that, despite significant differences on the intermediate stages, the final states of matter are rather insensitive to the equation of state. Comparison with the three–fluid model calculations shows that the transparency effects are not so important in central collisions at $E_{lab} < 30$ AGeV. It is shown that the deconfinement phase transition leads to broadening of proton rapidity distributions, increase of elliptic flow and formation of the pion antiflow. Our analysis shows that larger effects of the phase transition may be expected at $E_{lab} \sim 10$ AGeV, when the system spends the longest time in the mixed phase.
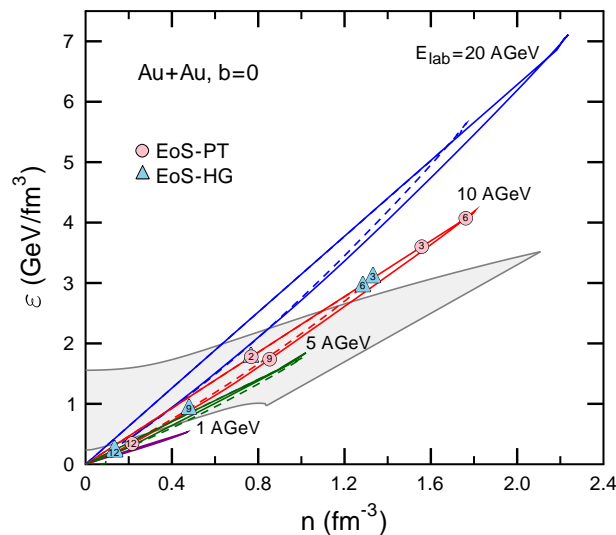
Time evolution of matter in central Au+Au collision at different E_{lab}. Shown are values of energy and baryon densities averaged over the central box $|x|, |y|, \gamma_0|z| < 1$ fm. Dashed and solid lines correspond to EoS–HG and EoS–PT, respectively. Numbers in triangles and circles give the c.m. time in fm/c. Shading shows the mixed phase region of deconfinement phase transition.

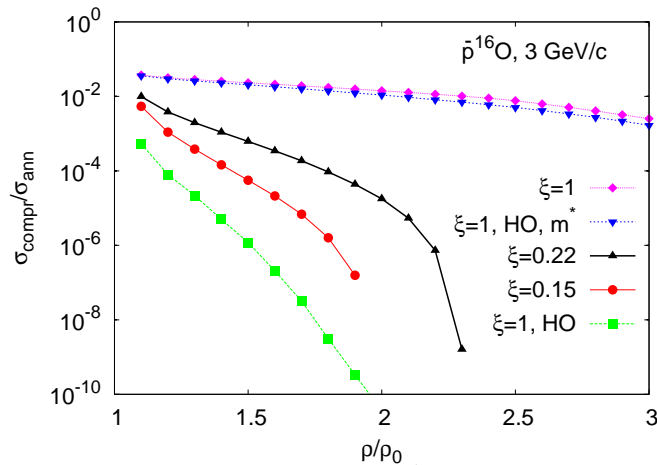**Related talks and publications in 2010:**

1. Igor Mishustin, *Hydrodynamic modeling of deconfinement phase transition in heavy-ion collisions*, ALICE Group seminar, Niels Bohr Institute, Copenhagen, 23 March 2010.

2. Andrey Merdeev, *Hydrodynamic modeling of phase transitions in heavy-ion collisions at FAIR energies*, Hydro-group meeting, ITP, Goethe University, June 21, 2010.

3. I.N. Mishustin, A.V. Merdeev, and L.M. Satarov, *Hydrodynamic modeling of deconfinement phase transition in nuclear collisions*, arXiv:1012.4364 [hep-ph].

Nuclear compression induced by a moving antiproton

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

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

Due to the strongly attractive real part of the $\bar{p}$-nucleus optical potential, an antiproton slowly moving in the nuclear interior may create a local zone with enhanced nucleon density. We have considered this possibility with a help of the GiBUU model. For this purpose a standard parallel ensemble simulation of the high-energy antiproton induced reaction has been performed. The antiproton momentum and position at the annihilation time moment have been stored in each parallel ensemble (or event). Assuming then, that the compression proceeds mainly on the short piece of the $\bar{p}$ trajectory before its annihilation, the antiproton has been reinitialized in every annihilation event with the same momentum and position as at its annihilation. Then a new GiBUU calculation with *switched off* annihilation has been done. Due to the coherent initialization of the antiproton at the same position in all parallel ensembles, the mean field effects have been taken into account in full strength in this calculation, which allows to calculate the nuclear response in a proper way. The survival probability of the antiproton during the compressional evolution was calculated via the time-integrated annihilation width. On the basis of these simulations we have evaluated the probability of $\bar{p}$-annihilation within a compressed zone (ACZ) where maximum nucleon density $\rho_{\max}$ exceeds a given value ρ. The results of calculations are shown in the figure below. The various curves demonstrate how the results depend on model parameters characterizing the $\bar{p}$ optical potential, in particular the scaling factor ξ of the $\bar{p}$ mean field ($\xi = 1$ corresponds to the G-parity transformed nucleon mean fields). For the phenomenologically preferable value $\xi = 0.22$ (leading to $\text{Re}(V_{\text{opt}}) = -153$ MeV) we find that annihilations at densities above $2\rho_0$ are predicted on the level of $10^{-4} \div 10^{-5}$. Such events can be detected in the future FAIR experiments with the $\overline{\text{PANDA}}$ detector. With expected $\bar{p}$-beam luminosity $L = 2 \cdot 10^{32}$ cm^{-2} s^{-1}, the ACZ rate can be estimated on the level of a few hundred events per second. Triggering on a fast proton in final state can, in principle, enhance the ACZ event fraction by about one order of magnitude, while suppressing the rate by factor 10^3. Certainly, further theoretical studies are needed in order to find the best experimentally realizable ways to observe nuclear compression in $\bar{p}$-nucleus collisions.

Event-averaged probability of $\bar{p}$ annihilation at $\rho_{\max} > \rho$ vs ρ for $\bar{p}^{16}O$ collisions at $p_{\text{lab}} = 3$ GeV/c. The default choice of parameters corresponds to $\xi = 0.22$.

Related talks and publications in 2010:

1. A.B. Larionov, I.N. Mishustin, L.M. Satarov, and W. Greiner, *Possibility of cold nuclear compression in antiproton-nucleus collisions*, Phys. Rev. C 82, 024602 (2010).

2. A.B. Larionov, I.N. Mishustin, L.M. Satarov, and W. Greiner, *Dynamical compression of the ^{16}O nucleus by a moving antiproton*, talk given at the meeting of the German Physical Society (DPG), Bonn, March 16, 2010.

Statistical approach for supernova matter

A.S. Botvina[1,2], I.N. Mishustin[1]

[1] Frankfurt Institute for Advanced Studies, [2] Institute for Nuclear Research, RAS, Moscow

We formulate a statistical approach for description of nuclear composition and equation of state of stellar matter at subnuclear densities and temperature up to 20 MeV, which are expected during the collapse and explosion of massive stars. The model includes nuclear, electromagnetic and weak interactions between all constituents of matter, under condition of statistical equilibrium. We construct a realistic ensemble of nuclear species, and demonstrate the differences from the models employing a single-nucleus approximation for heavy nuclei. Thermodynamical characteristics, isentropic trajectories, EOS, and nuclear composition of supernova matter are calculated for different values of the lepton fraction. In the figure one can see the evolution of the nuclear composition with increasing temperature for different baryon densities. At low temperatures ($T < 1$ MeV) the matter is mainly composed of heavy nuclei. With increasing temperatures the heavy nuclei gradually disintegrate into α's, neutrons and protons. At low densities this disintegration happens already at moderate temperatures $T \sim 1$–2 MeV, while at subnuclear densities ($\rho \sim 0.1 \cdot \rho_0$) the heavy nuclei survive even at higher temperatures, though they become very excited.

In our work we emphasize that the physical conditions of supernova matter are essentially determined by the state of hot nuclear matter at subnuclear densities investigated in multifragmentation reactions in the laboratory. Further studies of such reactions are especially important because supernova explosions may be considered as breeders for creating heavy and super-heavy elements. In our paper special attention is paid to a possible in-medium reduction of the nuclear symmetry energy, as suggested by nuclear multifragmentation experiments. We demonstrate that this effect may lead to significant modifications of the nuclear composition and electron capture rates, which are important for stellar dynamics and nucleosynthesis.
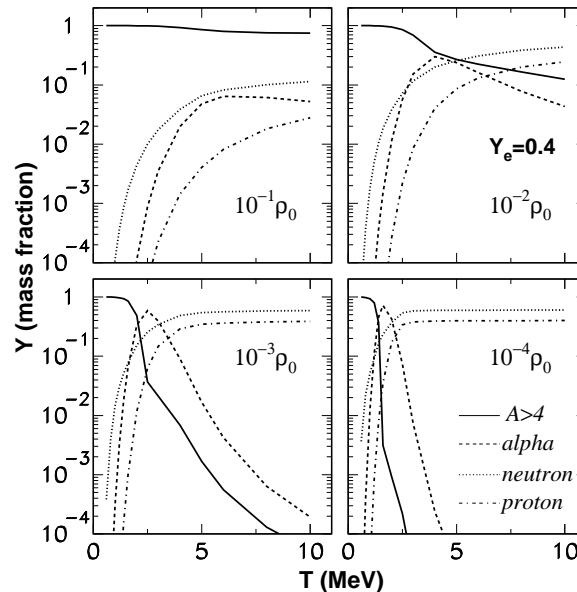
Mass fractions of nuclear species for stellar matter at Y_e=0.4 as functions of temperature. The results for baryon densities of 10^{-1}, 10^{-2}, 10^{-3}, $10^{-4} \rho_0$ are presented in the corresponding panels. Solid lines are for heavy nuclei ($A > 4$), dashed lines – α-particles, dotted lines – neutrons, dot-dashed lines – protons.

Related publications and talks in 2010:

1. A.S. Botvina, I.N. Mishustin, *Statistical approach for supernova matter,* Nucl. Phys. A 843, 98-132 (2010).
2. A.S. Botvina and I.N. Mishustin, *Statistical approach for supernova matter and nuclear multifragmentation*, International Conference on Nuclear Physics "NUCLEUS 2010" (ICNP2010): Methods of nuclear physics for femto- and nanotechnologies, Saint-Petersburg, Russia, July 6-9, 2010.

# Strong electric fields induced on a sharp stellar boundary

Collaborators: I.N. Mishustin[1], C. Ebel[1], W. Greiner[1],

[1] Frankfurt Institute for Advanced Studies

Due to a first order phase transition, a compact star may have a discontinuous distribution of baryon as well as electric charge densities, as e.g. at the surface of a strange quark star or inside of a hybrid star. If the matter is composed of several species with opposite electric charges and different masses, the presence of a sharp discontinuity should lead to a charge separation and generation of an electric field. For a macroscopic object like a star the condition of global charge neutrality must hold to a very high precision. Therefore, the positive charge of quarks or protons must be fully neutralized by the negative charge of electrons. However, since electrons are light and interact only via the electromagnetic force, they will penetrate through the phase boundary and generate a local charge disbalance around the discontinuity surface. The induced electrostatic potential $\phi(z)$ is determined from the 1d Poisson equation

$$\frac{d^2\phi}{dz^2} = -e\left[\rho_p(z) - \rho_e(z)\right] , \qquad (1)$$

where $e = \sqrt{4\pi\alpha}$=0.3028 is the proton charge and α is the fine-structure constant. For a given proton distribution the electron charge distribution $\rho_e(z)$ should be determined self-consistently. For this purpose we use the relativistic Thomas-Fermi approximation which should work well for an extended object like a heavy nucleus or star. We have solved numerically this equation assuming a Woods-Saxon distribution for the positive charge density. It is demonstrated that the strength of the electric field depends strongly on the diffuseness parameter a characterizing this distribution. For a<10 pm even supercritical electric fields may be produced in the vicinity of such a discontinuity. In a rotating star, the relative motion of electrons against of the positively-charged core may lead to the generation of a magnetic field which strength is proportional to the rotation frequency (see more in [2]).
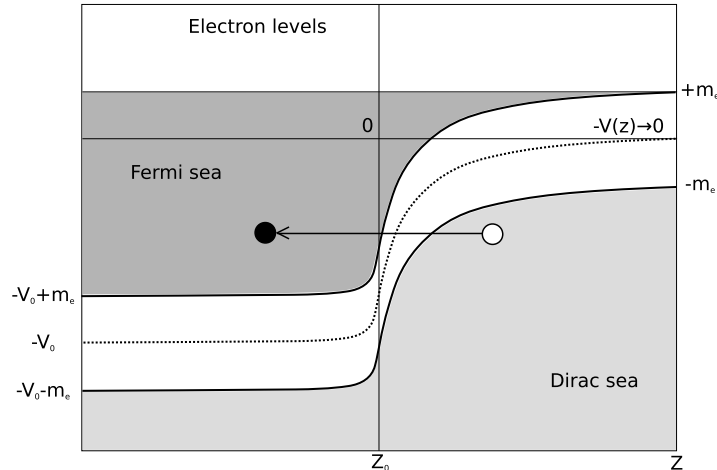
Schematic view of the electron energy levels in a strong electrostatic potential $-V(z) \equiv -e\phi(z)$. The electron states above (Fermi sea) and below (Dirac sea) the mass gap (white area) are shown by dark and grey shadowing. Despite the fact that the field is supercritical ($\Delta V > 2m_e$), the transitions from Dirac to Fermi sea (long arrow) are not allowed because all states in the Fermi sea are occupied.

## Related publications and talks in 2010:

1. Igor N. Mishustin, Claudio Ebel and Walter Greiner, *Strong electric fields induced on a sharp stellar boundary*, J. Phys. G: Nucl. Part. Phys. 37, 075201 (2010); arXiv:1002.2541v1 [astro-ph.SR].

2. Rodrigo Picanco Negreiros, Igor N. Mishustin, Stefan Schramm, Fridolin Weber, *Properties of Bare Strange Stars Associated with Surface Electric Fields*, Phys. Rev. D 82, 103010(6) (2010); arXiv:1008.0277 [astro-ph.HE].

Inner crusts of neutron stars in strongly quantising magnetic fields

Collaborators: I.N. Mishustin[1], W. Greiner[1], R. Nandi[2], D. Bandyopadhyay[2]

[1] Frankfurt Institute for Advanced Studies, [2] Saha Institute of Nuclear Physics, Calcutta, India

We study the properties and stability of nuclei in the inner crust of neutron stars in the presence of strong magnetic fields $B \sim 10^{17}$ G. Because of their larger magnetic moment, only electrons are affected by the magnetic fields of this strength. Landau quantization in the presence of strong magnetic fields leads to the modification of the electron phase-space occupation, that results in the decreasing electron chemical potential at given baryon density. This in turn leads to enhancement of electron as well as proton fractions at baryon densities ~ 0.001 fm^{-3}. It is assumed that each nucleus is residing in a Wigner-Seitz cell on the background of uniform neutron and electron gases. The calculations are done within the Thomas-Fermi approximation at zero temperature. The properties of nuclei (mass and charge numbers) are determined by using the subtraction procedure proposed by Bonche, Levit and Vautherin. The equilibrium nucleus at each average baryon density is found by minimising the free energy of the system with respect to all variational parameters including the WZ cell radius. It turned out that the total free energy of matter in the presence of strong magnetic field is lower as compared with the field free case. As one can see from the figure, nuclei with larger mass and charge numbers are obtained in the presence of strong magnetic fields. One can notice that our results in certain cases show oscillations around the field free level. This may be attributed to the fact that the population of Landau levels jumps from a few levels to zero in the above mentioned fields as baryon density decreases from higher to lower values.
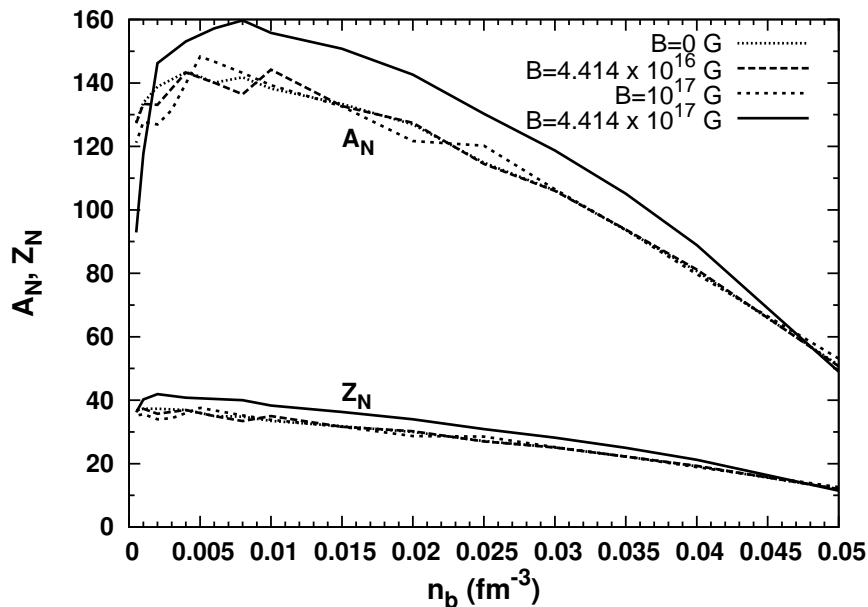
Total nucleon (A_N) and proton numbers (Z_N) in a nucleus are plotted as a function of average baryon density for magnetic fields $B = 0$, 4.414×10^{16}, 10^{17} and 4.414×10^{17} G. As one can see, in the strongest field up to 5 additional protons and 20 additional neutrons may be kept in the nuclei at average baryon densities around 0.01 fm^{-3}.

Related publications in 2010:

1. Rana Nandi, Debades Bandyopadhyay, Igor N. Mishustin and Walter Greiner, *Inner crusts of neutron stars in strongly quantizing magnetic fields*, submitted to Astrophys. J.; arXiv:1012.5970 [astro-ph.HE].

Possibility of synthesizing superheavy elements in nuclear explosions

Collaborators: I.N. Mishustin[1], W. Greiner[1], A. Botvina[1,2], V. Zagrebaev[1,3]

[1] Frankfurt Institute for Advanced Studies, [2] Institute for Nuclear Research, RAS, Moscow, [3] Joint Institute of Nuclear Research, Dubna

We study the possibility of synthesizing heavy and superheavy elements by using intensive neutron fluxes generated by nuclear explosions. Actually, this method was already partially employed alongside with nuclear reactors. However, because of some technical and political constraints it was abandoned later. Nevertheless, this method provides the highest neutron densities which are not possible to reach with other terrestrial techniques. The typical fusion reactions like ^{238}U + ^{48}Ca lead to proton-rich compound nuclei which lie above the β-stability line. On the other hand, the multiple neutron-capture reactions in nuclear explosions may bring the ^{238}U nuclei to the neutron drip-line. Then, after the neutron flux ceased, these nuclei undergo multiple β-decay and come close to the island of stability from the neutron-rich side. If a single explosion is insufficient, then, in principle, a properly delayed second explosion can do the job.
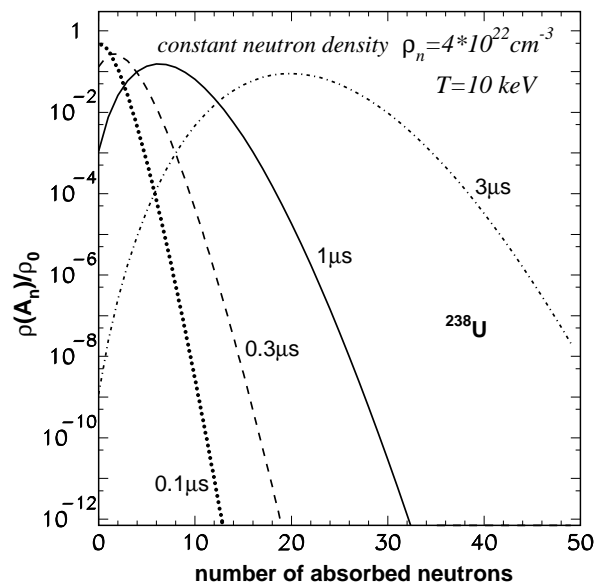
Relative abundances of neutron-rich nuclei produced after capture of neutrons normalized to the initial number of ^{238}U nuclei. It is assumed that a ^{238}U target is irradiated by a constant neutron flux of about $7 \cdot 10^{30}$ n/(s·cm^2) corresponding to neutron density and temperature given in the figure. Calculations are done for different exposure times (in microseconds) indicated at the corresponding curves.

Related publications in 2010:

1. Alexander Botvina, Igor Mishustin, Valeri Zagrebaev and Walter Greiner, *Possibility of synthesizing superheavy elements in nuclear explosions*, Int. J. Mod. Phys. 19,2063-2075 (2010);

2. Igor Mishustin, *Production of heavy and superheavy nuclei in explosive processes*, invited talk at the International Symposium "Advances of Nuclear Physics in Our Time" (Goa, India, Nov. 28 - Dec. 2, 2010), to be published in Proceedings.

# Modeling nuclear fragmentation reactions for cancer therapy applications

Collaborators: I.N. Mishustin[1], W. Greiner[1], I.A. Pshenichnov[1,2], A.S. Botvina[1,2]

[1] Frankfurt Institute for Advanced Studies, [1] Institute for Nuclear Research, RAS, Moscow

Recent developments of the Monte Carlo Model for Heavy-Ion Therapy (MCHIT) developed in FIAS were presented in two journal publications [1,2] and in a conference talk [3]. The major advancement of the model concerns the modelling of violent fragmentation reactions induced by light projectiles by means of the Fermi break-up model, and by heavy projectile nuclei by means of the Statistical multifragmnetation model.

By means of MCHIT we study the dose distributions from therapeutic beams of carbon nuclei in tissue-like materials, like water and PMMA. The contributions to the total dose from primary beam nuclei and from charged secondary fragments produced in nuclear fragmentation reactions are calculated. The build-up of secondary fragments along the beam axis is calculated and compared with available experimental data. Finally, we demonstrate the impact of violent multifragment decays on energy distributions of secondary neutrons produced by carbon nuclei in water.

With the MCHIT we are able to calculate not only the 3d distributions of the energy deposition but also the characteristics of secondary fragments which determine the tail beyond the Bragg peak. Further improvements are introduced into the MCHIT model to calculate the dose distributions on cellular (micrometer) scales. First results of microdosimetry simulations are in a good agreement with recent GSI measurements.
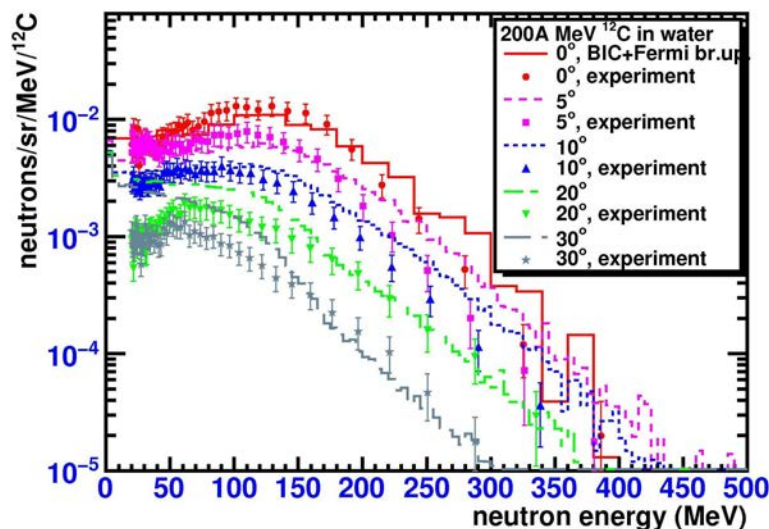
Calculated energy spectra of neutrons produced by 200 A MeV ^{12}C beam in a water phantom (various histograms) at 0°, 5°, 10°, 20° and 30° to the beam axis. The MCHIT results obtained with the Light-Ion Binary cascade model connected with the Fermi break-up model are shown. Experimental data by Gunzert-Marx et al., 2004, are shown by various symbols explained in the legend.

Related publications and talks in 2010:

1. I. Pshenichnov, A. Botvina, I. Mishustin, W. Greiner, *Nuclear fragmentation in extended media studied with Geant4 toolkit*, Nucl. Instr. Meth. Phys. Research B 268 (2010) 604; arXiv:0911.2017v1 [physics.med-ph].

2. I. Mishustin, I. Pshenichnov, W. Greiner, *Modelling heavy-ion energy deposition in extended media*, Eur. Phys. J. D 60 (2010) 109.

3. Igor Mishustin, *Monte Carlo Simulations of Ion-beam Cancer Therapy: from Nuclear Fragmentation to Microdosimetry*, International Conference "Dynamics of Systems on the Nanoscale", NRC, Rome, Italy, November 16-19, 2010.
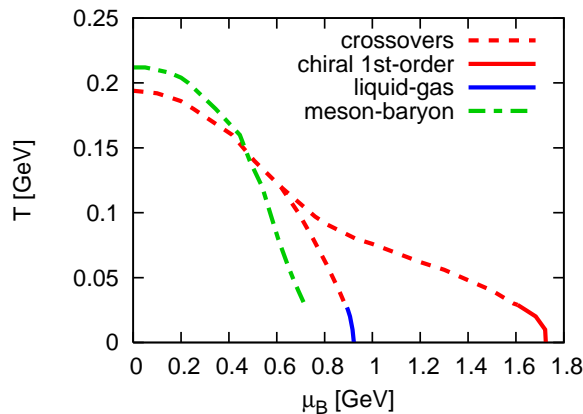
Thermodynamics of dense hadronic matter in chiral models

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

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

Model studies of hot and dense matter have suggested a rich phase structure of QCD at temperatures and quark chemical potentials of order Λ_{QCD}. Our knowledge on the phase structure however remains limited and in particular, properties of baryons near the chiral symmetry restoration are poorly understood. The realistic modeling of dense baryonic matter must take into account the existence of the nuclear matter saturation point, i.e. the bound state at baryon density $\rho_0 = 0.16$ fm^{-3}, like in Walecka type models. In this work we applied a parity doublet model to a hot and dense hadronic matter and explored the phase structure of a chiral symmetry restoration as well as a liquid-gas transition of nuclear matter. In the Figure we show the phase diagram of this model in mean field approximation. The liquid-gas transition survives up to $T = 27$ MeV. Above this temperature there is no sharp phase transition but the order parameter is still attracted by the critical point: the order parameter typically shows a double-step structure and this makes an additional crossover line terminating at the liquid-gas critical point. Another crossover line corresponding to the chiral symmetry restoration follows the steepest descent of the second reduction in $\langle\sigma\rangle$. With increasing temperature the two crossover lines become closer and finally merge.

In contrast, the trajectory of a meson-to-baryon "transition" defined from the ratio of particle number densities is basically driven by the density effect with the hadron masses being not far from their vacuum values. The line is almost independent of the parameter set and goes rather close to the liquid-gas transition line. The chiral crossover and the meson-baryon transition lines intersect at $(T, \mu_B) \sim (150, 450)$ MeV. The parity doublet model thus describes 3 domains: a chirally broken phase with mesons thermodynamically dominating, another chirally broken phase where baryons are more dominant and the chirally restored phase, which can be identified with quarkyonic matter. It is worthy to note that this intersection point is fairly close to the estimated triple point at which hadronic matter, quarkyonic matter and quark-gluon plasma may coexist.

In the mirror assignment of chirality to nucleons, dynamical chiral symmetry breaking generates a mass difference between parity partners and the chiral symmetry restoration does not necessarily dictate the chiral partners to be massless. The origin of a nucleon mass constrained by the scale anomaly in QCD is currently under investigation.

The phase diagram of a two-flavored parity doublet model.

Related publication in 2010:

1) C. Sasaki and I. Mishustin, *Thermodynamics of dense hadronic matter in a parity doublet model*, Phys. Rev. C 82, 035204 (2010).

Vector mesons at finite temperature and QCD sum rules

Collaborators: Y. Kwon[1], C. Sasaki[2], W. Weise[1]

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In this work we have constructed finite energy sum rules (FESR) in order to study the behavior of ρ and a_1 mesons as well as their mixing at finite temperature, with the aim of exploring the pattern of chiral symmetry restoration. The sum rules for the lowest two spectral moments of vector and axial vector spectral functions involve only the leading QCD condensates as corrections. With inclusion of perturbative QCD terms up to order α_s^3, these sum rules permit a reliable quantitative analysis, unaffected by the large uncertainties from condensates of higher dimension such as the four-quark condensates.

In the large-N_c limit, schematic distributions with delta-function resonances and a step-function parametrization of the high-energy continuum, when inserted in the FESR analysis, reproduce the well-known current algebra and chiral sum rules. As an interesting feature one finds that, at zero temperature, the continuum threshold s_V in the vector channel is identified with the scale characteristic of spontaneous chiral symmetry breaking: $\sqrt{s_V} = 4\pi f_\pi$. Above this scale chiral symmetry is restored in its Wigner-Weyl realization. In the resonance region below this scale, the symmetry is in the spontaneously broken Nambu-Goldstone realization.

When realistic spectral functions with large widths are implemented, this 'clean' separation of scales is no longer rigorously maintained, but the FESR analysis is still useful, with the pole mass in the vector correlator now replaced by the normalized first moment of the spectral distribution. Within its range of applicability (up to temperatures of about 140 MeV), the sum rule analysis consistently shows an almost constant behavior of this average vector meson spectral mass. The primary temperature dependence of the spectral function comes from $\rho - a_1$ mixing in the thermal pionic medium. The a_1 mass, again identified with the normalized first moment of the axial-vector spectral distribution, decreases with rising temperature. This indicates the expected tendency of the ρ and a_1 spectra becoming identical (degenerate) when chiral symmetry is restored. The continuum threshold scale s_V in the vector channel (even when smoothed by a ramping function) systematically moves downward in energy as the temperature increases. This feature is observed in all cases studied. However, while the identification of $\sqrt{s_V}$ with the chiral scale $4\pi f_\pi$ emerges naturally at $T = 0$, the downward evolution with temperature of $\sqrt{s_V}$ is significantly slower than that of $f_\pi(T)$ deduced from chiral perturbation theory.
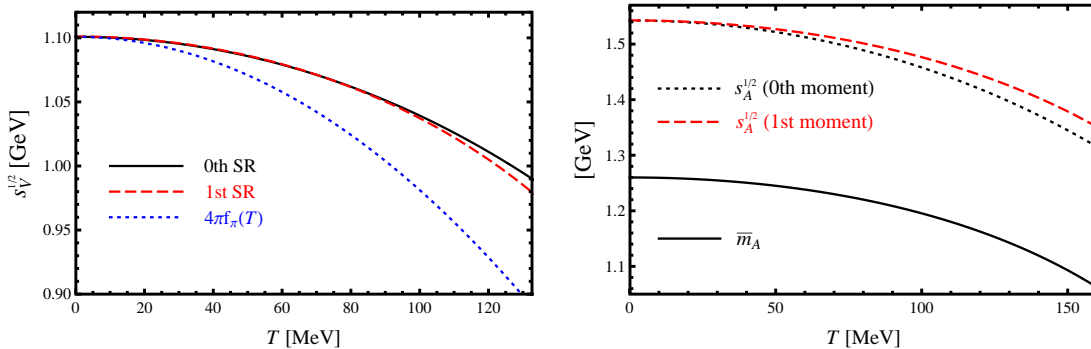
Left: Continuum threshold $\sqrt{s_V}$ in the vector meson channel as a function of T obtained from the sumrules for the 0th (black solid line) and 1st (red dashed line) moment of the spectral function. The T-dependence of chiral scale $4\pi f_\pi(T)$ (blue dotted line) is also displayed. Right: Same in the axial-vector channel. In contrast to the ρ meson, the a_1-meson mass (black dotted line) decreases with rising temperature.

Related publication in 2010:

1) Y. Kwon, C. Sasaki and W. Weise, *Vector mesons at finite temperature and QCD sum rules*, Phys. Rev. C 81, 065203 (2010).

Lattice QCD calculation of Taylor expansion coefficients with respect to chemical potential

Collaborators: O. Kaczmarek[1], F. Karsch[1,2,3], E. Laermann[1], C. Miao[2], S. Mukherjee[2], P. Petreczky[2] C. Schmidt[3,4], W. Söldner[3,4], W. Unger[3,4]

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Lattice QCD calculations at nonzero chemical potential by means of standard Monte Carlo methods are impossible due to the notorious sign problem. In order to extent first principle lattice QCD calculations to small but nonzero chemical potentials and circumvent the sign problem, we perform a calculation of Taylor expansion coefficients of the pressure and the chiral condensate (chiral order parameter). Numerical calculations have been performed with an improved staggered fermion action (p4) for (2+1)-flavor QCD. The heavier strange quark mass is kept close to its physical value, while the degenerate light quark masses are decreased towards the massless limit.

The Taylor expansion coefficients of the pressure (as shown in the left plot) are of direct interest to the phenomenology of heavy ion collisions, as they are directly connected to moments of the fluctuation of conserved charges such as baryon number, electric charge and strangeness. Of great interest are also ratios of these moments, such as e.g. the kurtosis. Here the dependence on the interaction volume as well as on the mass spectrum of the theory is completely suppressed. The leading order dependence of the kurtosis on the baryon chemical potential along the freeze-out curve as a function of the center of mass energy is shown in the right plot.
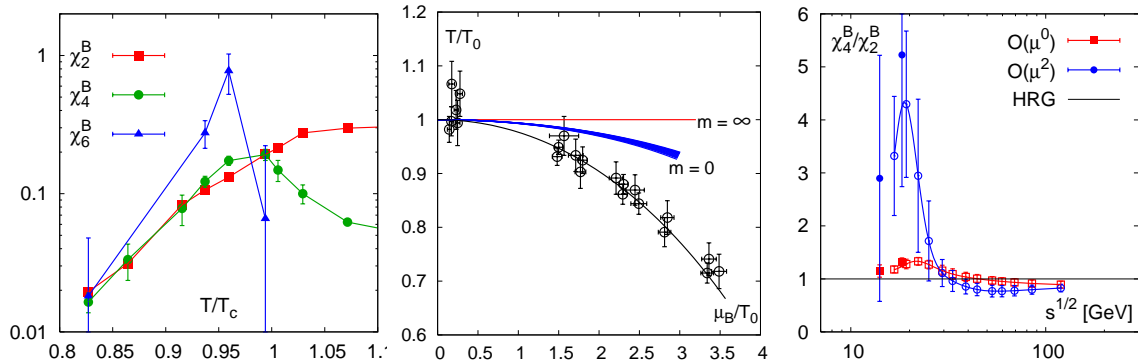
Moments of the baryon number fluctuations (left), phase boundary in the chiral limit and freeze-out line (middle) and ratio of baryon number fluctuations (kurtosis) along the freeze-out curve (right).

The Taylor expansion coefficients of the chiral condensate provide access to the critical behavior of QCD. By matching the order parameter and its (mixed) susceptibilities to corresponding scaling functions we obtain the scaling fields. The mixing of the reduced temperature and the chemical potential yields the curvature of the critical line in the chiral limit as show in the middle plot. As a result we obtain $T_c(\mu_B)/T_c(0) = 1 - 0.0066(7)(\mu_B/T)^2 + \mathcal{O}((\mu_B/T)^4)$. We thus find that the curvature of the critical line is about a factor of 3-4 smaller than the experimentally obtained freeze-out curve (also shown in the middle plot).

Related publications in 2010:
1) F. Karsch, E. Laermann, C. Miao, S. Mukherjee, P. Petreczky, C. Schmidt, W. Soeldner, W. Unger, to be published in Phys. Rev. D; [arXiv:1011.3130[hep-lat]].
2) M. Cheng, *et al.* [RBC-Bielefeld Collaboration]; arXiv:1010.1216 [hep-lat].
3) C. Schmidt, arXiv:1012.2230[hep-lat].
4) C. Schmidt and S. Mukherjee, PoS (Lattice 2010) 214; [arXiv:1012.2231[hep-lat]].
5) C. Schmidt, Prog. Theor. Phys. Supplement No. 186 (2010) 563; [arXiv:1007.5164 [hep-lat]].

# Determination of the chiral critical line of (2+1)-flavor QCD

Collaborators: P. de Forcrand[1], O. Philipsen[2], C. Schmidt[3,4], D. Smith[3,4]

[1] ETH Zürich, Switzerland, [2] Goethe-Universität, Frankfurt am Main, Germany, [3] GSI, Darmstadt, Germany, [4] FIAS, Frankfurt am Main, Germany.

The project aims on an analysis of the critical behavior of QCD. We utilize the framework of lattice QCD and perform simulations with two light and one heavy quark flavor. Within this quark mass plane we plan to map out the critical line that separates the region where the QCD transition is of first order, from the region where the transition is a crossover. In previous works this line has been determined on coarse lattices, with four points in time direction. With this project we want to analyze the cutoff effects of the critical line by going to finer lattices. It will be interesting to estimate the tri-critical point, which is the endpoint of this line in the chiral limit of the two light flavors. Only if the mass of tri-critical point (the heavy flavor mass) is of the order of the physical strange quark mass or larger, it has a change to affect the critical behavior of QCD at the physical quark mass point.

Furthermore, we want to analyze the dependence of this critical line on a chemical potential. In order to do so we plan to investigate the response of several thermodynamical quantities on a small baryon chemical potential. By a comparison with well known scaling functions and fitting all non-universal constants we will be able to determine the curvature of the critical surface. This completely new method can be confronted with results from the previously used Binder cummulant method.

The simulations will be performed on GPUs. A code for dynamical staggered fermions have been developed using CUDA. It will be used on the GPU-Scout cluster at the Center for Scientific Computing (CSC) at the Goethe University of Frankfurt. We are currently porting the code to OpenCL in order to gain more flexibility in the GPU type. This will enable us to effectively use the new LOEWE cluster at CSC.
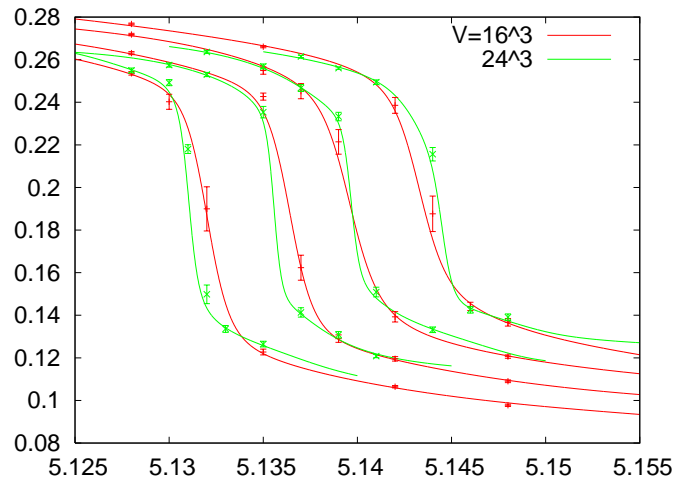
The chiral condensate as a function of the inverse coupling $\beta = 6/g^2$ on $N_\tau = 4$ lattices. The degenerated quark masses are $am_q = am_s = 0.024, 0.026, 0.028, 0.030$ (from left to right). The reproduction of previous $N_\tau = 4$ results proves the correctness of the CUDA code.

Related publication in 2010:

1) D. Smith, *Effective potential for Polyakov loops from a center symmetric effective theory in three dimensions*, Phys. Rev. D 82, 034503 (2010) [arXiv:0911.4037 [hep-lat]].

An effective chiral Hadron-Quark Equation of State

Collaborators: J. Steinheimer[1], S. Schramm[1], H. Stöcker[1,2,3]

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We developed an approach for modeling an EoS that respects the symmetries underlying QCD, and includes the correct asymptotic degrees of freedom, i.e. quarks and gluons at high temperature and hadrons in the low-temperature limit. We achieve this by including quarks degrees of freedom and the thermal contribution of the Polyakov loop in a hadronic chiral sigma-omega model. The hadrons are suppressed at high densities by excluded volume corrections. Nevertheless, we observe a substantial hadronic contribution to the EoS up to temperatures of 2 times T_c. We can show that the properties of the EoS are in qualitative agreement with lattice data at $\mu_B = 0$. Various quantities, like the pressure and energy density, are in good agreement with lattice data. Deviations from lattice results can be explained by the hadronic contributions and volume corrections. In spite of a continuous phase transition, we obtain a considerably smaller value for the speed of sound when compared to lattice calculations. At finite baryon density, the transition from deconfined to confined matter proceeds as a smooth crossover for all values of μ_B. The same is true for the chiral phase transition (except the liquid gas phase transition, which is of first order at very low temperatures). At high chemical potentials and low temperatures we find a very interesting phase structure. In this region chiral symmetry is partially restored, while deconfinement is not yet realized, thus creating an exotic form of matter.
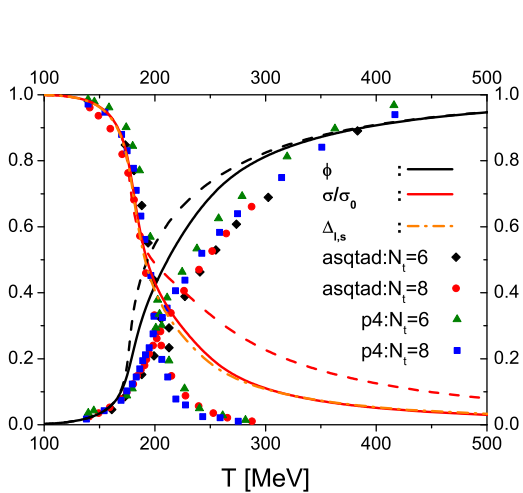

Figure 1: *The normalized order parameters for the chiral (red lines), and deconfinement (black line) phase transition as a function of T at $\mu_B = 0$. The symbols denote lattice data.*
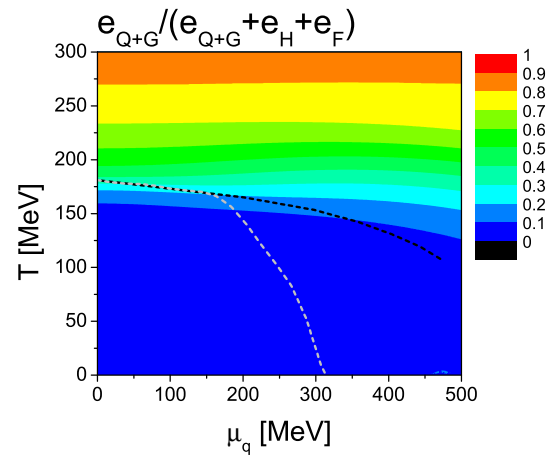

Figure 2: *Contour plot of the fraction of the total energy density which comes from the quark contribution and the Polyakov loop potential. The dashed grey line indicates the crossover of the chiral condensate while the solid black line shows the crossover for the Polyakov loop.*

Related publications in 2010:
J. Steinheimer, S. Schramm, H. Stöcker, *An Effective chiral Hadron-Quark Equation of State*, to be published in J. Phys. G; arXiv:1009.5239 [hep-ph].
S. Schramm, J. Steinheimer, V. Dexheimer, H. Stöcker, *Phase structure of strongly interacting matter and simulations of heavy-ion collisions using a quark-hadron model*, J. Phys. G 37, 094041 (2010).
J. Steinheimer, S. Schramm, *The problem of repulsive quark interactions – Lattice versus mean field models*, to be published in Phys. Lett. B; arXiv:1005.1176 [hep-ph].

Mach Shock Waves in Nuclear Collisions

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

[1] Frankfurt Institute for Advanced Studies, [2] Institut für Theoretische Physik, Goethe Universität Frankfurt, [3] Center for Scientific Computing, Frankfurt, [4] GSI – Helmholtzzentrum für Schwerionenforschung, Darmstadt.

We study the formation and propagation of high density compression waves in asymmetric nucleus-nucleus collisions. Therefor we use a (3+1)-dimensional ideal relativistic hydrodynamics code with different freeze-out methods to study Ne+U collisions at 0.5–20 AGeV and compare the results to UrQMD transport model calculations. In the hydrodynamic picture a Mach shock wave is formed and leads to a conical particle emission scheme with distinct peaks at Mach angles. In the transport model binary nucleon-nucleon scattering results in a particle emission pattern which approximates the shape of a boosted thermal distribution. We state that a Cooper Frye freeze-out kills the Mach cone signal by superimposing a major boosted thermal distribution (see figure, lhs).

For the calculation of an equation of state that ensures a realistic description of strongly interacting matter as a substantial input for hydrodynamic calculations we use an effective chiral hadronic model that includes all known hadrons and resonances up to 2.2 GeV. This framework allows us to study the influence of baryonic resonances on the phase structure, i.e. in particular on the order and location of a phase transition and the possible existence of a critical endpoint (see figure, rhs).

(a)　　　　　　　　　(b)
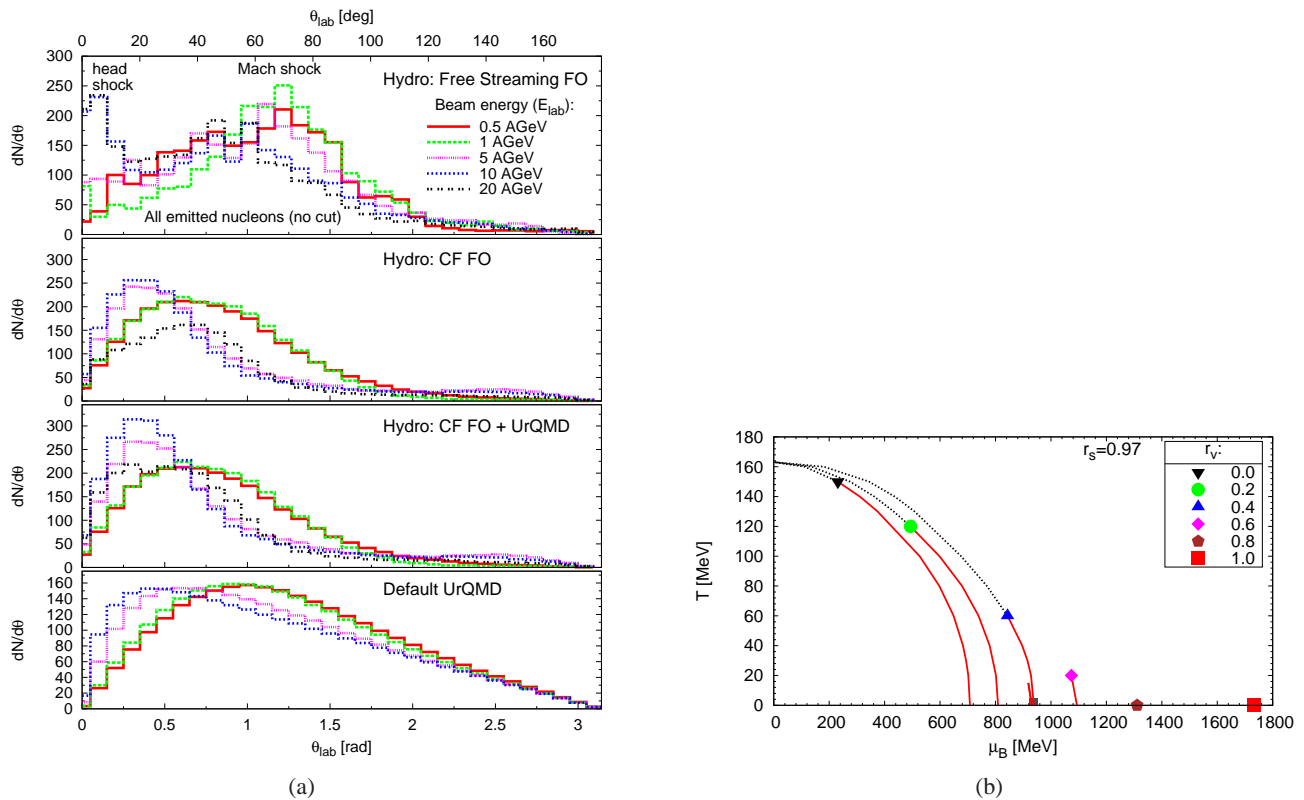
a: Angular spectra from Ne+U from hydrodynamics with different freeze-out methods and from UrQMD transport. b: Phase diagram from chiral hadronic model with varied vector couplings.

Related publications in 2010:

1) P. Rau, J. Steinheimer, B. Betz, H. Petersen, M. Bleicher, H. Stöcker, *Conical Emission from Shock Waves in Ne(1-20 AGeV)+U Collisions*, arXiv:1003.1232 [nucl-th].
2) P. Rau, J. Steinheimer, S. Schramm, H Stöcker, *Chiral Hadronic Model for the QCD Equation of State*, paper in preparation.

Research Report by Marcus Bleicher

Collaborators: M. Bleicher, E. Bratkovskaya, E. Santini, G. Moschelli, M. Hauer, B. Bäuchle, M. Nahrgang, C. Herold, J. Steinheimer, G. Graef, V. Lindenstruth, J. Gerhard, H. Stöcker, I. Mishustin

Hybrid+Boltzmann approach
A new modular hybrid transport approach was successfully developed and used to simulate heavy-ion reactions in the FAIR/SPS energy domain. The model is based on the combination of a kinetic theory to describe the early and late phase of the collision with an effective hydrodynamic model for the high density phase. It incorporates a phase transition to the Quark Gluon Plasma (QGP) by means of different equations of state. The model was used for several studies of QCD-Matter at FAIR energies. Among the observables studied were the production of phi mesons and direct photons, Hanburry-Brown-Twiss correlations, event-by-event fluctuations and elliptic flow of hadrons. New insights were gained by comparing the results of simulations with and without a phase transition to a QGP. First studies were made to combine the hybrid model with a parton cascade.

Multi-particle interactions
Various techniques and implementations of multi-particle interactions have been performed within the Boltzmann Approach to Multi-Particle Scattering (BAMPS) framework. A strong influence of the three-particle interactions on the chemical equilibration times, the elliptic flow and the effective viscosity of the QCD medium has been found. First steps towards an implementation of multi-particle interactions into the hadronic cascade model Ultra-relativistic Quantum Molecular Dynamics (UrQMD) have been done. Here parton rearrangement processes were implemented and the resulting effects were studied.

Modeling of the phase transition out of equilibrium
A new model to study fluctuations at the critical point was developed. It is based on the coupling of the chiral field equations to hydrodynamic simulations. First studies have shown that the correlation length might be shorter than previously expected because of a more realistic modeling of the collision dynamics.

Off-shell transport approach with quasi particles
A hybrid-transport model, Parton-Hadron-String Dynamics (PHSD) has been developed. It includes an equation of state for the QGP adopted from lattice QCD calculations of the Bielefeld group. The basic idea is to describe the properties of QCD adequately within the dynamical quasi-particle model (DQPM). In this case the dressed propagator for quarks and gluons is given explicitly by means of complex self-energies. The latter include a real part, which describes dynamical mass generation as well as an imaginary part for the interaction rate of the effective degrees of freedom. The time-like part of the eight-dimensional distribution functions can be propagated within the light-cone using off-shell transport theory once the self-energies have been fixed in the DQPM. The hadronization process is described by means of Lorentz invariant transition rates based on Kadanoff-Baym dynamics. Applications to relativistic nucleus-nucleus collisions in the FAIR and SPS energy regime have been carried out.

Related publications in 2010:
1) E. Mount, G. Gräf, M. Mitrovski, M. Bleicher, M. Lisa: *Correspondence between HBT radii and the emission zone in non-central heavy ion collisions*, [arXiv:1012.5941]

2) F. Wang, M. Bleicher: *Nuclear absorption effects on Lambda-bar/p-bar ratio in heavy ion collisions*, [arXiv:1011.4289]

3) M. Nahrgang, M. Bleicher: *Non-equilibrium fluctuations at the QCD phase transition*, [arXiv:1011.5379]

4) K. Werner, Iu. Karpenko, T. Pierog, M. Bleicher, K. Mikhailov: *Evidence for Hydrodynamic Evolution in Proton-Proton Scattering at LHC Energies*, [arXiv:1010.0400]

5) Q. Li, C. Shen, M. Bleicher: *System-size dependence of the pion freeze-out volume as a potential signature for the phase transition to a Quark Gluon Plasma*, [arXiv:1009.3334]

6) E. Santini, M. Bleicher: *Low mass dimuons within a hybrid approach*, [arXiv:1009.5266]

7) B. Bäuchle, M. Bleicher: *Direct Photons from a Hybrid Approach − Exploring the parameter space*, [arXiv:1008.1862]

8) B. Bäuchle, M. Bleicher: *Direct photon calculations in heavy-ion collisions at $\sqrt{s_{NN}}$ = 62.4 - 200 AGeV in a (3+1) dimensional hybrid approach*, Phys. Rev. C82, 064901 (2010), [arXiv:1008.2332]

9) B. Bäuchle, M. Bleicher: *Transport and hydrodynamic calculations of direct photons at FAIR*, to be published in Phys. Lett. B, [arXiv:1008.2338]

10) K. Werner, Iu. Karpenko, T. Pierog, M. Bleicher, K. Mikhailov: *Event-by-Event Simulation of the Three-Dimensional Hydrodynamic Evolution from Flux Tube Initial Conditions in Ultrarelativistic Heavy Ion Collisions*, Phys. Rev. C82, 044904 (2010), [arXiv:1004.0805]

11) P. Rau, J. Steinheimer, B. Betz, H. Petersen, M. Bleicher, H. Stöcker: *Conical Emission from Shock Waves in Ne(1-20 AGeV)+U Collisions*, [arXiv:1003.1232]

12) B. Bäuchle, M. Bleicher: *Direct photon emission in Heavy Ion Collisions from Microscopic Transport Theory and Fluid Dynamics*, PoS BORMIO2010:062 (2010), [arXiv:1003.5454]

13) H. Petersen, M. Bleicher: *Eccentricity fluctuations in an integrated hybrid approach: Influence on elliptic flow*, Phys. Rev. C81, 044906 (2010). [arXiv:1002.1003]

14) S. Vogel, J. Aichelin, M. Bleicher: *Resonances as a possible observable of hot and dense nuclear matter*, J. Phys. G37, 094046 (2010). [arXiv:1001.3260]

15) G. Gräf, E. Santini, H. Petersen, J. Steinheimer, M. Mitrovski, M. Bleicher: *Strangeness production in hadronic models and recombination models*, J. Phys. G37, 094010 (2010), [arXiv:1001.4937]

16) B. Bäuchle, M. Bleicher: *Calculations of direct photon emission in Heavy Ion Collisions at $\sqrt{s_N N}$ = 200 GeV*, J. Phys. Conf. Ser. 230, 012033 (2010), [arXiv:1008.1866]

17) J. Steinheimer, H. Petersen, M. Mitrovski, M. Bleicher: *Strangeness production at SPS energies in a (3+1)-dimensional Boltzmann+hydrodynamics approach*, J. Phys. G37, 094038 (2010)

Dynamical equilibration of the strongly interacting parton-hadron matter

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

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

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 transition from initial pure partonic matter to hadronic degrees of freedom (or vice verse) occurs dynamically by interactions, if the energy local density is below critical. The size of box is fixed to 9^3 fm^3. We start with light quarks, antiquarks and gluons with random space positions and the momenta distributed according to the Fermi-Dirac distribution, see Fig. 1(a). Note that the system is out of equilibrium initially.

For the equilibrated system we can extract a 'temperature' by fitting the particle energy spectra with the thermal distribution:

$$\frac{d^3 N_i}{dp^3} \sim A(E_i, p_i) \exp(-E_i/T),$$

where $E_i = \sqrt{p_i^2 + m_i^2}$ is the energy of each particle. In the thermal equilibrium the spectra of all particle species can be characterized by one single slope. This is illustrated in Fig. 1(b). The deviations from the Boltzmann distribution at low energy are due to the broad spectral functions of partons.
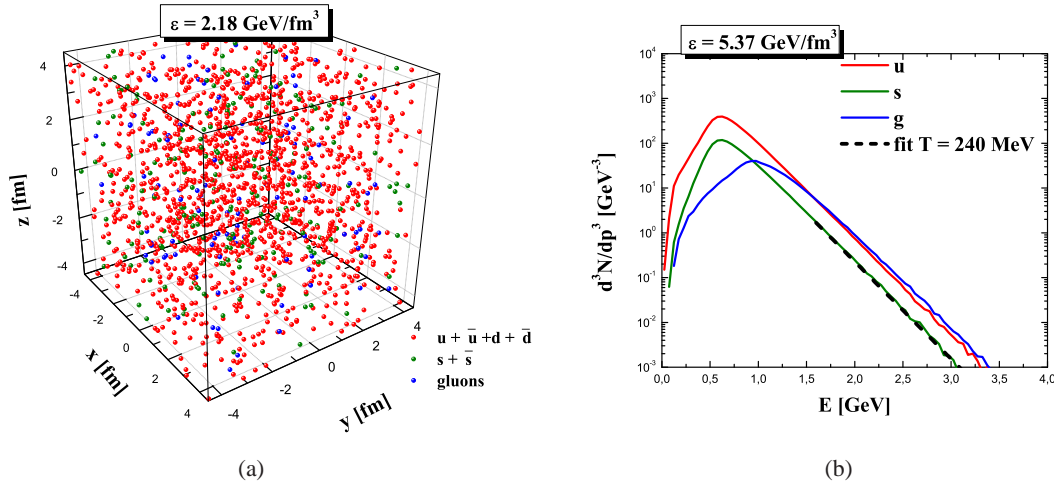

(a)   (b)

Figure 1: *(a) The systems, initialized by solely partons at an energy density of 2.18 GeV/fm^3. The positions of light (anti-)quarks are shown by red dots, of strange (anti-)quarks by green dots and of gluons with blue dots. (b) The energy spectra for the off-shell u (red) and s quarks (green) and gluons (blue) in equilibrium for a system initialized at an energy density of 5.37 GeV/fm^3.*

Related publication in 2010:
1)V. Ozvenchuk, E. Bratkovskaya, O. Linnyk, M. Gorenstein, W. Cassing, *Dynamical equilibration in strongly-interacting parton-hadron matter*, e-Print: arXiv:1101.0218 [nucl-th]

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

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

[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

To address the dilepton production in a hot and dense medium – as created in heavy-ion collisions – we employ an up-to-date relativistic transport model, i.e. the Parton Hadron String Dynamics (PHSD) that incorporates the explicit partonic phase in the early reaction region. The approach consistently describes the full evolution of a relativistic heavy-ion collision from the initial hard scatterings and string formation through the dynamical deconfinement phase transition to the quark-gluon plasma (QGP) as well as hadronization and to the subsequent interactions in the hadronic phase. Dilepton radiation by the quasiparticles proceeds dominantly via the following elementary processes: $q + \bar{q} \to \gamma^*$, $q(\bar{q}) + g \to \gamma^* + q(\bar{q})$, and $q + \bar{q} \to g + \gamma^*$. Note that in our calculations the running coupling α_S (which depends on the local energy density according to a parametrization of lQCD data) is of the order $O(1)$ and thus the contribution of the higher order diagrams is not subleading! Also, we take into account the non-perturbative spectral functions and self-energies of quarks and gluons thus going beyond the leading twist. By implementing the off-shell partonic processes into the PHSD transport approach, we calculate the dilepton spectra in $Au + Au$ at $\sqrt{s}$=200 GeV and compare to the PHENIX data in Figs. 1(a) and 1(b). In Fig. 1(a) we show the our results for low masses ($M = 0 - 1.2$ GeV); in this region, the yield in PHSD is dominated by hadronic sources and essentially coincides with the HSD result. There is a discrepancy between the PHSD calculations and the data in the region of masses from 0.2 to 0.6 GeV. The discrepancy is not amended by accounting for the radiation from the QGP, since the latter is 'over-shone' by the radiation from hadrons integrated over the evolution of the collision. In contrast, the partonic radiation is visible in the mass region $M = 1 - 4$ GeV as seen in Fig. 1(b). The dileptons generated by the quark-antiquark annihilation in the sQGP constitute about half of the observed yield in the mass range between the masses of the ϕ and the J/Ψ mesons. Thus, accounting for partonic radiation in PHSD fills up the gap between the hadronic model results and the data at $M > 1$ GeV.
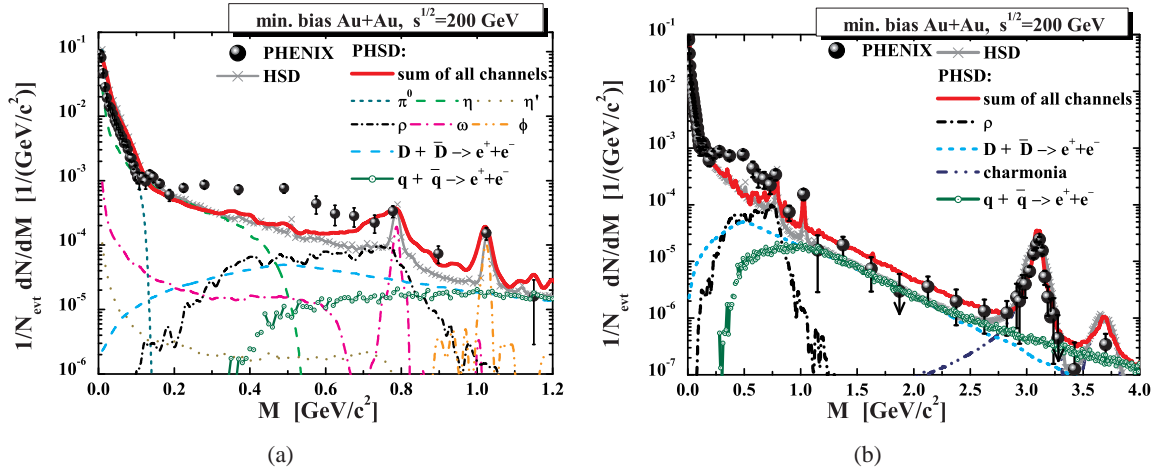

Figure 1: *(a) The PHSD results for the mass differential dilepton spectra in case of inclusive $Au + Au$ collisions at $\sqrt{s} = 200$ GeV in comparison to the data from PHENIX in the low mass region ($M = 0 - 1.2$ GeV). (b) The PHSD results for the mass differential dilepton spectra in case of inclusive $Au + Au$ collisions at $\sqrt{s} = 200$ GeV in comparison to the data from PHENIX for $M = 0 - 4$ GeV.*

Related publications in 2010:
1) O. Linnyk, W. Cassing, E. L. Bratkovskaya, J. Manninen, submitted to Nucl. Phys. A
2) O. Linnyk, arXiv:1004.2591
3) E. L. Bratkovskaya, O. Linnyk, W. Cassing, J. Phys.: Conf. Ser. 230 (2010) 012032
4) O. Linnyk, E. L. Bratkovskaya, W. Cassing, AIP Conf. Proc. 1257 (2010) 700
5) O. Linnyk, E. L. Bratkovskaya, J. Manninen, and W. Cassing, accepted to J. Phys.: Conf. Ser.

Di-jet correlations in heavy-ion collisions within the HSD transport approach

Collaborators: V.P. Konchakovski[1,2], E.L. Bratkovskaya[3,4], W. Cassing[1], M.I. Gorenstein[3,4]

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A systematic study of correlations in pseudorapidity and azimuthal angle for high-p_T charged hadrons in heavy-ion collisions at the top RHIC energy has been performed within the Hadron String Dynamics (HSD) transport approach. The study shows that a significant part of the high p_T hadron attenuation seen experimentally can be attributed to inelastic interactions of 'leading' pre-hadrons with the dense hadronic environment. It turns out that the 'far-side' correlations are suppressed by up to 60% in central collisions due to the pre-hadronic interactions in line with earlier studies. Since a much larger suppression is observed experimentally in central reactions there should be strong additional partonic interactions in the dense QGP medium created in Au+Au collisions at RHIC. Furthermore, our calculations do not show a 'ridge' in $\Delta\eta$ on the near-side which also indicates additional non-hadronic correlations.

The di-jet correlations are measured as a function of azimuthal angle $\Delta\phi$ and pseudorapidity $\Delta\eta$ between the trigger and associated particles: $C(\Delta\eta, \Delta\phi) = (1/N_{trig})(d^2 N_{assoc}/d\Delta\eta\ d\Delta\phi)$, where N_{trig} is the number of trigger particles. To obtain the di-jet correlations one has to subtract a background distribution. In our calculations we use the mixed events method which allows to properly subtract the background by taking associated particles for each trigger particle from another randomly chosen event.
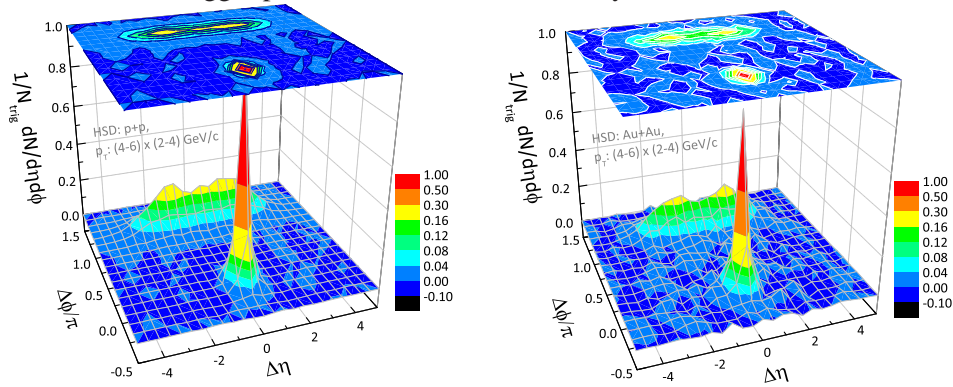
The associated particle $(\Delta\eta, \Delta\phi)$ distribution for p+p (top) and central Au+Au (bottom) collisions at $\sqrt{s} = 200$ GeV within the HSD transport approach.

In the figure we present the HSD results for p+p and Au+Au collisions for the associated differential particle $(\Delta\eta, \Delta\phi)$ distribution. We use the same cuts as the STAR Collaboration, $4 < p_T^{trig} < 6$ GeV/c and $2 < p_T^{assoc} < 4$ GeV/c. In the HSD transport calculations we obtain on average 0.5 trigger particle in an event for this set of cuts. The away side structure is suppressed in Au+Au collisions in comparison to p+p, however, HSD doesn't provide enough high p_T suppression to reproduce the Au+Au data. The additional suppression should be attributed to a QGP produced at relativistic heavy-ion collisions. The di-jet correlations obtained in the HSD transport simulations of Au+Au collisions (cf. Figure), furthermore, do not show a ridge structure in the pseudorapidity for the near-side jet as in the data.

We conclude that the HSD hadron-string medium does not show enough suppression for the away-side jet-associated particles. For the first time the medium response on the interactions has been taken into account in the present non-perturbative HSD calculations. The non-perturbative calculations, however, do not reproduce the long-range rapidity correlations for the near-side jet while supporting the results from perturbative investigations. It is interesting to check in future whether the recently proposed Parton Hadron String Dynamics model (PHSD) – incorporating explicit partonic degrees of freedom and dynamical hadronization – will be able to reproduce the observed structures.

Related publications in 2010:
1) V. P. Konchakovski, E. L. Bratkovskaya, W. Cassing and M. I. Gorenstein, Phys. Rev. C 82, 037902 (2010).
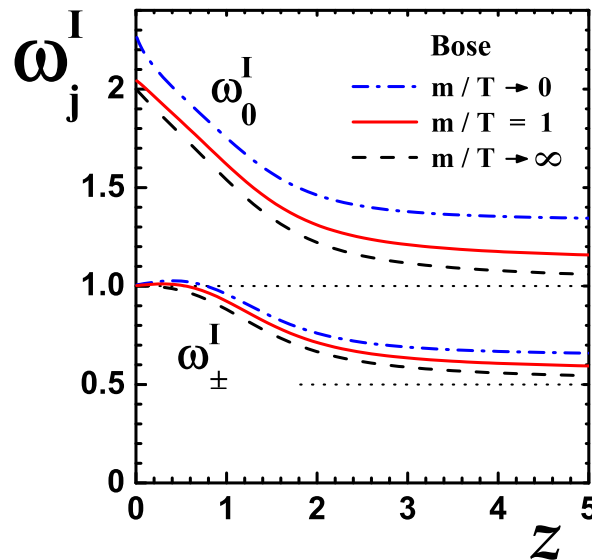
Pion Number Fluctuations and Correlations in the Statistical System with Fixed Isospin

Collaborators: V.V. Begun[1,2], M.I. Gorenstein[1,2], O.A. Mogilevsky[1]

[1] Bogolyubov Institute for Theoretical Physics, Kiev, Ukraine, [2] Frankfurt Institute for Advanced Studies

Successful application of the statistical model to the description of mean hadron multiplicities in high-energy collisions has stimulated investigations of properties of statistical ensembles. It was recently found that even in the thermodynamic limit, results for the scaled variance $\omega = (\langle N^2 \rangle - \langle N \rangle^2)/\langle N \rangle$ are different in different ensembles. Hence the equivalence of ensembles holds for mean values in the thermodynamic limit, but does not extend to fluctuations. Our primary interest in the present study is to analyze an influence of non-Abelian (non-additive) charge conservation on the particle number fluctuations. We restrict our consideration to the simplest statistical system with non-Abelian symmetry – an ideal pion gas with zero isospin $I = 0$.

We have found that for finite systems, one observes a suppression of the average total pion number and an increase of the pion number fluctuations. The suppression effects due to isospin conservation are the same for average numbers of π^0, π^+, and π^-. However, we find quite different behavior of the corresponding scaled variances. For neutral pions, there is the enhancement of the fluctuations; whereas for charged pions, the isospin conservation suppresses fluctuations.

Scaled variances for neutral ω_0^I and charged pions $\omega_\pm^I$ in the Bose gas with $I = 0$ as a function of one-particle partition function that is proportional to the system size and multiplicity. The solid lines correspond to mass to the temperature ratio $m/T = 1$, dashed-dotted lines to $m/T \to 0$, and dashed lines to $m/T \to \infty$.

Related publication in 2010:
1) V.V. Begun, M.I. Gorenstein and O.A. Mogilevsky, *Pion Number Fluctuations and Correlations in the Statistical System with Fixed Isospin*, Phys. Rev. C82 (2010) 024904.

Related talks in 2010:
1) V.V. Begun, *Pion Number Fluctuations and Correlations in the Statistical System with Fixed Isospin*, International Workshop "Statistical Particle Production", Bad Liebenzell, Germany, 25-28 April 2010.
2) V.V. Begun, *Statistical Fluctuations and Correlations in Hadron-Resonance Gas*, International Workshop "Statistical Particle Production", Bad Liebenzell, Germany, 25-28 April 2010.
3) V.V. Begun, *Fluctuations and correlations in pion system with fixed isospin*, Sixth Workshop on Particle Correlations and Femtoscopy (WPCF2010), Kiev, Ukraine, 14-18 September 2010.

## Modified Bag Models for the Quark Gluon Plasma Equation of State

Collaborators: V.V. Begun[1,2], M.I. Gorenstein[1,2], O.A. Mogilevsky[1]

[1] Bogolyubov Institute for Theoretical Physics, Kiev, Ukraine, [2] Frankfurt Institute for Advanced Studies

The modified versions of the bag model equation of state (EoS) are considered. They are constructed to satisfy the main qualitative features observed for the quark-gluon plasma EoS in the lattice QCD calculations:

$$\varepsilon(T) = \sigma T^4 - C T^2 + B, \quad p(T) = \frac{\sigma}{3}T^4 - C T^2 - A T - B, \tag{1}$$

where $\varepsilon(T)$ is energy density and $p(T)$ is pressure density. A quantitative comparison with the lattice results at high temperatures T are done in the SU(3) gluodynamics and in the full QCD with dynamical quarks. Our analysis advocates a negative value of the bag pressure constant B.
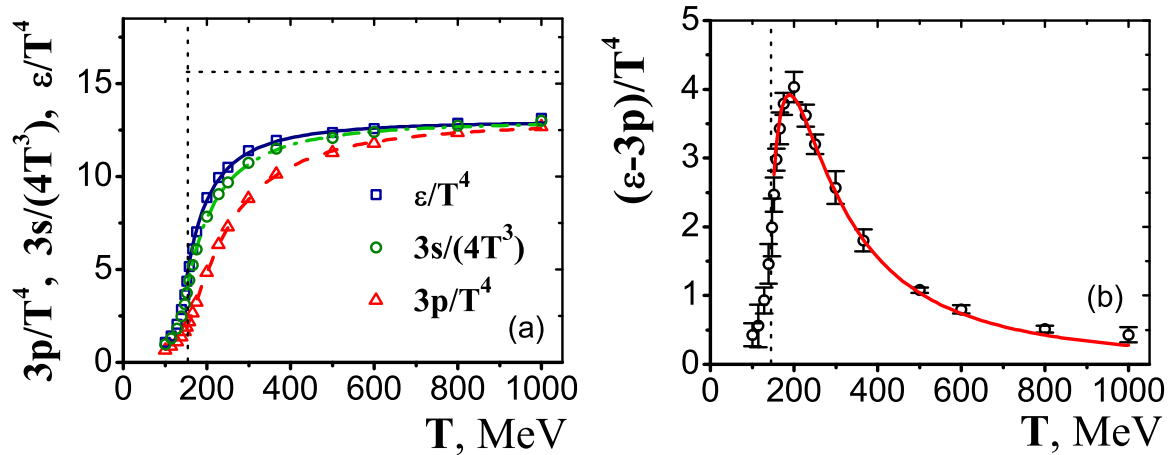
The symbols are recent Monte Carlo lattice results from Wuppertal-Budapest Collaboration for the $2+1$ QCD equation of state. The vertical dotted lines show the inflection point of the interaction measure $(\varepsilon - 3p)/T^4$ $T_i = 152$ MeV and horizontal line shows the Stefan-Boltzmann constant $\sigma_{SB} \simeq 15.63$. The model parameters are $\sigma = 13.01$, $A \simeq 0$, $C = 6.06 T_i^2$, and $B = -2.34 T^4$.

Related publications in 2010:

1) V.V. Begun, M. I. Gorenstein and O. A. Mogilevsky, *Equation of State of the Quark Gluon Plasma within the Quasi-particle Approach*, Ukrainian Journal of Physics, 55, (2010) 1049.

2) V.V. Begun, M.I. Gorenstein and O.A. Mogilevsky, *Modified Bag Models for the Quark Gluon Plasma Equation of State*, arXiv:1004.0953 [hep-ph].

Related talks in 2010:

1) V.V. Begun, *Modified Bag Models for the Quark Gluon Plasma Equation of State*, International Workshop "Statistical Particle Production", Bad Liebenzell, Germany, 25-28 April 2010.

Hadron production in $p+p$, $p+Pb$ and $Pb+Pb$ collisions at the LHC energies with HIJING2.0 model

**Collaborators:** Wei-Tian Deng[1,2], Xin-Nian Wang[3,4], Rong Xu[3]

[1] Frankfurt Institute for Advanced Studies, [2] Shandong University, China, [3] Huazhong Normal University, China, [4] Lawrence Berkeley National Laboratory, California,

HIJING Monte Carlo model is updated with modern parton distribution functions for the nucleons and the new set of parameters within the two-component model for mini-jet production in high-energy nucleon-nucleon collisions. Because of the large gluon distribution at small x in the GRV parameterization of the nucleon's PDFs used in HIJING 2.0, one has to introduce an energy-dependent transverse momentum cut-off p_0 for the mini-jet production and the soft parton interaction cross section σ_{soft} in order to describe the energy-dependence of the total, inelastic cross sections and the central rapidity hadron density in high-energy $p+p(\bar{p})$ collisions.

The updated HIJING 2.0 model is shown to describe the existing experimental data on hadron production from ISR energy up to Fermilab Tevatron energy. The HIJING 2.0 results are also shown to be in good agreement with the recently published hadron spectra in $p+p$ collisions at the LHC energies ($\sqrt{s}$=0.9, 2.36 TeV). The HIJING 2.0 predictions for $p+p$ collisions at $\sqrt{s}=7$ and 14 TeV are also given.

With a model parameterization for nuclear modification of the parton distribution functions, The range of gluon shadowing parameter $s_g = 0.20 - 0.23$ in the new HIJING parameteriztion of parton shadowing enables us to predict the centrality dependence of the charged hadron rapidity density with reduced uncertainty in $Pb+Pb$ collisions at $\sqrt{s} = 2.75$ and 5.5 TeV/n. The centrality dependence is surprisingly independent of colliding energy for most centralities strting at $N_{part} = 50(100)$ for $\sqrt{s} = 2.76(5.5)$ TeV. However, the centrality dependence in the peripheral collisions becomes stronger at higher colliding energies.
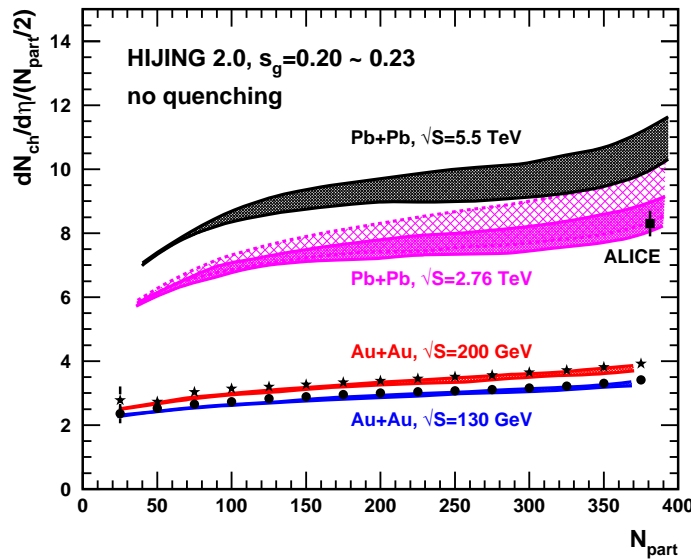
Charged hadron multiplicity density in mid-rapidity per particepant pair $2\mathrm{d}N_{ch}/\mathrm{d}\eta/N_{part}$ as a function of N_{part} from HIJING2.0 calculation with gluon shadowing parameter $s_g = 0.20 - 0.23$ (solidshade) and $s_g = 0.17 - 0.22$ (dash-shade) as compared to combinde RHIC data for $Au+Au$ collisions and ALICE data at LHC.

Related publications in 2010:

1) W.-T. Deng, X.-N. Wang and R. Xu, *Hadron production in p+p, p+Pb, and Pb+Pb collisions with the HIJING 2.0 model at energies available at the CERN Large Hadron Collider*, to be published in Phys. Rev. C; arXiv:1008.1841 [hep-ph]

2) W.-T. Deng, X.-N. Wang and R. Xu, *Gluon shadowing and hadron production in heavy-ion collisions at LHC*; arXiv:1011.5907 [nucl-th]

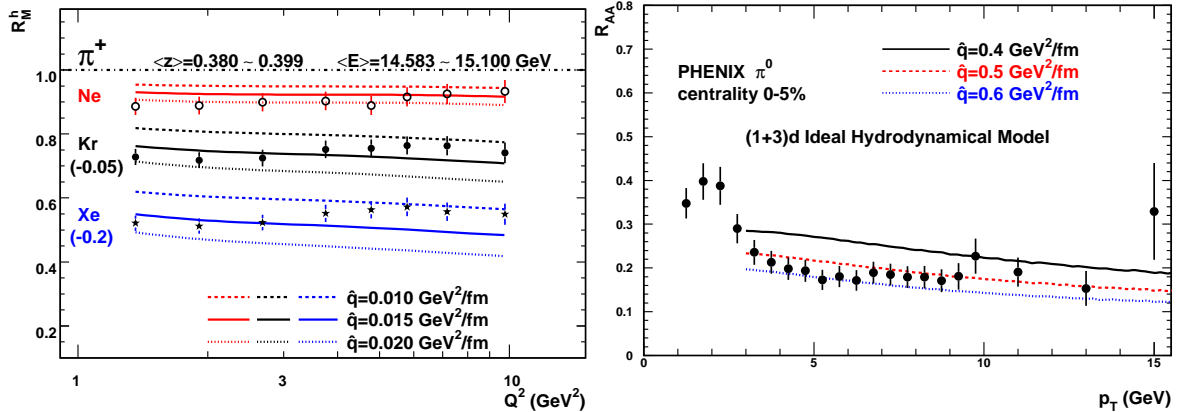# Modified DGLAP Evolution for Fragmentation Functions in Nuclei and QGP

Collaborators: Wei-Tian Deng[1,2], Ning-Bo Chang[2], Xin-Nian Wang[3]

[1] Frankfurt Institute for Advanced Studies, [2] Shandong University, China, [3] Lawrence Berkeley National Laboratory, California

We have extended the modified DGLAP evolution equations to include induced gluon radiation for gluon jet and quark-anti-quark pair creation from gluon fusion within the framework of generalized factorization for higher-twist contribution to multiple parton scattering. The effective parton splitting functions are proportional to a path integration of the jet transport parameter $\hat{q}$ over the propagation length. We then numerically solve the coupled mDGLAP equations for medium modified fragmentation functions for different static profile of medium and different values of the jet transport parameter $\hat{q}$.

The mDGLAP evolution is applied to quark propagation in the deeply inelastic scattering (DIS) of a large nucleus. The calculated nuclear modification of the effective fragmentation functions are in good agreement with experimental data in the intermediate z region. In modeling the initial condition for modified fragmentation functions, we have chosen to include medium induced radiation and parton energy loss below the initial scale Q_0^2. In this case, most of the medium modification comes from mDGLAP evolution in the low Q^2 region while large Q^2 contribution is power-suppressed. This leads to a weak Q^2 dependence of the medium modification of the fragmentation functions which is consistent with the experimental data in DIS.

One can extend the calculation for medium modified parton fragmentation functions in DIS to hot medium like QGP or hot hadronic matter created in high-energy heavy-ion collisions. To take into account both the longitudinal and transverse expansion of the hot matter, we use a 3D ideal hydrodynamic simulations which give us information on each of the hot matter evolution. If we neglect nuclear effect such as the shadowing effect on the initial parton distribution function, we can get the nuclear modification factor R_{AA} for a fixed parameter b. From our results, one is suggested that the gluon density in QGP is about 30 times larger than which in cold nucleon.

Left: Comparison of the modified multiplicity ratios as a function of Q^2 for Ne, Kr and Xe targets.
Right: Comparison of the nucleon modification factor R_{AA} for π^0 in $0-5\%$ biased events.

Related publications in 2010:

1) W.-T. Deng, N.-B. Chang, X.-N. Wang, *Modified DGLAP Evolution for Fragmentation Functions in Nuclei and QGP*, arXiv:1012.1514 [nucl-th]

Structure and Thermal Evolution of Compact Stars

Collaborators: R. Negreiros[1], S. Schramm[1], I. Mishustin,[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. The density inside these objects is many times higher than the density of atomic nuclei (possibly up to 15 times more dense). At such extraordinary densities, atomic nuclei are squeezed so tightly together that novel states of matter, ordinarily not seen in our earthly environment, are created. These new states range from hyperons ($\Sigma^{+,0,-}, \Lambda, \Xi^{0,-}$) to meson condensates ($\pi^-, K^-$) and to deconfined quarks. It is also theorized that neutron stars may be made of absolutely stable quark matter, a configuration of matter that is hypothesized to be more stable than the most stable atomic nuclei: ^{56}Fe. 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.

In our research we use state of the art microscopic models to investigate the structure and thermal evolution of compact stars. The structure of the star is calculated by numerically solving Einstein's equations for a rotating compact, which provide us with information about the macroscopic structure of the star (gravitational mass, radius, mass-shedding frequency, pressure and density profiles). By combinining this information with the underlying microscopic model being used, we are able to calculate the thermal evolution of the star. This provides us with a wealth of data that can be compared with observed data on compact stars, allowing us to appraise the underlying model for the equation of state.
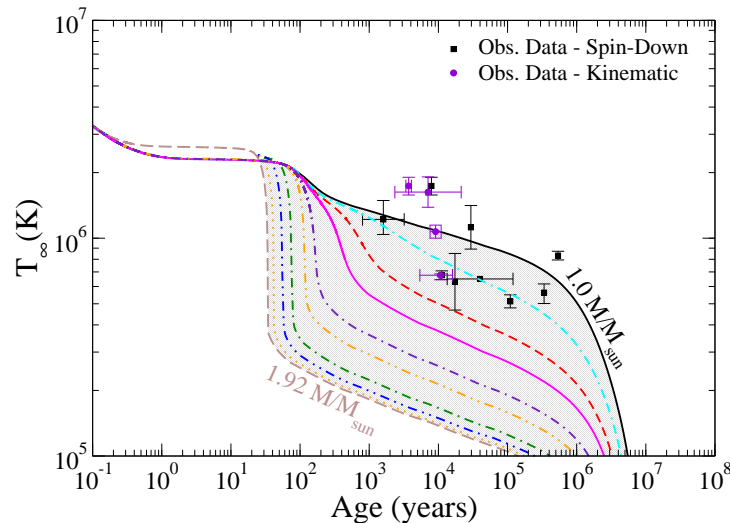
Thermal evolution for a compact stars calculated with an SU(3) non-linear σ model.

Related publications in 2010:

1) R. Negreiros, I. Mishustin, S. Schramm, *Properties of bare strange stars associated with electric fields*, Phys. Rev. D82 (2010) 103010.

2) R. Negreiros, V. Dexheimer, S. Schramm, *Modeling hybrid stars with an SU(3) non-linear sigma model*, Phys. Rev. C82 (2010) 035803.

3) R. Negreiros, V. Dexheimer, S. Schramm, *Quark core impact on hybrid star cooling*, arXiv:0907.5537 (2010).

4) F. Weber, O. Hamil, K. Mimura, R. Negreiros, *From crust to core: A brief review of quark matter in neutron stars*, Int. J. Mod. Phys. D19 (2010) 1427.
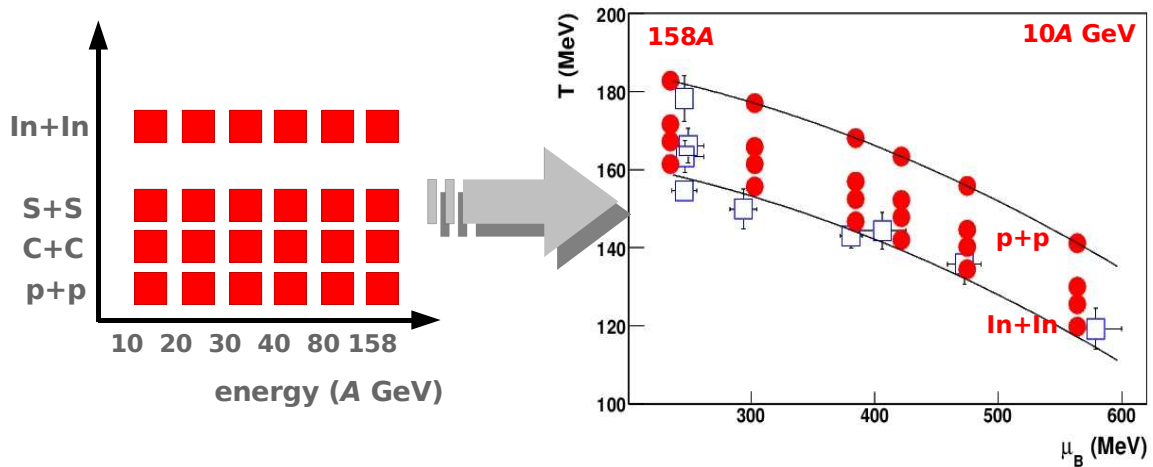
Fluctuations and Correlations in Nucleus-Nucleus Collisions within Transport Models

Collaborators: E.L. Bratkovskaya[1], M.I. Gorenstein[1,2], W. Greiner[1], V.P. Konchakovski[1,2]

[1] Frankfurt Institute for Advanced Studies, [2] Bogolyubov Institute for Theoretical Physics, Kiev, Ukraine

The event-by-event fluctuations in high energy nucleus-nucleus (A+A) collisions are expected to be closely related to the transitions between different phases of QCD matter. By measuring the fluctuations one should observe anomalies from the onset of deconfinement and dynamical instabilities when the expanding system goes through the 1-st order transition line between the quark-gluon plasma (QGP) and the hadron gas. Furthermore, the QCD critical point may be signaled by a characteristic pattern in enhanced fluctuations. An ambitious experimental program for the search of the QCD critical point has been started by the NA61 Collaboration at the CERN SPS. The program includes a variation in the atomic number A of the colliding nuclei as well as an energy scan. This allows to explore the phase diagram in the temperature – baryonic chemical potential plane near the critical point. One expects to 'locate' the position of the critical point by studying its 'fluctuation signals'. A specific combination of atomic number A and bombarding energy E_{lab} could move the chemical freeze-out of the system close to the critical point and show a 'spike' in the multiplicity fluctuations. The microscopic transport approach – Hadron-String-Dynamics (HSD) – operates from lower SIS to top RHIC energies. This model is very helpful in the interpretation of the upcoming experimental data.

The influence of participant number fluctuations on hadron multiplicity fluctuations has been emphasized and studied in detail. One needs to make a very rigid selection – 1% or smaller – of the 'most central' collision events. The present HSD results for the particle number fluctuations provide a general trend of their dependencies on A and E_{lab} and indicate quantitatively the systematic uncertainties. The expected enhanced fluctuations – attributed to the critical point and phase transition – can be observed experimentally on top of a monotonic and smooth 'hadronic background'. The most promising signature of the QCD critical point would be an observation of a non-monotonic dependence of the scaled variances with bombarding energy E_{lab} for central A+A collisions with fixed atomic mass number.

Left: The data sets on central A+A collisions planned to be registered by NA61 in a search for the critical point of strongly interacting matter. *Right:* Hypothetical positions of the chemical freeze-out points of the reactions (In+In, S+S, C+C and p+p from bottom to top at 158*A*, 80*A*, 40*A*, 30*A*, 20*A* and 10*A* GeV from left to right) to be studied by NA61 in the (temperature)-(baryon-chemical potential) plane are shown by full dots. The open squares show the existing Pb+Pb data.

Related publications in 2010:
1) V.P. Konchakovski, M.I. Gorenstein, E.L. Bratkovskaya, W. Greiner, *Fluctuations and Correlations in Nucleus-Nucleus Collisions within Transport Models*, J. Phys.G 37, 073101 (2010).
2) V.P. Konchakovski, M.Hauer, M.I. Gorenstein, E.L. Bratkovskaya, *K/π, K/p and p/π Ratio Fluctuations within the HSD Transport Approach*, J. Phys. G 37, 094045 (2010).

Stability Peninsulas on the Neutron–Rich Part of the Nuclear Chart

Collaborators: D. K. Gridnev[1], S. Schramm[1], K. A. Gridnev[1,2], V. N. Tarasov[3], Walter Greiner[1]

[1] Frankfurt Institute for Advanced Studies, [2] Saint Petersburg State University, Russia, [3] NSC, Kharkov Institute of Physics and Technology, Ukraine

The general theoretical approach for locating the neutron drip line is to take a nucleus and load it with neutrons until one reaches the saturation point, where the nucleus gets rid of extra neutrons through hadronic decay. Using Hartree-Fock calculations with Skyrme forces we show that in this way one may overlook the formation of stability peninsulas, where nuclei regain their stability when more neutrons are added to them, see the Figure below. Performing the calculations we analyze the mechanism and conditions for formation of such peninsulas, predict new isotopes and study their properties. These peninsulas appear near "magic" neutron numbers or near the so–called quenched "magic" numbers. Some of these stable nuclei have an interesting decay mode: to transform into an energetically favorable state they must sometimes release more than 8 neutrons at a time (such decays were not experimentally observed so far). We try to understand this decay mode and calculate the corresponding lifetimes.
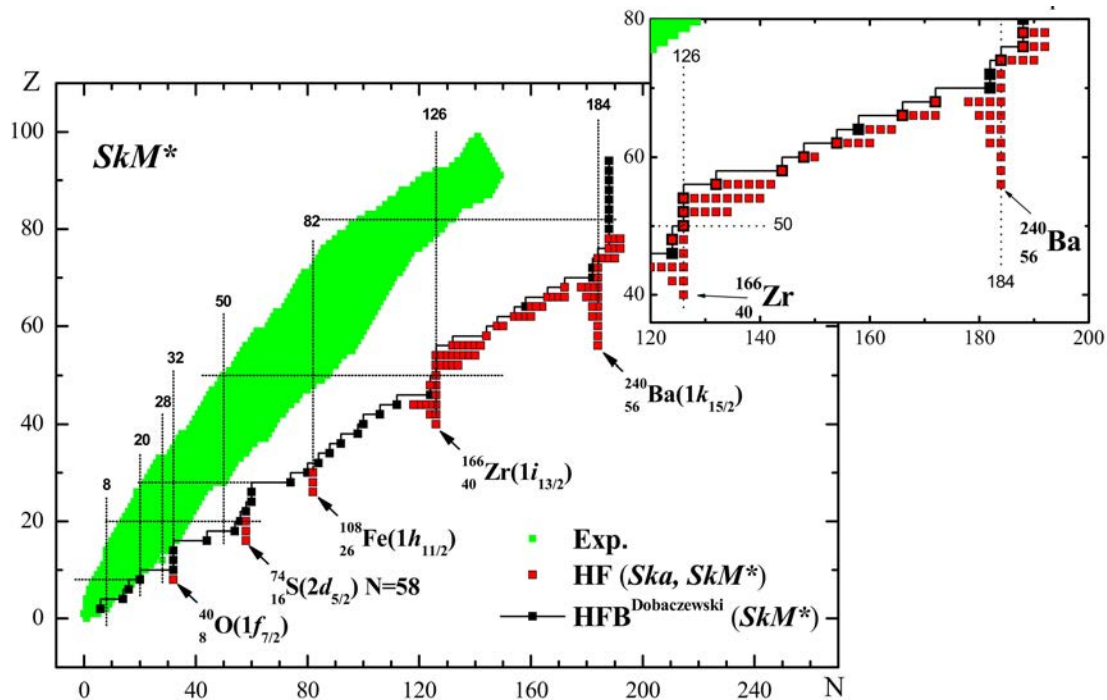
Nuclear Chart. Green area shows the so far experimentally found stable isotopes. Black squares show the 1n drip line in HFB calculations and red squares show the isotopes, which are stable against one neutron emission in our calculations (Ska and SkM* forces are used). Red stability peninsulas stretch along the Z axis and are located at "magic" and quenched "magic" neutron numbers.

Related publications in 2010:

1) K.A. Gridnev, V.N. Tarasov, D.V. Tarasov, D.K. Gridnev, V.V. Pilipenko, W. Greiner, *Theoretical prediction of extremely neutron rich Zr and Pb*, Int. J. Mod. Phys. E19 (2010) 449

2) V.N. Tarasov, K.A. Gridnev, D.K. Gridnev, V. I. Kuprikov, D.V. Tarasov, W. Greiner and X. Vinyes, *Investigation of Neutron Stability of Neutron-Rich O, Ar, Kr, and Rn Isotopes*, Bull. Russ. Acad. Sciences 74, No. 11, (2010) 1624

3) S. Schramm, D.K. Gridnev, V.N. Tarasov, K.A. Gridnev and W. Greiner, *Stability Peninsulas near Neutron Drip Line*, to be submitted to Phys. Rev. Lett.

True ternary fission of superheavy nuclei

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

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

The term "ternary fission" is commonly used to denote the process of formation of light charged particle accompanied fission. This is a rare process (less than 1%) relative to binary fission. The probability of such a process decreases sharply with increasing mass number of third particle. Experiments show that there is extremely small probability of the ternary fission of actinide nuclei with the mass of the third particle $A_3 > 20$ [F. Gönnenwein et al., 1999]. In contrast to such a process, the term "true ternary fission" is used for a simultaneous decay of heavy nucleus into three fragments of not very different mass. Such decays of low excited heavy nuclei were not observed yet, but being discovered it becomes a new type of radioactivity. Early theoretical considerations based on the liquid drop model [W.J. Swiatecki, 1958; H. Diehl and W. Greiner, Nucl. Phys. A (1974)] and a more sophisticated three-center shell model [J. Maruhn and W. Greiner, Z. Phys. A (1972)] showed that the potential energy landscape and, in particular, the fission barrier plays a decisive role for the ternary fission process. It was also found that the shell effects may significantly reduce the ternary fission barriers even for much less probable oblate (triangle) deformations of very heavy nuclei.
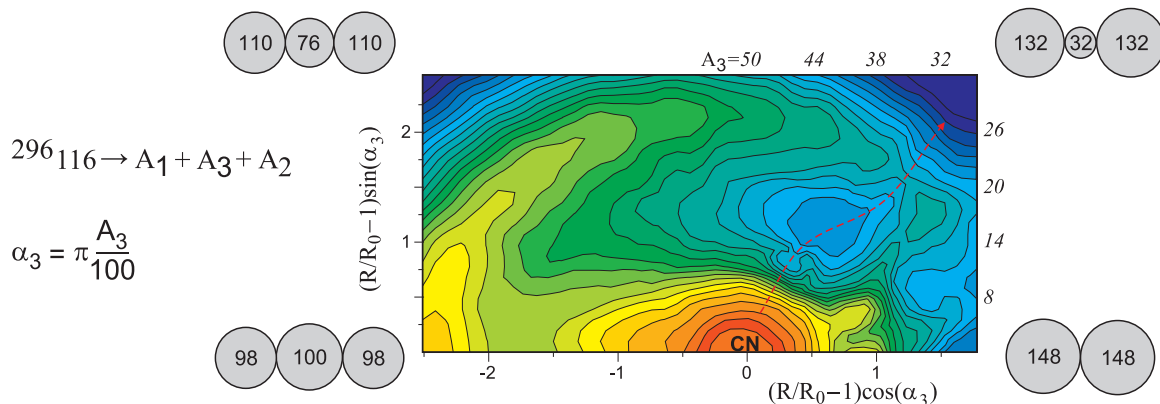
Potential energy surface for ternary fission of $^{296}116$ nucleus depending on elongation R and mass of the third fragment A_3 (shown by italic numbers). Contour lines are drawn over 5 MeV.

Since then there was no any significant progress in theoretical and experimental investigation of ternary fission. However today it becomes possible to study experimentally the properties and dynamics of formation and decay of superheavy nuclei, for which, as we found, the ternary fission could be rather probable. Basing on the developed three-center shell-model we showed that the true ternary fission is quite possible for superheavy nuclei due to the strong shell effects. The potential energy (see the Figure) has a well-distinguishable ternary fission valley which corresponds to a three-body clusterization with the two double-magic tin-like cores plus the supplementary third fragment ($^{296}116 \rightarrow ^{132}_{50}\text{Sn} + ^{32}_{16}\text{S} + ^{132}_{50}\text{Sn}$). The fission barrier in this ternary exit channel was found to be quite comparable with those for the binary fission. The simplest way to discover this phenomenon in decays of excited superheavy nuclei is a detection of two tin-like clusters with appropriate kinematics in low-energy collisions of medium mass nuclei with actinide targets. In addition, we found that the ternary quasi-fission process could be even more pronounced for giant nuclear systems formed in collisions of heavy actinide nuclei. For example, in collision of two ^{233}U nuclei the shell effects make rather favorable a three-body clusterization with the formation of two double-magic led nuclei and magic calcium nucleus as a third particle ($^{233}_{92}\text{U} + ^{233}_{92}\text{U} \rightarrow ^{208}_{82}\text{Pb} + ^{50}_{20}\text{Ca} + ^{208}_{82}\text{Pb}$). In this case a three-body clusterization might be proved experimentally by detecting two coincident lead-like fragments in low-energy U+U collisions.

Related publication in 2010:
1) V. I. Zagrebaev, A. V. Karpov, and Walter Greiner, *True ternary fission of superheavy nuclei*, Physical Review C81 (2010) 044608.

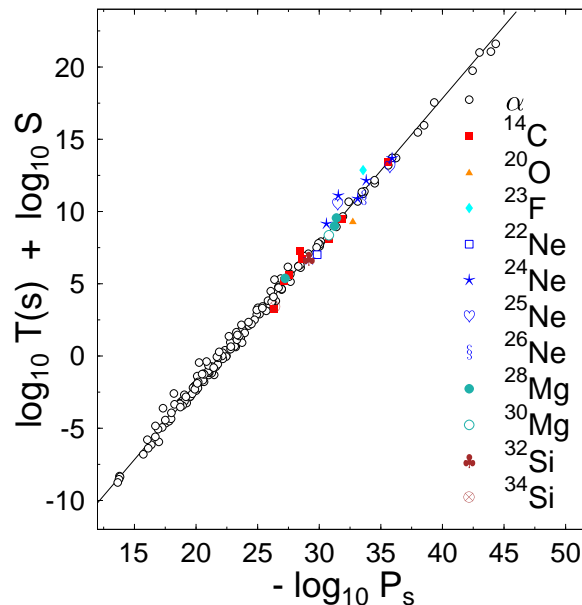# One universal curve for cluster radioactivities and α decay

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

The field of heavy-particle radioactivity was developed during the last 30 years. Four years after the theoretical prediction in 1980 (see http://www.britannica.com/EBchecked/topic/465998/) Rose and Jones discovered experimentally ^{14}C radioactivity of ^{223}Ra. In 1991 we introduced universal curves for every kind of cluster decay mode and for α decay. They are based on the quantum mechanical tunneling process relationship of the disintegration constant $\lambda = \nu S P_s$, valid in both fission-like or α-like theories. ν is the frequency of assaults on the barrier per second, S is the preformation probability of the cluster at the nuclear surface (equal to the penetrability of the internal part of the barrier in a fission theory) and P_s is the quantum penetrability of the external potential barrier.

In 2010 we developed a new type of plot, UNIV, in which one straight line accomodates all kinds of cluster radioactivities and α decay. An example of such a curve is shown in the Figure. The points correspond to 163 even-even α emitters and 27 cluster radioactivities data experimentally determined (8 ^{14}C, 6 ^{24}Ne, 3 ^{28}Mg, 2 ^{25}Ne and only one for each of the ^{20}O, ^{23}F, ^{22}Ne, ^{26}Ne, ^{30}Mg, ^{32}Si, and ^{34}Si radioactivities). The experimental data on α decay of even-even emitters and cluster radioactivities of even-even, even-odd, and odd-even nuclei could be described by a single universal curve by plotting $\log_{10} T(s) + \log_{10} S = f(-\log_{10} P_s)$.

The hindrance factor is a free parameter which may be determined by fitting the experimental data in order to obtain the minimum values of the standard root-mean-square deviation of $\log_{10} T$ values. The overall standard deviation obtained by taking one value of $h_{UNIV} = 0.040$ for even-even α-emitters and all types (even-even, even-odd and odd-even) of cluster emitters was $\sigma = 0.428$. There is no successful experiment on cluster radioactivity of an odd-odd parent nucleus. The experimental data on heavy cluster decay in three groups of even-even, even-odd, and odd-even parent nuclei are reproduced with comparable accuracy by two types of universal curves, UNIV and UDL, derived using fission-like and α-like theories.

One single universal curve for α decay and cluster radioactivities.

Related publications in 2010:
1) D. N. Poenaru, W. Greiner, *Cluster Radioactivity*, in Clusters in Nuclei 1. Lecture Notes in Physics, 818, Ed. C. Beck (Springer, Berlin, 2010), pp. 1-56.
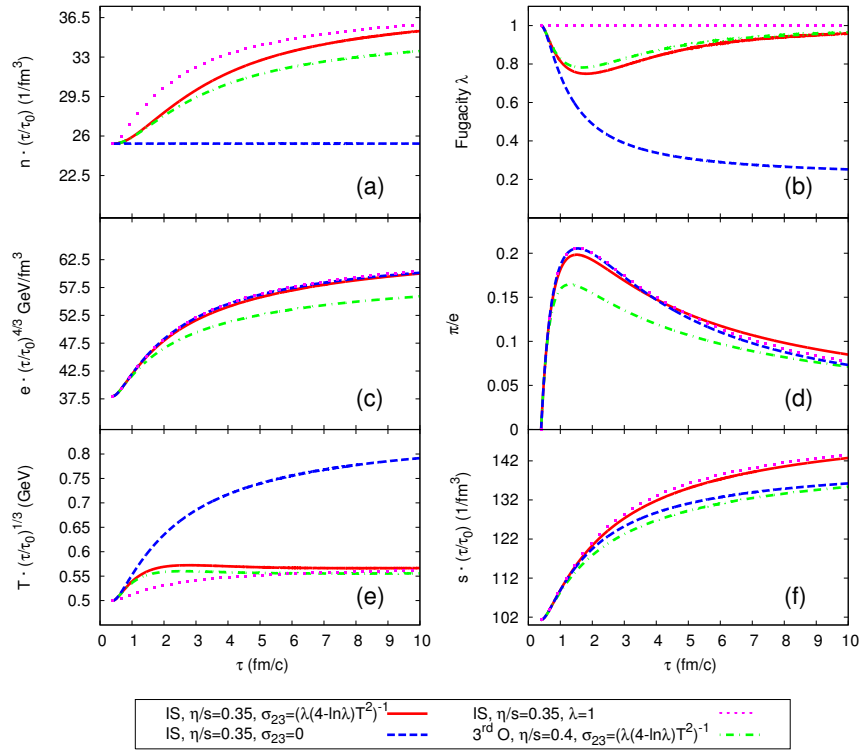2) D. N. Poenaru, R. A. Gherghescu, W. Greiner, Phys. Rev. C, to be published.

A relativistic dissipative hydrodynamic description for systems including particle number changing processes

Collaborators: A. El[2], A. Muronga[3], Z. Xu[1], C. Greiner[2]

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In this work we have presented an extended set of viscous hydrodynamic equations, in which particle number changing processes are taken into account via a rate equation. The rate equation of the particle number density is derived from the Boltzmann equation employing the Grad's approximation. A one-dimensional boost-invariant expansion is considered for simplifying the derivation of the hydrodynamic equations. We have demonstrated that a proper treatment of particle number evolution is essential for a hydrodynamic description of the gluon system, especially for describing chemical equilibration and for determining the temperature and the momentum spectra of the system.

We have compared the results between the hydrodynamic and transport calculations including inelastic $2 \leftrightarrow 3$ processes. The energy density and the shear pressure obtained from the third-order hydrodynamic equations agree well with the results from the transport approach using BAMPS even at large $\eta/s = 0.75$, while the results from the Israel-Stewart hydrodynamics deviate from the BAMPS results by $10\% - 20\%$ for $\eta/s = 0.35 - 0.75$. Both the IS and the third-order hydrodynamic calculations fail to meet the BAMPS results on the particle number density at large η/s. The reason is that at large η/s the viscous effect is so large that the Grad's ansatz for the off-equilibrium distribution should be modified beyond the second order in momentum, in order to give a more accurate rate equation of the particle number density.

Time evolution of (a) the particle number density, (b) fugacity, (c) energy density, (d) shear pressure to energy density ratio, (e) temperature and (f) entropy density.

Related publications in 2010:

A. El, A. Muronga, Z. Xu, C. Greiner, *A relativistic dissipative hydrodynamic description for systems including particle number changing processes*, Nuclear Physics A 848 (2010) 428
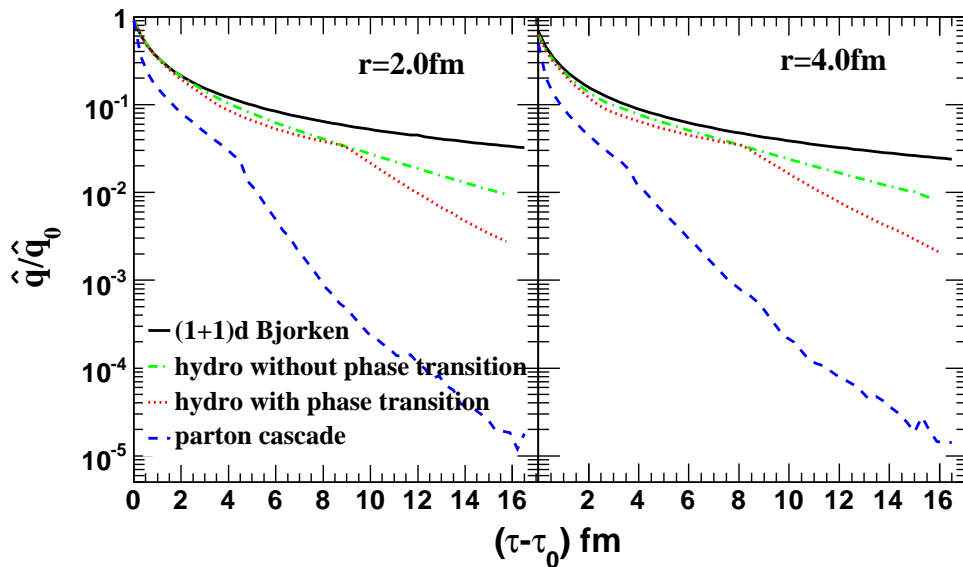
Bulk matter evolution and extraction of jet transport parameters at RHIC

Collaborators: X.-F. Chen[1,3], C. Greiner[2], E. Wang[3], X.-N. Wang[2,4], and Z. Xu[1]

[1] Frankfurt Institute for Advanced Studies, [2] Institut für Theoretische Physik, Goethe-Universität Frankfurt, [3] Institute of Particle Physics and Key Laboratory of Quark & Lepton Physics, Huazhong Normal University, Wuhan, China, [4] Nuclear Science Division, Lawrence Berkeley National Laboratory, Berkeley, USA

Within the picture of jet quenching induced by multiple parton scattering and gluon bremsstrahlung, medium modification of parton fragmentation functions and therefore the suppression of large transverse-momentum hadron spectra are controlled by both the value and the space-time profile of the jet transport parameter along the jet propagation path. Experimental data on single-hadron suppression in high-energy heavy-ion collisions at the Relativistic Heavy Ion Collider (RHIC) energy are analyzed within the higher-twist (HT) approach to the medium-modified fragmentation functions and the next-to-leading order perturbative QCD parton model.

Assuming that the jet transport parameter $\hat{q}$ is proportional to the particle number density in both quark gluon plasma (QGP) and hadronic phase, experimental data on jet quenching in deeply inelastic scattering off nuclear targets can provide guidance on $\hat{q}_h$ in the hot hadronic matter. One can then study the dependence of the extracted initial value of jet-quenching parameter $\hat{q}_0$ at initial time τ_0 on the bulk medium evolution. Effects of transverse expansion, radial flow, phase transition, and nonequilibrium evolution are examined. The extracted values are found to vary from $\hat{q}_0 \tau_0 = 0.54$ GeV^2 in the $(1 + 3)$d ideal hydrodynamic model to 0.96 GeV^2 in a cascade model, with the main differences coming from the initial nonequilibrium evolution and the later hadronic evolution. The overall contribution to jet quenching from the hadronic phase, about 22%-44%, is found to be significant. Therefore, a realistic description of the early nonequilibrium parton evolution and later hadronic interaction will be critical for accurate extraction of the jet transport parameter in the strongly interacting QGP phase in high-energy heavy-ion collisions.

Time evolution of the scaled jet transport parameter at position of radius of 2 fm and 4 fm.

Related publications in 2010:

Xiao-Fang Chen, Carsten Greiner, Enke Wang, Xin-Nian Wang, and Zhe Xu, *Bulk matter evolution and extraction of jet transport parameters in heavy-ion collisions at energies available at the BNL Relativistic Heavy Ion Collider (RHIC)*, Physical Review C 81 (2010) 064908

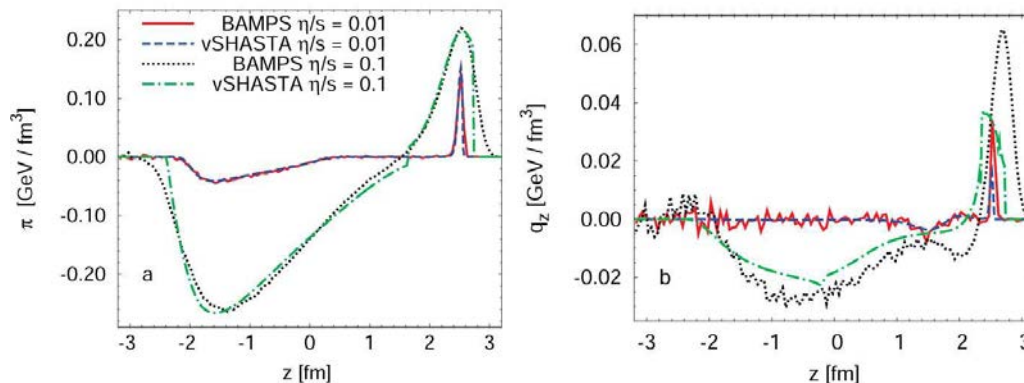# Investigation of shock waves in the relativistic Riemann problem

Collaborators: I. Bouras[2], E. Molnár[1,3], H. Niemi[1], Z. Xu[1], A. El[2], O. Fochler[2], C. Greiner[2], and D. H. Rischke[1,2]

[1] Frankfurt Institute for Advanced Studies, [2] Institut für Theoretische Physik, Goethe-Universität Frankfurt, [3] KFKI, Research Institute of Particle and Nuclear Physics, Budapest, Hungary

We have studied the formation and evolution of relativistic shock waves in dissipative matter with nonzero shear viscosity and heat conductivity by solving the relativistic Riemann problem. This was accomplished by using both relativistic kinetic theory and relativistic dissipative fluid dynamics. The relativistic kinetic approach solves the Boltzmann equation by using the BAMPS code. The fluid-dynamical approach is based on Israel and Stewart (IS) theory and was solved numerically by the vSHASTA method for hyperbolic equations. When the viscosity is zero, both give equivalent results and reproduce the analytic solutions of the Riemann problem in the perfect-fluid limit.

As the viscosity increases the agreement between the approaches starts to deteriorate. For cases when the viscosity is small, the agreement is still excellent. For even larger values of the η/s ratio, IS theory develops discontinuities which survive even after long times. These substructures are not supported by the kinetic simulations. They are an artifact of the method of moments on which IS theory is based. Part of this discrepancy can be understood to result from the inapplicability of IS theory for large Knudsen numbers Kn_e. We found that for $Kn_e < 1/2$ the difference between kinetic theory and IS theory is less than $\sim 10\%$.

The shear pressure profile was reasonably well described by the IS equations from small to moderate viscosities. The results are quite insensitive to the second-order terms in the IS equation for the shear viscosity. However, the same is not true for heat flow. At very small viscosities the heat flow was quite well described, including all terms in the IS equation. At larger viscosity the results are very sensitive to the coupling term between the heat flow and shear viscosity. In the Riemann problem studied here, the heat flow is an order of magnitude smaller than the shear pressure, and the coupling to shear dominates the behavior of the heat flow. This coupling gives a too large contribution in the heat-flow component, which is not supported by the kinetic calculations.

Numerical solutions of the relativistic Riemann problem for the shear pressure (a) and heat flow (b).

Related publications in 2010:
I. Bouras, E. Molnár, H. Niemi, Z. Xu, A. El, O. Fochler, C. Greiner, and D. H. Rischke, *Investigation of shock waves in the relativistic Riemann problem: A comparison of viscous fluid dynamics to kinetic theory*, Physical Review C 82 (2010) 024910

Hydrodynamical modeling of ultrarelativistic heavy-ion collisions

Collaborators: G. S. Denicol[1], K. J. Eskola[2,3], H. Holopainen[2,3], P. Huovinen[1], E. Molnár[4,5], H. Niemi[4], D. H. Rischke[1,4]

[1] Institute für Theoretische Physik, Johann Wolfgang Goethe-Universität, Frankfurt am Main, Germany, [2] Department of Physics, University of Jyväskylä, Finland, [3] Helsinki Institute of Physics, University of Helsinki, Finland, [4] Frankfurt Institute for Advanced Studies, Frankfurt am Main, Germany, [5] KFKI Research Institute for Particle and Nuclear Physics, Hungary

One of the most important goals in the high-energy heavy-ion collision experiments is to extract properties of strongly interacting elementary particle matter, the Quark Gluon Plasma (QGP). Once the QGP is created in these collisions, it will cool down and hadronize very fast. Clearly, connecting the properties of the QGP to the experimental data requires a good understanding of dynamics of the created system.

Hydrodynamics provides a convenient framework to study the dynamics of such systems, since the matter properties near thermal equilibrium, like the equation of state, bulk and shear viscosities and thermal conductivity, are direct input to the hydrodynamical calculations. We used relativistic dissipative hydrodynamics to investigate the effects of temperature dependent shear viscosity to entropy ratio η/s on the transverse momentum spectra and elliptic flow of hadrons in ultrarelativistic heavy ion collisions.

We found that the elliptic flow coefficients in the $\sqrt{s_{NN}} = 200$ GeV Au+Au collisions, at the Relativistic Heavy Ion Collider (RHIC), are insensitive to the value of η/s in the high temperature quark-gluon plasma (QGP), as long as it has the same minimum value near the QCD phase transition. In contrast, we found that the elliptic flow is very sensitive to the η/s of the hadron gas. On the other hand, we found that sensitivity of the elliptic flow to the high-temperature η/s increases with increasing multiplicity and simultaneosly sensitivity to the hadronic viscosity decreases. This makes Pb+Pb collisions at the Large Hadron Collider (LHC) more suitable system to extract transport properties of the QCD matter at high-temperature.

One of the key inputs for the hydrodynamical models is an initial state. We investigated the effects of fluctuations in the initial energy density distribution in the elliptic flow and transverse momentum spectra. Event-by-event hydrodynamics with fluctuating initial conditions allows us to analyze the elliptic flow in the same way as the experimental collaborations. This procedure gives a good description of the centrality dependence of the elliptic flow in the Au+Au collisions at RHIC, which is otherwise very difficult to reproduce using average (non-fluctuating) initial conditions.

Related publications in 2010:

1) H. Niemi, G. S. Denicol, P. Huovinen *et al.*, *Influence of the shear viscosity of the quark-gluon plasma on elliptic flow in ultrarelativistic heavy-ion collisions*, [arXiv:1101.2442 [nucl-th]].

2) H. Holopainen, H. Niemi, K. J. Eskola, *Event-by-event hydrodynamics and elliptic flow from fluctuating initial state*, [arXiv:1007.0368 [hep-ph]].

3) H. Holopainen, H. Niemi, K. J. Eskola, *Elliptic flow from event-by-event hydrodynamics with fluctuating initial state*, [arXiv:1012.0180 [hep-ph]].

Research Report by Giorgio Torrieri

Project 1: The large N_c limit of the nuclear liquid-gas transition

Collaborator: I. Mishustin (FIAS)

In [1] we have investigated the scaling, with the number of colors N_c, of the low-energy liquid gas phase transition in the Van Der Waals approximation. Under very reasonable assumptions, the phase diagram grows from one covering a very small region ($\ll \Lambda_{QCD}$ where Λ_{QCD} is the characteristic QCD scale, the constituent quark mass) at $N_c = 3$ to one $\sim \Lambda_{QCD}$ at $N_c \gg 3$ (Fig. 1) . We therefore conjecture that the recently proposed new "quarkyonic phase", based on large N_c arguments, is simply the large N_c limit of the well-studied liquid-gas nucelar phase transition.
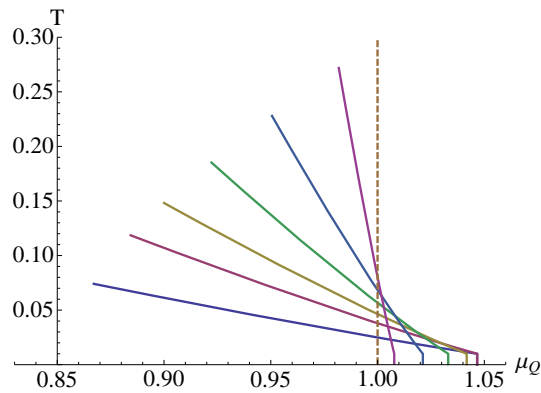

Figure 1: *The phase diagram of liquid-gas matter as a function of the number of colors N_c*

Project 2: Mach-cone like signal generation in heavy ion collisions

Collaborators: B. Betz[1], M. Gyulassy[1], J. Noronha[1], D. Rischke[2]

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

In [2] We have shown that initial fluctuations in jet production, together with hydrodynamic flow, can generate a signal which looks very much like the experimentally observed signal often interpreted as a "Mach cone". We suggested the experimental measurement for heavy quark tagged cones to falsify this mechanism and experimentally distinguish the "fake" from the true Mach cone.

Project 3: Bulk viscosity of mixtures

Collaborator: S. Pratt[1] (Michigan State University)

Viscosity is a pretty non-trivial concept, even for relatively simple systems. It has long been known that even an ideal gas has a zero bulk viscosity provided the masses of its particles are either zero or infinity. In [3] we have explored a mixture of light and heavy particles, and calculated its viscosity. We have also explored the influence of viscous corrections on particle distributions when the fluid freezes out.

Project 4: Hydrodynamic response to heavy Quarks in the Quark-Gluon Plasma

Collaborator: J. Noronha[1] (Columbia University, New York)

In [4], we have shown that the speed of sound depends on the admixture of charm quarks in a way that is both rigorously calculable and dependent on non-perturbative characteristics of QCD, such as confinement. As Fig. 2 shows, correlations due to the presence of heavy quarks systematically distort the medium's speed of sound. At the LHC, where charm quarks will be abundantly produced, this effect can be tested thoroughly by correlating charm quark abundance to flow.
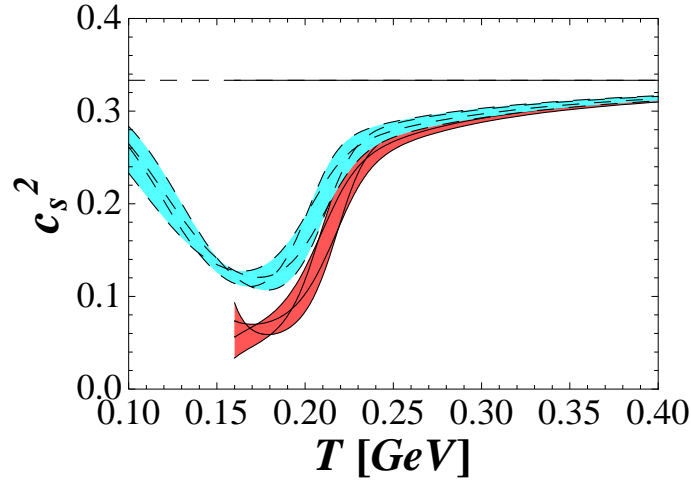
Figure 2: *The speed of sound in a medium where the charm over entropy ratio is 0.1 (lower band) compared to the speed of sound of a purely light-quark plasma (upper band)*

Project 5: Phenomenology of AdS/CFT solutions

Collaborators: M. Gyulassy[1], J. Noronha[1]

[1] Columbia University, New York

The AdS/CFT correspondence seems to give a viscosity qualitatively compatible with the one measured at RHIC. In [5], we investigate whether the same coupling constant can describe both viscosity and opacity to heavy quarks. As Fig. 3 shows, this is indeed the case, although future measurements with detailed heavy quark tagging will provide a more stringent test for quark gluon plasma models inspired by string theory. Fig. 3 also shows the weakly coupled calculation, which can adequately describe opacity but fails to describe viscosity by an order of magnitude.
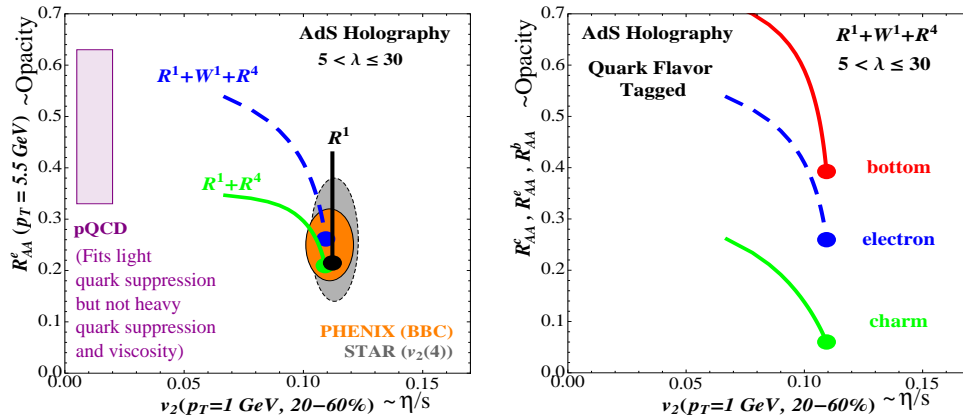

Figure 3: *A unified description of viscosity and heavy quark opacity in the strongly coupled limit using AdS/CFT duality*

Project 6: Fluctuations and resonances in heavy ion collisions

Collaborators: R. Bellwied[1], G. Westfall[2], Ch. Markert[3]

[1] University of Houston, [2] Michigan State University, [3] University of Texas at Austin

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The measurement of fluctuations in heavy ion collisions, combined with the direct measurement of resonances, gives us a way to gauge the effect of hadronic reinteractions between chemical and thermal freezeout. In [6] we have performed this analysis with fluctuation and resonance data from the STAR collaboration. Results seem to indicate that the K^* does not in fact reinteract much between production and freezeout.
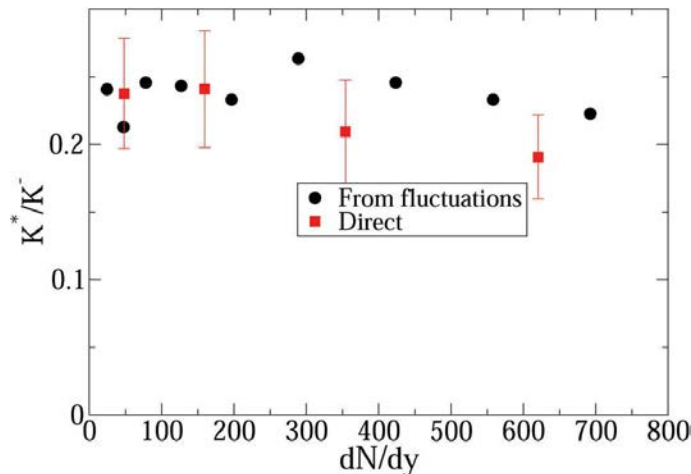

Figure 4: *A comparison of the K^* resonance probed at chemical freezeout from fluctuations and from thermal freezeout by direct measurement*

Project 7: Scaling of flow observables in hydrodynamics

Experimental data has now been obtained in heavy ion systems at many different energies and system sizes. In [7] I use, to constrain currently popular models (such as hydrodynamics) the scaling of flow observables with rapidity, multiplicity and energy. I find that these models typically are not able to reproduce the experimentally seen scalings, speculate for the reason of this discrepancy, and suggest ways of clarifying the situation.

Related publications in 2010:

[1] G. Torrieri and I. Mishustin, *The nuclear liquid-gas phase transition at large N_c in the Van der Waals approximation,* Phys. Rev. C **82**, 055202 (2010) [arXiv:1006.2471 [nucl-th]].

[2] B. Betz, J. Noronha, G. Torrieri, M. Gyulassy and D. H. Rischke, *Universal flow-driven conical emission in ultrarelativistic heavy-ion collisions,* Phys. Rev. Lett. **105**, 222301 (2010) [arXiv:1005.5461 [nucl-th]].

[3] S. Pratt and G. Torrieri, *Coupling relativistic viscous hydrodynamics to Boltzmann descriptions,* Phys. Rev. C **82**, 044901 (2010) [arXiv:1003.0413 [nucl-th]].

[4] G. Torrieri and J. Noronha, *Flavoring the Quark-Gluon Plasma with charm,* Phys. Lett. B **690**, 477 (2010) [arXiv:1004.0237 [nucl-th]].

[5] J. Noronha, M. Gyulassy and G. Torrieri, *Conformal holography of bulk elliptic flow and heavy quark quenching in relativistic heavy Ion collisions,* Phys. Rev. C **82**, 054903 (2010) [arXiv:1009.2286 [nucl-th]].

[6] G. Torrieri, R. Bellwied, C. Markert and G. Westfall, *Statistical hadronization phenomenology in K/π fluctuations at ultra-relativistic energies,* J. Phys. G **37**, 094016 (2010) [arXiv:1001.0087 [nucl-th]].

[7] G. Torrieri, *Rapidity scaling of multiplicity and flow in weakly and strongly interacting systems,* Phys. Rev. C **82**, 054906 (2010) [arXiv:0911.4775 [nucl-th]].

Dependence of elliptic flow on number of parton degrees of freedom

Collaborators: Z. Xu[1], C. Greiner[2]

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

Employing the on-shell parton cascade BAMPS we have studied the effect of an increasing number of parton degrees of freedom on the elliptic flow parameter v_2 generated in Au + Au collisions at the RHIC energy $\sqrt{s_{NN}} = 200$ GeV. The initial condition for BAMPS is assumed to be an ensemble of gluon minijets. The additional effective quark degrees of freedom during the further evolution are created by increasing the degeneracy factor d_G from 16 for a pure gluon system to 40 for a quark-gluon system with two quark flavors. This prescription indicates the assumption that quarks and gluons are identical particles. With this assumption for the BAMPS calculations, we have found that the p_T-averaged v_2 values and the total transverse energy at midrapidity are almost unchanged with or without quarks, which is a consequence of the almost same transport collision rates during the entire expansion. Second, incorporating quarks the parton multiplicities at freeze-out increase, which leads to a decrease of the mean parton transverse momenta $\langle p_T \rangle$ and a softening of the transverse spectra. Simultaneously, the differential elliptic flow $v_2(p_T)$ shifts toward lower momentum. Adding quarks with two flavors brings a 20% effect on $\langle p_T \rangle$ and $v_2(p_T)$, which is smaller than the maximum value of 26% owing to the incomplete chemical equilibration in the present studies. The incomplete chemical equilibration is also the reason for the slightly smaller η/s value in the QGP compared with the result for a pure gluon plasma.
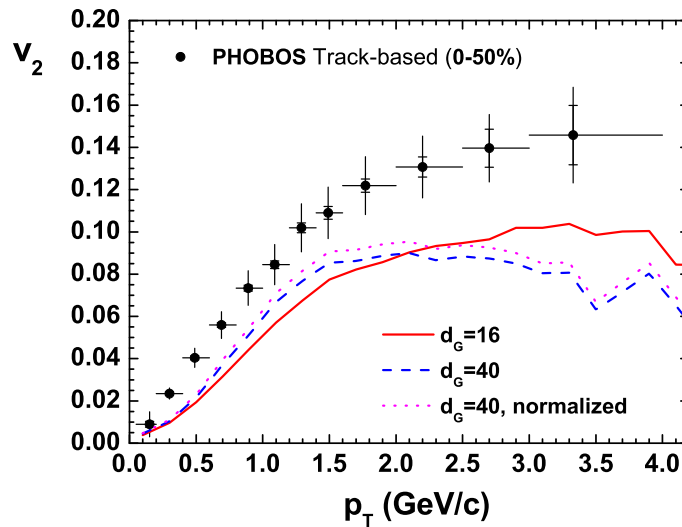
Momentum dependence of the elliptic flow $v_2(p_T)$ for the most central 50% collisions.

Related publications in 2010:
Z. Xu, C. Greiner, *Dependence of elliptic flow on number of parton degrees of freedom*, Physical Review C 81 (2010) 054901

Energy loss in a partonic transport model including bremsstrahlung processes

Collaborators: O. Fochler[2], Z. Xu[1], C. Greiner[2]

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

In this work, we have presented detailed results on the energy loss mechanisms for high-energy gluons within the microscopic parton transport model BAMPS. To this end we have investigated the evolution of high-energy gluons within thermal and static media of gluons.

We have discussed collisional energy loss ΔE as well as the contribution of radiative processes implemented in BAMPS via the Gunion-Bertsch matrix element. The inelastic $gg \rightarrow ggg$ processes are found to be the dominant source of energy loss for high-energy gluons in computations within the BAMPS model resulting in a strong differential energy loss that rises almost linearly with the jet energy. The strong mean energy loss in $gg \rightarrow ggg$ processes is due to a heavy tail in the ΔE distribution for single interactions, caused by the phase-space configurations of outgoing particles dictated by the Gunion-Bertsch matrix element in combination with the effective LPM cutoff. This prefers the emission of radiated gluons into the backward hemisphere with energies that in the center-of-momentum frame are comparable to that of the remaining outgoing particles, while they are small in the laboratory frame. The jet energy in these cases can be split into two particles yielding a large energy loss.

For a purely gluonic medium with T = 400 MeV the transport parameter $\hat{q}$ stemming from binary $gg \rightarrow gg$ interactions is found to be roughly constant at $\hat{q} = 2.3$ GeV^2/fm. When including inelastic $gg \leftrightarrow ggg$ processes, $\hat{q}$ as a measure of the accumulated transverse momentum exhibits a stronger dependence on the path length and is much larger than for elastic interactions, $\hat{q} = 12 - 23$ GeV^2/fm.

Extending our investigations of jet quenching in central Au + Au collisions at RHIC energies, we have presented the gluonic contribution to the nuclear modification factor for noncentral b = 7 fm collisions simulated in BAMPS. The gluonic R_{AA} in these off-central events is found to be flat at $R_{AA} \sim 0.13$ over a wide range in transverse momentum p_T for a critical energy density of $\varepsilon_c = 1.0$ GeV/fm^3, being in qualitative agreement with the experimental results.
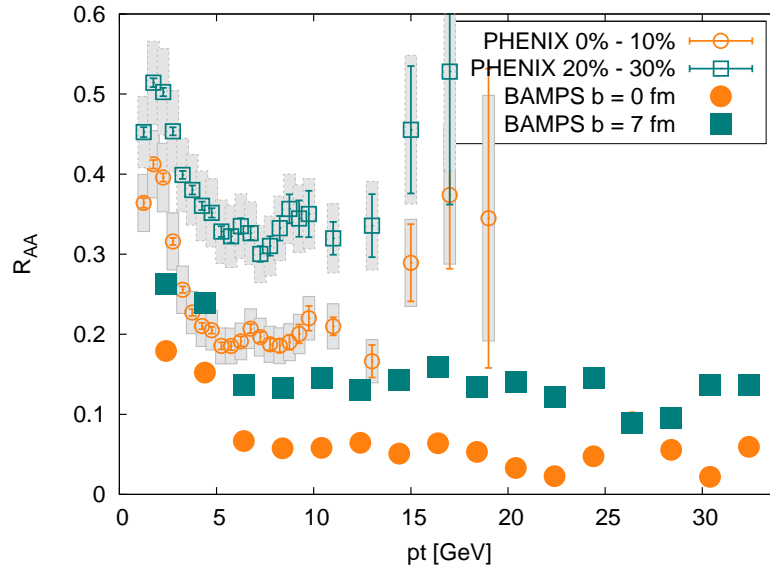
Gluonic nuclear modification factor at midrapidity from simulations of Au + Au collisions at 200A GeV.

Related publications in 2010:
O. Fochler, Z. Xu, C. Greiner, *Energy loss in a partonic transport model including bremsstrahlung processes*, Physical Review C 82 (2010) 024907

Israel-Stewart fluid dynamics and kinetic theory

Collaborators: B. Betz[1], I. Bouras[2], G. S. Denicol[2], A. El[2], O. Fochler[2], C. Greiner[2], T. Koide[3], F. Lauciello[2], E. Molnár[3,4], H. Niemi[3], F. Reining[2], D. H. Rischke[2,3], J. Uphoff[2], C. Wesp[2], Z. Xu[2,3]

[1] Department of Physics, Columbia University, New York, USA, [2] Institute für Theoretische Physik, Johann Wolfgang Goethe-Universität, Frankfurt am Main, Germany, [3] Frankfurt Institute for Advanced Studies, Frankfurt am Main, Germany, [4] KFKI Research Institute for Particle and Nuclear Physics, Budapest, Hungary

Interest in modeling high-energy heavy-ion collisions with dissipative hydrodynamics has been increased drastically within the last few years. However, straightforward generalization of the non-relativistic Navier-Stokes equations to relativistic flows is problematic as the resulting theory is not causal and it's solutions are not stable. One way to solve these problems is use so-called second order theories. One such theory is formulated by Israel and Stewart (IS).

The IS theory can be derived as an approximation to the Boltzann equation. Therefore, we can compare the two theories, kinetic theory and the IS hydrodynamics, using the same setup, i.e. with the same cross-sections and same initial conditions. This allows us to quantify how well the hydrodynamic solutions compares with the solutions of the full Boltzmann equation.

We tested the applicability of the IS theory by comparing the numerical solutions of the IS theory to the direct numerical solutions of the Boltzmann equation. We showed that the two theories agree well if the viscosity is small, and that the agreement starts to deteoriate when viscosity increases. The main quantity that characterize the applicability of the hydrodynamics is Knudsen number Kn, i.e. the ratio between microscopic and macroscopic lenght scales. We found that a good agreement between kinetic theory and IS theory requires $Kn < 1/2$.

Many of the terms in IS equations were neglected in the original derivation, where the IS theory was obtained from the Boltzmann equation by using so called moments method. We have completed the work, by including all the terms that appear in the equations in the 14-moment approximation.

We have further investigated the structure of the shock waves in the dissipative matter, by using kinetic theory.

Related publications in 2010:

1) E. Molnar, H. Niemi, D. H. Rischke, *Numerical tests of causal relativistic dissipative fluid dynamics* Eur. Phys. J. C65, 615-635 (2010). [arXiv:0907.2583 [nucl-th]].

2) I. Bouras, E Molnar, H. Niemi et al., *Investigation of shock waves in the relativistic Riemann problem: A Comparison of viscous fluid dynamics to kinetic theory*, Phys. Rev. C82, 024910 (2010), [arXiv:1006.0387 [hep-ph]].

3) B. Betz, G. S. Denicol, T. Koide et al., *Second order dissipative fluid dynamics from kinetic theory*, [arXiv:1012.5772 [nucl-th]].

4) I. Bouras, E. Molnar, H. Niemi et al., *Relativistic Shock Waves and Mach Cones in Viscous Gluon Matter*, J. Phys. Conf. Ser. 230, 012045 (2010). [arXiv:1004.4615 [hep-ph]].

5) I. Bouras, A. El, O. Fochler et al., *Mach Cones in Viscous Matter*, Proceedings "Hot Quarks 2010", [arXiv:1008.4072 [hep-ph]].

Equation of State for Neutron Stars

Collaborators: A. Kurkela[1], P. Romatschke[2], A. Vuorinen[3], B. Wu[2,3,4]

[1] ETH Zürich, [2] Frankfurt Institute for Advanced Studies, [3] University of Bielefeld, [4] Peking University

Compact stars offer a unique window of cold nuclear matter in the regime of extremely high densities. In particular, it has long been speculated that "exotic" phases of nuclear matter, such as quark matter could exist in the core of neutron stars. Lacking the tools to solve QCD accurately for densities expected in compact stars, simple toy models such as the MIT bag model for the QCD equation of state have been state of the art for the past 30 years.

Somewhat surprisingly, more reliable results can be obtained using recent results from perturbative QCD. In fact, matching modern quark matter to realistic hadronic equations of state, one can reproduce available observations of neutron stars without any fine-tuning of parameters. Hybrid stars with maximum masses of $2.1M_\odot$ are possible, which is in-line with the recent observation of the 1.97 ± 0.04 solar mass neutron star J1614-2230.
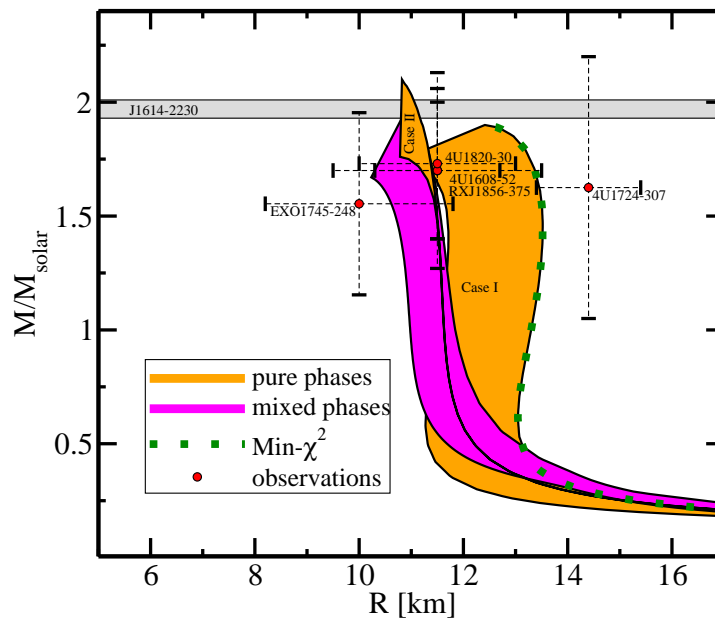
Star mass-radius curves for hybrid EoSs compared to observations (both assuming negligible spin frequencies).

Related publications in 2010:
1) A. Kurkela, P. Romatschke, A. Vuorinen, B.Wu, *Looking inside neutron stars: Microscopic calculations confront observations*, arXiv:1006.4062 [astro-ph.HE], submitted to Physical Review D

Neutron stars with small radii - the role of Δ resonances

Collaborators: Torsten Schürhoff[1,2], Stefan Schramm[1,2,3], Veronica Dexheimer[4]

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[2] Institute for Theoretical Physics, Goethe University, Frankfurt, Germany

[3] Center for Scientific Computing, Goethe University, Frankfurt, Germany

[4] Gettysburg College, Gettysburg, USA

Recent experimental measurements of both the mass and radius of neutron stars suggests that they may be smaller than previously considered, with radii between 8 and 10 kilometers and masses between 1.6 and 1.9 solar masses. Equations of state that contain only neutrons, protons, electrons and neutrinos cannot explain these low values.

In our approach, we use a well-tested flavor SU(3) sigma model and include both Δ resonances and hyperons in the equation of state. In addition, we vary the coupling strength of the Δ resonances to the vector mesons as a free parameter. If this coupling strength is only slightly smaller than the coupling between nucleons and vector mesons, by a factor of 0.9, we are able to reproduce the measured mass-radius-relationship and the extracted equation of state for these neutron stars. At certain densities, Δ resonances become the dominant particle species in such a star, while the addition of hyperons only plays a minor role for the mass-radius-relationship and equation of state.
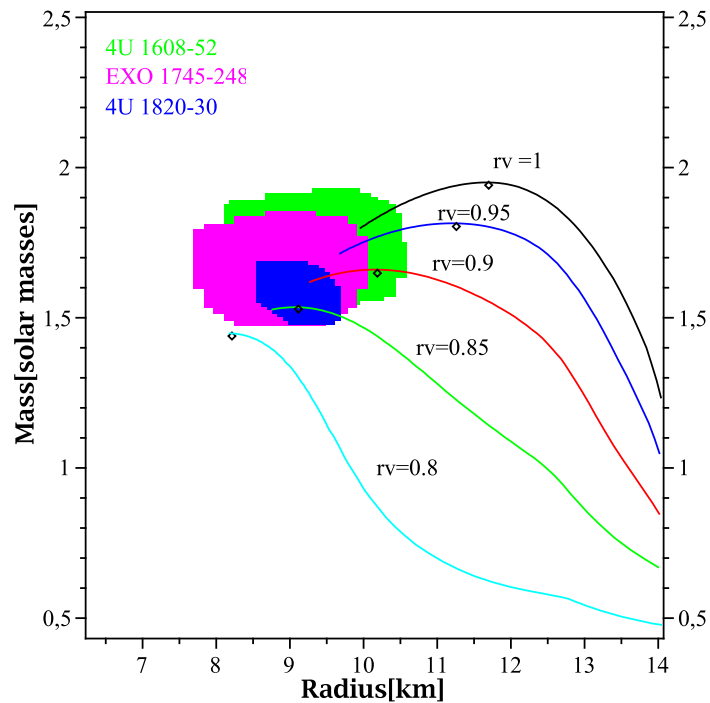
Mass-radius relationship for neutron stars with various coupling strength of the Δ resonances. Also shown is are the 1-σ confidence areas for the measured neutron stars.

Related publication in 2010:

1) T. Schürhoff, S. Schramm and V. Dexheimer, *Neutron stars with small radii - the role of Δ resonances*, Astrophys. J. Lett. 724 (2010), L74-77, arXiv:1008.0957 [astro-ph.SR]

Pseudo-General Relativity

**Collaborators:** P. O. Hess[1], W. Greiner[2], L. Maghlaoui[2] , G. Caspar[2], T. Schönenbach

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The standard Theory of General Relativity was extended to a pseudo-complex version, extending the space coordinates to pseudo-complex oness. Pseudo-complex coordinates ($X = x_1 + Ix_2$) are treated similar to complex coordinates with the difference that $I^2 = 1$. This permitted to formulate a theory of General Relativity, in two orthogonal spaces, which are related later via a modified variational principle. As a consequence, dark energy is included automatically. We discussed the cases of a central mass (pseudo-complex Schwarzschild solution) and the pseudo-complex Robertson-Walker model of the universe. In the Schwarzschild solution the central mass accumulates dark energy until the collaps is stopped due to the repulsion of the dark energy. As a consequence, neither an event horizon nor a central singularity exists in the pseudo-complex version of General Relativity. The solution behaves very similar to the standard Schwarzschild solution and differences appear only near to the former event horizon. We discussed changes in the perihelion shift of Mercury, which are at least one order of magnitude less than the actual measurements. For the pseudo-complex Roberson-Walker model of the universe we obtained additional solutions. All solution experiment in the early times of the universe a de-acceleration, which later on turns into an acceleration. However, the new solutions permit that this acceleration approaches a constant value or, after having reached a maximum acceleration, it tends to zero for infinite time. We also started to investigated charged (pseudo-complex Nordström-Reissner solution) and rotating (Kerr solution) black holes, which are still ongoing investigations.

Antigravitation in the center
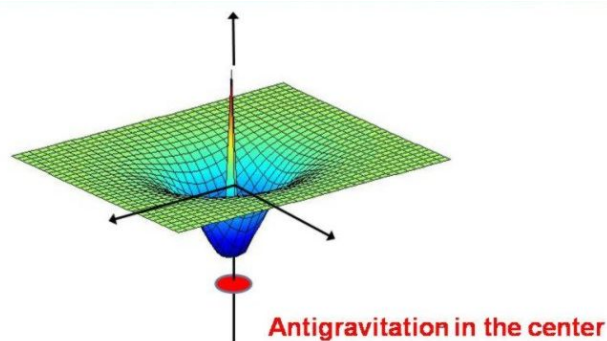
Related publications in 2009 and 2010:

1) P. O. Hess, W. Greiner, *Pseudo-Complex General Relativity*, Int. J. Mod. Phys. E 18 (2009), 51-77.
2) P. O. Hess, L. Maghlaoui and W. Greiner, *The Robertson-Walker Metric in a Pseudo-complex General Relativity*, Int. J. Mod. Phys. E 19 (2010), 1315-1339.
3) P. O. Hess, L. Maghlaoui and W. Greiner, *There are no Black Holes; Pseudo-Compex General Relativity – Review and some Predictions*, Int. J. Mod. Phys. D 19 (2010), 1217-1232.

Minimal length effects in quantum field theory and particle physics

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

[1] Frankfurt Institute for Advanced Studies, [2] Northeastern University, USA [4] University of Bergamo, Italy [2] University of Geneva, Switzerland

Even if efficient, well defined and accurate, renormalization can be considered not more than a mere artificial procedure to circumvent the problem of the ultraviolet completion of theories describing fundamental interactions. On pure physical grounds, one may hope that the spacetime itself, when probed at extreme energy scales, can provide a natural cutoff for any field theory. A similar way of reasoning is mandatory when gravity is concerned for its long standing problem of lack of renormalization. However one may think to reformulate all field theories in order to modify their behavior in the Planckian, trans-Planckian regimes. In this spirit, we initially calculate the radiation perceived by an accelerated detector (Unruh effect) by means of a noncommutative field theory: instead of the Planckian spectrum, we found a suppressed non-thermal radiation, i.e., a modification so drastic that can be explained only by accepting that noncommutative field theory can affect in some circumstances the infrared sector of fields according to a UV/IR duality. In this framework we formulate a new field theory endowed with two cutoffs, UV and IR, by assuming an extended representation of Hilbert spaces. Further studies concerned modifications of fields for the presence of un-particles, the conjectures conformal invariant hidden sector of the standard model which would show up at the Terascale. We obtained compelling deviations to Newton's law by employing entropic gravity arguments. Finally we applied noncommutative field theories in a variety of physical context, spanning from cosmology to quantum electrodynamics. As a special result we mention the derivation of modified neutrino oscillation frequencies, which would lead to estimates of the fundamental scale in future experiments.
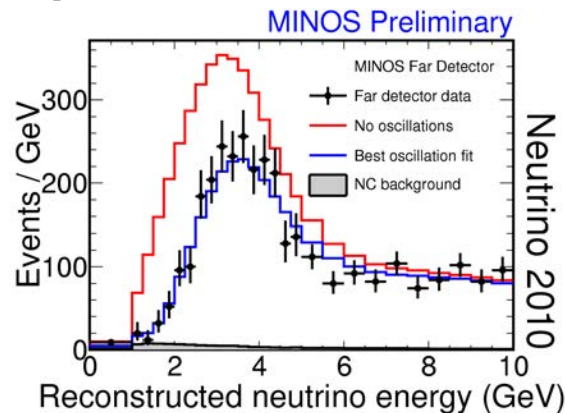
Measured energy distribution at the far detector of the MINOS experiment. Terascale noncommutative deviations are detectable for source-detector distances comparable to the Earth-Moon distance.

Related publications in 2010:

1) P. Nicolini and M. Rinaldi, *A minimal length versus the Unruh effect*, to be published in Phys. Lett. B; arXiv:0910.2860 [hep-th].

2) P. Nicolini, *Entropic force, noncommutative gravity and un-gravity*, Phys. Rev. D 82 (2010) 044030

3) M. Kober and P. Nicolini, *Minimal Scales from an Extended Hilbert Space*, Classical and Quantum Gravity 27 (2010) 245024

4) B. Barbiellini and P. Nicolini, *Enhancement of Compton Scattering by an Effective Coupling Constant*, submitted to Phys. Rev. A; arXiv:1005.5496 [cond-mat]

5) R. Garattini and P. Nicolini, *A Noncommutative approach to the cosmological constant problem*, under review on Phys. Rev. D; arXiv:1006.5418 [gr-qc]

6) M. Sprenger, P. Nicolini and M. Bleicher, *Neutrino oscillations as a novel probe for a minimal length*, submitted for publication; arXiv:1011.5225 [hep-ph]

Diffusive processes and microstructure of a quantum universe

Collaborators: P. Nicolini[1], B. Niedner[1,2], L. Modesto[3], E. Spallucci[4]

[1] Frankfurt Institute for Advanced Studies, [2] Imperial College London, UK [3] Perimeter Institute for Theoretical Physics, Canada [4] University of Trieste, Italy

Spacetime is expected to change its nature when high energies/short scales are concerned. In this regime spacetime has a fabric, whose meshes encode the local loss of resolution, i.e., the presence of the Planck length. 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 modelled by a fractal surface. A fractal has the important property of having a dimension that can be a non integer number, and thus smaller than the topological dimension of usual manifolds. This fact can be seen by defining the spectral dimension

$$D = -2 \frac{\partial \ln P_g(s)}{\partial \ln s}. \tag{1}$$

namely the spacetime dimension perceived by a diffusive process, where

$$P_g(s) = \frac{\int d^d x \sqrt{\det g_{ab}} \, K(x,x;s)}{\int d^d x \sqrt{\det g_{ab}}} \tag{2}$$

is the diffusion return probability, s is the diffusion time and $K(x,y;s)$ is the heat kernel, representing the probability density of diffusion from x to y. If at the Planck scale the spectral dimension equalled two, this could be a signature of a renormalizable character of gravity. In such a context, by employing an original representation of the heat kernel motivated by noncommutative geometry arguments, we showed that, for the case of flat space, the spectral dimension equals two as expected. This has been a major breakthrough in the field since calculations did not need any numerical simulation, but were carried analytically in a clean way. This work has been generalized in two cases: the diffusion of unparticles which has disclosed a scenario for fractals in the trans-Planckian regime and the Haussdorff dimension, a complementary indicator of the amount of fuzziness of a quantum spacetime.
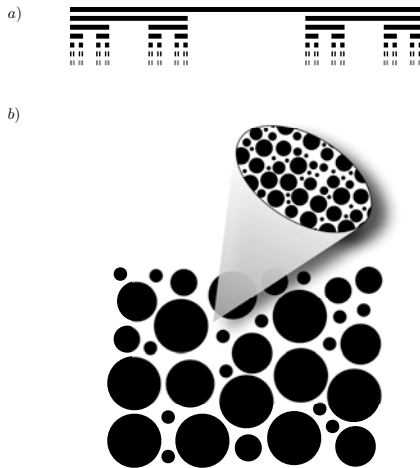
In (a) we have a Cantor set, i.e. a fractal surface which resembles the quantum spacetime.
In (b), there is an artistic picture of the spacetime, whose holed structure shows a fractal self-similarity.

Related publications in 2010:
1) L. Modesto and P.Nicolini, *Spectral dimension of a quantum universe*, Phys. Rev. D 81 (2010) 104040
2) P. Nicolini and E. Spallucci, *Un-spectral dimension and quantum spacetime phases*, to be published in Phys. Lett. B; arXiv:1005.1509 [hep-th]
3) P. Nicolini and B. Niedner, *Hausdorff dimension of a particle path in a quantum manifold*, to be published in Phys. Rev. D; arXiv:1009.3267 [gr-qc]

Black holes at the LHC and ultraviolet complete quantum gravity

Collaborators: M. Bleicher[1], P. Nicolini[1], L. Modesto[2], J. W. Moffat[2], D. Batic[3]

[1] Frankfurt Institute for Advanced Studies, [2] Perimeter Institute for Theoretical Physics, Canada [3] University of West Indies, Jamaica

After more than 30 years of intensive debate about an efficient formulation of a quantum theory of gravity, we still have an even more fundamental and concrete problem: the absence of any quantum gravity data. Against this background, a major breakthrough is given by the possibility for spacetime of being endowed with more than the usual four dimensions: this fact would make the gravitational coupling strong at scales now accessible to current particle accelerators. On the phenomenological ground this implies the possibility of smashing matter at distances for which the gravitational collapse into a black hole would be more than realistic. In this framework, we focused our studies on the specific issue of the Hawking radiation, a foreseen thermal radiation that would be plentifully emitted by elementary particle size black holes. More specifically we reviewed the conventional derivation of this effect at the light of recent nonlocal field theories and ultraviolet complete quantum gravity formulations. As a result, in contrast to an expected divergent terminal phase of the Hawking emission we showed that a black hole undergoes a final cooling down towards a zero temperature remnant configuration. We analysed phenomenological consequences of the presence of black hole remnants in particle detectors and we extended our analysis to the difficult but crucial problem of deriving a quantum gravity corrected microscopic charged, spinning black hole, the more realistic model for describing products of hadron collisions. As a result we showed that quantum gravity effects at the Terascale are able to cure conventional curvature singularities occurring in Einstein gravity black hole models.
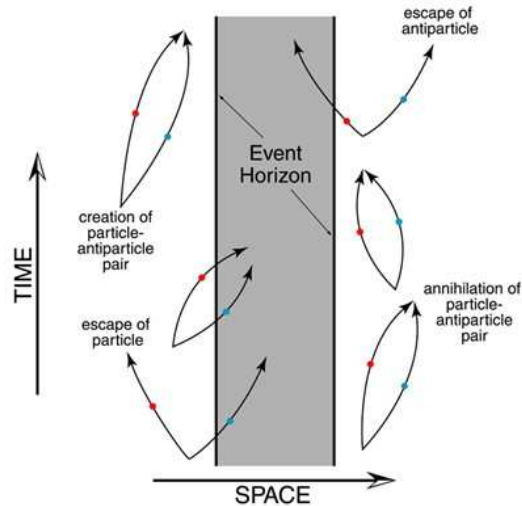
The Hawking radiation as a quantum vacuum effect in the presence of an event horizon.

Related publications in 2010:

1) M. Bleicher and P. Nicolini, *Large extra dimensions and small black holes at the LHC*, J. Phys. Conf. Ser. 237 (2010) 012008
2) D. Batic and P. Nicolini, *Fuzziness at the horizon*, Phys. Lett. B 692 (2010) 32
3) L. Modesto and P. Nicolini, *Charged rotating noncommutative black holes*, Phys. Rev. D 82 (2010) 104035
4) L. Modesto, J. W. Moffat and P. Nicolini, *Black holes in an ultraviolet complete quantum gravity*, to be published in Phys. Lett. B; arXiv:1010.0680 [gr-qc]

4.2 Neuroscience

Expectation Truncation and the Benefits of Preselection in Training Generative Models

Collaborators: J. Lücke[1], J. Eggert[2]

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

Data interpretation in many applications of artificial and biological systems is challenging because of noise, the complexity of the input and because of its ambiguity. Optimal inference based on probabilistic generative models is in general intractable in such situations because it involves the evaluation of all potential interpretations of the input. To approximate optimal inference, a fast initial stage of processing has therefore long since been suggested. In this paper we show how such a preselection of hidden variables can be used to efficiently train generative models with binary hidden variables. The approach is based on Expectation Maximization (EM) and uses an efficiently computable approximation to the sufficient statistics of a given model. The computational cost to compute the sufficient statistics is strongly reduced by selecting, for each data point, the relevant hidden causes. The approximation is applicable to a wide range of generative models and provides an interpretation of the benefits of preselection in terms of a variational EM approximation.

To empirically show that the method maximizes the data likelihood, it is applied to different types of generative models including: a version of non-negative matrix factorization (NMF), a model for non-linear component extraction (MCA), and a linear generative model similar to sparse coding. The derived algorithms are applied to both artificial and realistic data, and are compared to other models in the literature. We find that the training scheme can reduce computational costs by orders of magnitude and allows for a reliable extraction of hidden causes.
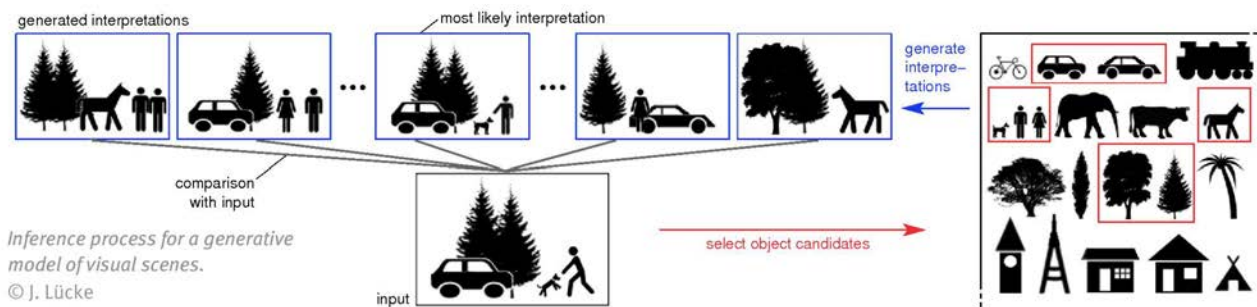
Inference model for a generative model of visual scenes

Model averaging as a developmental outcome of reinforcement learning

Collaborators: T.H. Weisswange[1], C.A. Rothkopf[1], T. Rodemann[2], J. Triesch[1]

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

To make sense of the world, humans have to rely on the information they receive from their sensors. Due to noise on one side and redundancies on the other side, it is possible to improve estimates of the signal's causes by integrating over multiple sensors. In recent years it has been shown that humans do so in a way that can be matched by optimal Bayesian models. Such an integration is only beneficial for signals originating from a common source and there is evidence that human behavior takes into account the probability for a common cause. For the case in which the signals can originate from one or two sources, it is so far unclear, whether human performance is best explained by model selection, model averaging, or probability matching. Furthermore, recent findings show that young children are often not integrating different modalities, indicating that this has to be learned during development. But which mechanisms are involved and how interaction with the environment could determine this process remains unclear.

Here we use a reinforcement learning (RL) algorithm that is trained to perform an audio-visual orienting task. Two signals originate from either one or two sources and provide noisy information about the position of objects. The agent receives rewards if the action brings him close to the objects. The agent quickly learns to act in a way that closely approximates the behavior of a Bayesian observer. It behaves differently depending on the probability for a single cause and on the reliabilities of the cues. When we test with signals for which the behavior of model selection and model averaging differ most, the agent obtains significantly more reward than a Bayesian model selecter and matches very closely the reward obtained by the Bayesian model averager.

Our results show that a RL agent can learn when and how to do cue integration, without explicitly computing with probability distributions. This suggests that RL based mechanisms could at least support the development of such behavior.
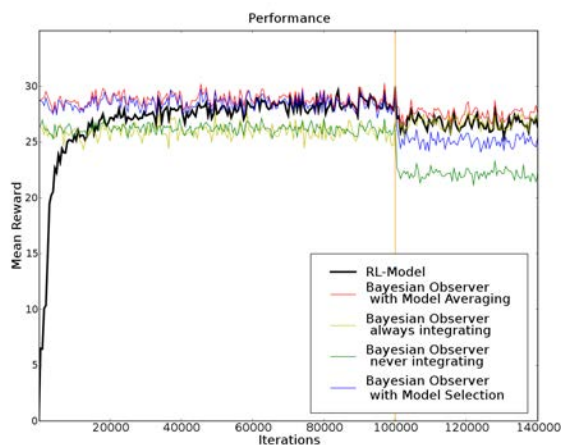
Performance of the RL agent and the optimal Bayesian models. Performance behind the orange line shows test case restricted on inputs with largest difference between model averaging and model selection.

Related publications in 2010:

1) C.A. Rothkopf, T.H. Weisswange and J. Triesch, *Computational modeling of multisensory object perception*, in "Multisensory Object Perception in the Primate Brain", M. Naumer and J. Kaiser (ed.), Springer, 2010, 21-53

2) J. Triesch, C.A. Rothkopf and T.H. Weisswange, *Coordination in Sensory Integration*, in "Dynamic Coordination in the Brain", C. von der Malsburg, W.A. Phillips and W. Singer (ed.), MIT Press, 2010, 229-234

3) T.H. Weisswange, C.A. Rothkopf, T. Rodemann and J. Triesch, *Model averaging as a developmental outcome of reinforcement learning*, in Proceedings: Computational and Systems Neuroscience (COSYNE 2010), 2010

A stable, activity-dependent plasticity rule for homeostatic synaptic scaling

Collaborators: P. Joshi, J. Triesch

Frankfurt Institute for Advanced Studies

Hebbian mechanisms in the form of long-term potentiation (LTP) and long-term depression (LTD) are essential for selectively modifying the synaptic efficacies in order to learn a new task. While Hebbian mechanisms are important for learning, they are known to be unstable due to the positive feedback process which leads the circuit into hyper- or hypo-active regimes. Recent neurophysiological experiments have identified several forms of homeostatic plasticity mechanisms that stabilize the neural circuits. These include mechanisms for modulating the intrinsic excitability of the cell and for controlling the total synaptic drive. A new synaptic plasticity mechanism is presented here that enables a neuron to obtain homeostasis of its firing rate over longer timescales while leaving the neuron free to exhibit fluctuating dynamics in response to input variance. Mathematical results demonstrate that the plasticity rule described here is globally asymptotically stable. It is shown that the synaptic scaling rule is multiplicative in nature as is suggested by recent neurobiological experiments. A key prediction made by this model is that multiplicative synaptic scaling happens not on the population level but on the level of individual synapses. Performance of the rule is benchmarked under different input conditions from single neuron to network level and a comparison of the rule is presented with other rules. Finally a model is presented which shows that the synaptic scaling rule presented here can lead to ocular dominance shift following monocular deprivation, suggesting that the synaptic scaling mechanisms could be the biophysical substrate behind this change in binocular organization.
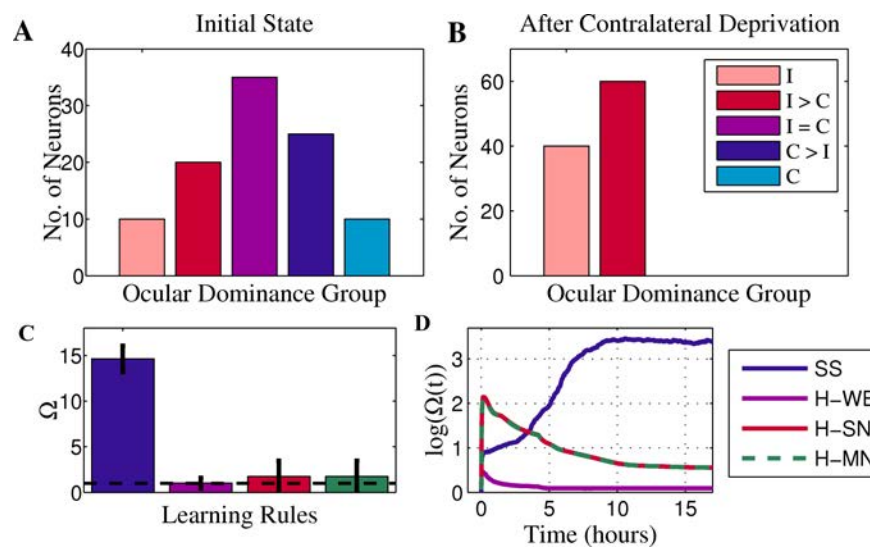
Ocular dominance shift in a model V1 neurons strip following monocular deprivation. (**A**) *Ocular dominance histogram showing the distribution of V1 neurons into the five ocular dominance categories during the baseline phase, and* (**B**) *after contralateral deprivation. Most of the neurons are driven binocularly in the baseline phase, whereas monocular deprivation makes neurons unresponsive to the deprived eye. Comparison of the synaptic scaling rule with other plasticity rules (SS → Synaptic Scaling, H-WB, H-SN, H-MN → Hebbian rule with weight bounds, subtractive and multiplicative normalization respectively) that can potentially cause OD shift following monocular deprivation.* (**C**) *Value of Ω for each rule after deprivation.* (**D**) *Temporal evolution of $\Omega(t)$ during the deprivation phase for the plasticity rules. Dashed line in panel E and F ($\Omega = 1$) indicates no ocular dominance.*

Related publication in 2010:

1) P. Joshi and J. Triesch, *A stable, activity-dependent plasticity rule for homeostatic synaptic scaling and the emergence of ocular dominance shift through monocular deprivation in model V1 neurons* , Submitted, 2010

The timescale of informative multineuronal spike patterns in visual cortex

Collaborators: Ovidiu Jurjuț[1], Danko Nikolić[1], Wolf Singer[1], Raul Mureşan[2]

[1] FIAS and MPI für Hirnforschung, Frankfurt, [2] Center for Cognitive and Neural Studies, Cluj-Napoca, Romania

The project pushes forward our current understanding of how collections of neurons process information in the cortex. The strategy we investigate is neuronal coding trough spatiotemporal spike patterns, i.e. constellations of spikes distributed across multiple neurons over a given time window. First, we question if spike patterns can convey information about external stimuli by selectively occurring for some stimuli and/or at specific moments in time. Second, we aim to identify the timescales of informative spike patterns and investigate how they relate to the temporal properties of the stimuli.

To address these questions, we use spiking signals recorded from the primary visual cortex of anesthetized cats while the animals were presented with stimuli of various temporal dynamics. In addition, we developed a set of classifiers that are able to identify and quantify the occurrence of spike patterns on arbitrary timescales (Jurjuț et al.). By taking into account different properties of spike pattern occurrence (e.g. stimulus specificity or stimulus time-locking), classifiers can determine the timescales that are most informative for discriminating between visual stimuli.

Our results thus far suggest that informative spike patterns evolve on a continuum of coexisting timescales, which strongly depend on the temporal dynamics of the stimuli.
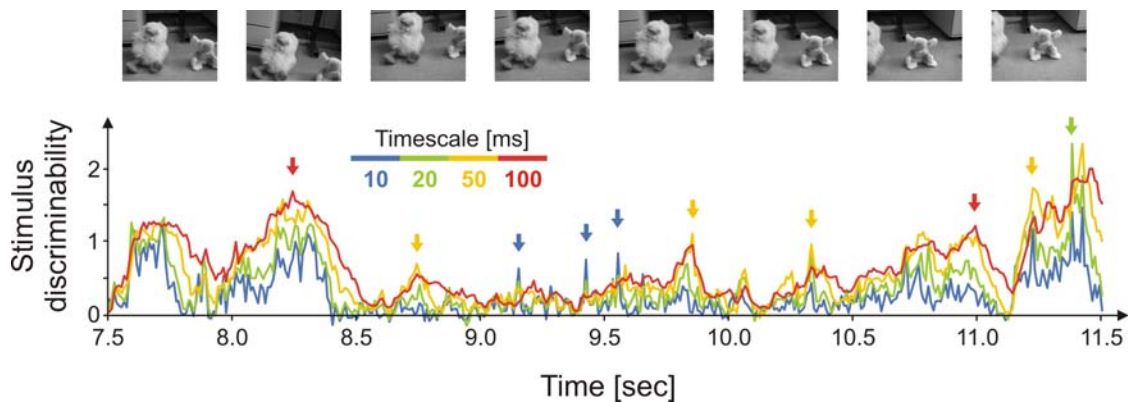
Figure. Discriminating a visual stimulus from a set based on the activity of 22 neurons at various timescales. Stimuli were movies showing natural scenes. The arrows point moments in time where one timescale was more informative than the others in discriminating the stimulus from the set (from Jurjuț et al.).

Related publication:
O.F. Jurjuț, D. Nikolic, W. Singer, S. Yu, M.N. Havenith, R.C. Mureşan, *Timescales of Multineuronal Activity Patterns Reflect Temporal Structure of Visual Stimuli*. PLoS ONE 6(2): e16758 (2011)

Learning Bayesian priors in self-organizing recurrent networks

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

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

The mechanisms by which recurrent cortical networks implement Bayesian computations are not understood. We explore the role of local plasticity rules in learning statistical priors in a self-organizing recurrent neural network (SORN). The network 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. After learning, the network exhibits spontaneous activity that matches the stimulus-evoked activity during training and thus can be interpreted as samples from the network's prior probability distribution over evoked activity states. Furthermore, we show how learning the frequency and spatio-temporal characteristics of the input sequences influences the network's performance in several classification tasks. These results establish a novel connection between low level learning mechanisms in recurrent networks and high level concepts of statistical inference and learning.
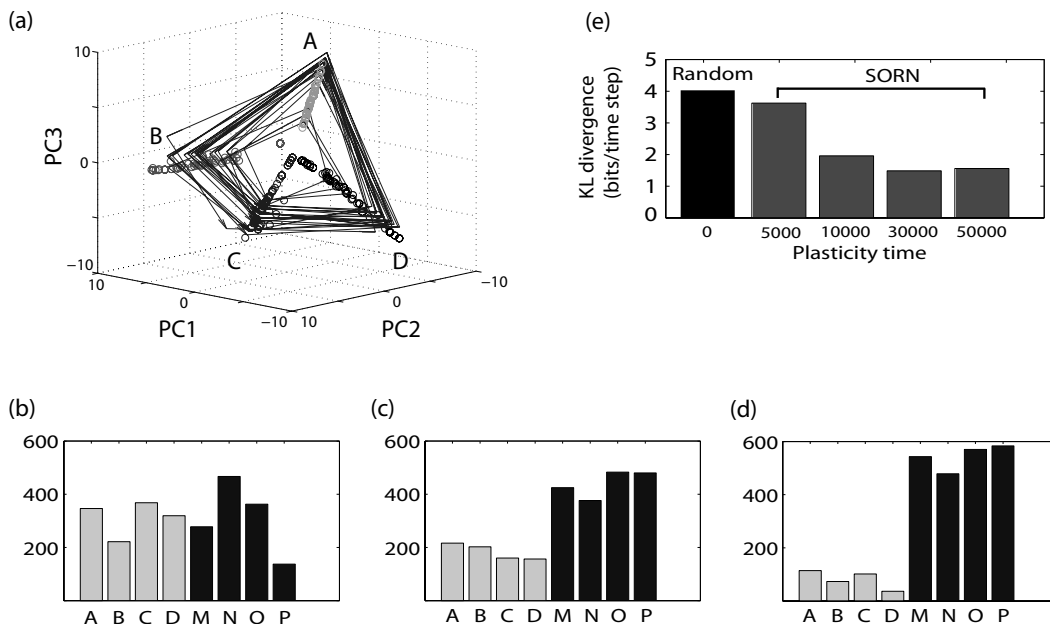
Spontaneous and evoked activity become similar in SORNs: (a) Result of PCA on SORN's internal representations during evoked activity to a sequence of letters (circles), and spontaneous activity in the absence of input (lines). (b) Distribution of spontaneous states for random networks in the absence 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.

Publications and conferences 2010:

1) A. Lazar, G. Pipa and J. Triesch, *Spontaneous Activity in a Self-Organizing Recurrent Network Reflects Prior Learning*, Conference Abstract: Computational and Systems Neuroscience 2010, I-39.
2) A. Lazar, G. Pipa and J. Triesch, *Learning Bayesian priors in a recurrent network with STDP*, Conference Abstract: Neuroscience 2010, 414.
3) A. Lazar, *Self-Organizing Recurrent Neural Networks*, PhD Thesis.

Development of Coordinated Eye and Head Movements in Primates

Collaborators: S. Saeb[1], C. Weber[2], J. Triesch[1]

[1] Frankfurt Institute for Advanced Studies, [2] University of Hamburg.

Gaze shifts of primates are characterized by coordinated eye and head movements. Although much effort has been put forth to reveal the neural substrate underlying the gaze shift control system or to find the optimality principle behind its dynamics, it remains unclear how such a control scheme develops in primates.

In this theoretical study, we start by assuming a simple cost function and a plausible neural learning model. The cost function depends on the instantaneous visual error signal integrated over time, plus a regularization term. We proceed by training the neural model with respect to the proposed cost function using learning rules that are biologically plausible. While these learning mechanisms adjust the connection strengths of the neural model, we manipulate the free parameters of the model to match its behavior to experimental observations. Using a set of such parameters for head-restrained (HR) and another for head-free (HF) gaze shift conditions, our model is able to reproduce many of the gaze shift characteristics observed in experiments. These characteristics include the saccadic main sequence and the bell-shaped velocity profiles in HR, and the relative contribution of eye and head to the gaze shift as well as its dependence on initial eye position in HF conditions. Furthermore, our model reproduces the early fixation phase of the eyes in HR and the so-called vestibulo-ocular reflex (VOR) phase in HF conditions. All of these results are gradually achieved through incremental learning, which implies that the visuomotor system may incorporate a similar kind of learning to constantly calibrate its control circuitry with respect to a cost function. The model can be generalized to other ballistic motor control tasks beyond gaze shifts by finding appropriate motor plant models and cost functions.
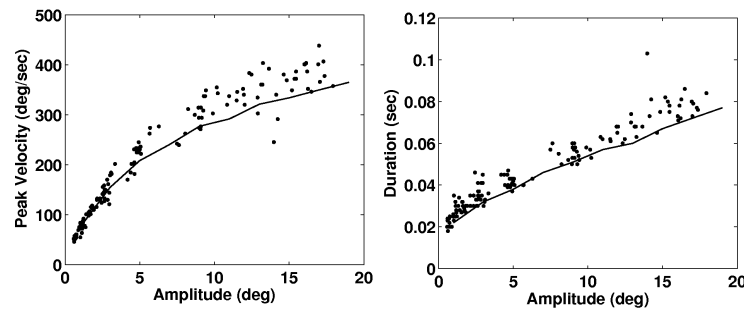
Comparing model results (solid lines) to experimental data (dots) in HR condition.
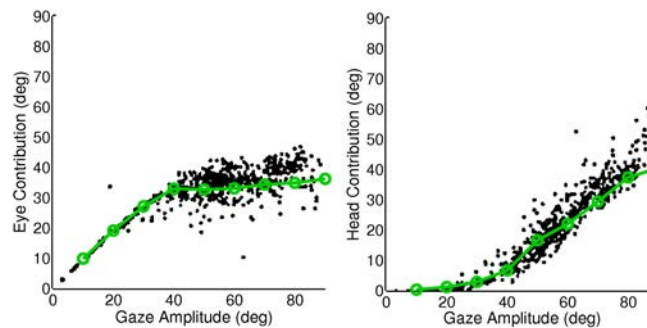
Comparing model results (solid lines) to experimental data (dots) in HF condition.

Related publications in 2010:
1) S. Saeb, C. Weber, and J. Triesch, *Learning coordinated eye and head movements: unifying principles and architectures*, Front. Comput. Neurosci. Conference Abstract: Bernstein Conference on Computational Neuroscience (2010).
2) S. Saeb, C. Weber, and J. Triesch, *Learning the optimal control of coordinated eye and head movements*, Submitted to PLoS Computational Biology (2010).

Orientation discrimination under memory and perceptual loads

Collaborators: L. Scocchia[1], G. M. Cicchini[2], J. Triesch[1]

[1] Frankfurt Institute for Advanced Studies, [2] University of Florence, Italy

Maintaining a complex object in visual working memory (VWM) slows processing of similar visual stimuli during the maintenance period (Robinson, Manzi & Triesch, 2008). In this study, we explored the interaction between the processing of low-level features of simple visual objects and the contents of visual working memory (VWM). Participants were required to memorize the orientation of a Gabor patch (a 2D sinusoidal grating embedded in gaussian noise) and to perform an orientation discrimination task during the retention interval. The discrimination task consisted of judging whether a Gabor patch was oriented 'upward' or 'downward' relative to 45°, twice consecutively after the presentation of the memory stimulus. In order to distinguish VWM from perceptual effects, participants were also tested in a similar control condition that did not require memorization. Significantly lower accuracy and slower reaction times were observed in the VWM than in the control condition, thus indicating that holding in memory an oriented stimulus interfered with orientation discrimination performance significantly more than simply attending to it. Furthermore, discrimination performance was strongly affected by the orientation of the memorized stimulus: VWM loads closer to the vertical selectively disrupted performance when the discrimination stimulus was relatively more vertically oriented (i.e: 41° from vertical), whereas VWM loads closer to the horizontal selectively disrupted performance when the discrimination stimulus was relatively more horizontally oriented (i.e: 49° from vertical). The control condition showed a similar pattern of results at the first but not at the second of the two subsequent discriminations. This result indicates that the interference of an oriented memory trace with orientation discrimination performance is visual in nature and can be disrupted by perceptual interference unless it is actively maintained in VWM.
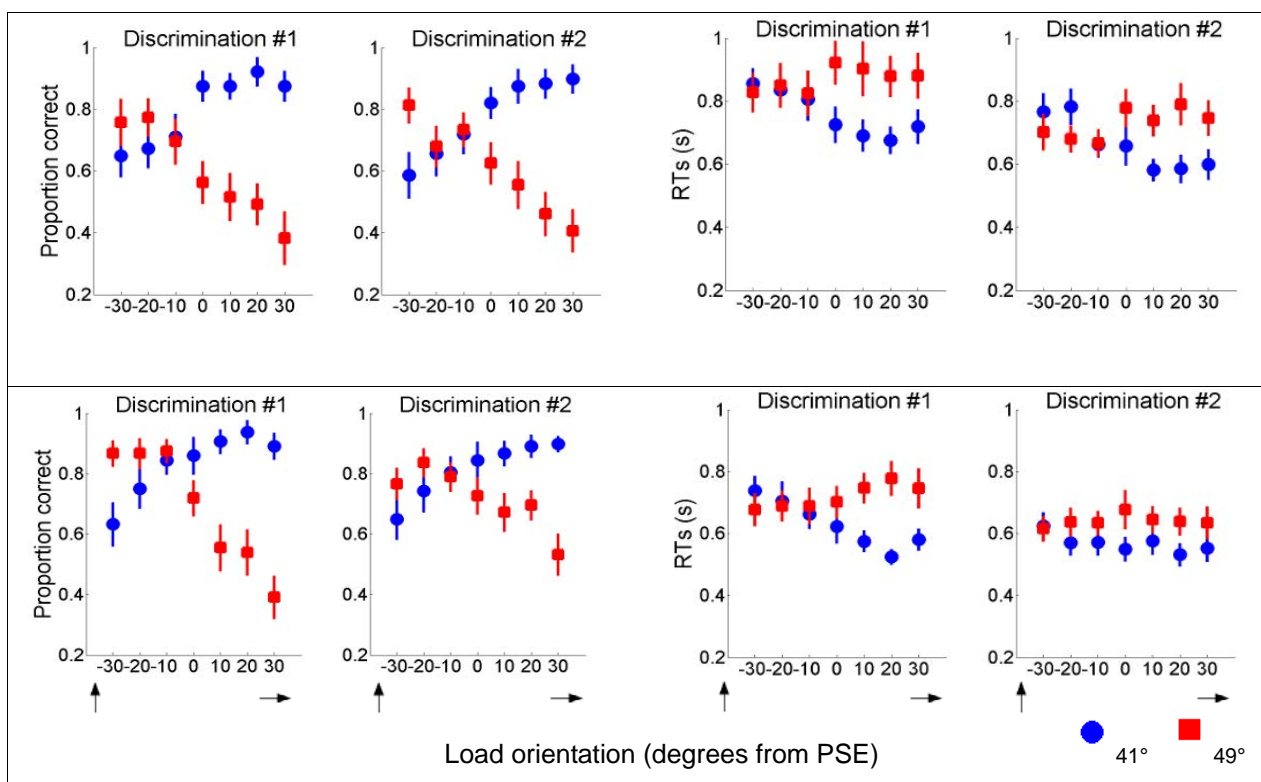
Performance at the two tasks. *Upper row*: memory condition, *lower row*: perceptual control condition.

Related publication in 2010:

L. Scocchia, G. M. Cicchini, and J. Triesch, *What's 'up'? Orientation discrimination while holding orientations in memory*, Perception 39, ECVP Abstract Supplement (2010) 38.

Working memory development through reward-dependent STDP – role of structural plasticity during learning

Collaborators: C. Savin and J. Triesch

Instead of being fixed, hard-wired structures, cortical networks are capable of significant reorganization. As we learn new skills or adapt to changes in the environment, brain structure changes as well (Yoshida et al 2003, Hihara et al, 2006)- existing synapses are eliminated and new synapses are grown. These structural changes can sometimes be homeostatic, maintaining the stability of the system, while in other cases they may play an important role in shaping the network function (Zito and Svoboda, 2002). Moreover, it was suggested that such cooperative synaptic formation is important for explaining the statistics of synaptic connections observed in rat cortex, which could not emerge by random sparse connections alone (Fares and Stepanyants, 2009). However, the functional implications of this form of structural plasticity remain unclear.

We investigated this question in the context of our previous working memory model (Savin and Triesch, 2009) in which a neural network learns to store input-specific information for a certain time, through reward-sependent learning. In addition, structural plasticity was implemented in two steps. First, very weak synapses are pruned, as dendritic spines are known to retract in absence of synaptic activity (Lamprecht and LeDoux, 2004). Second, new synapses are grown between neurons which exhibit correlated activity, but are not yet synaptically connected. Moreover, the two processes are balanced, such that the overall connectivity of the network is preserved.

When comparing networks implementing structural plasticity to networks with fixed random connectivity, we see that the performance can be significantly improved by network reorganization. The sparseness of the connectivity matrix, with values similar to those observed in the cortex, ensures appropriate dynamics for the network, but makes the performance critically dependent on the particular instance of the fixed weight matrix. In contrast, the activity-dependent synaptic reorganization will correct a "bad" initial choice of weights, such that the network can encode the input stimuli more reliably. Our results suggest that activity-dependent structural plasticity could play an important role in optimizing the sparse cortical connectivity to best encode information.

Related publication in 2010:
Savin, C. and Triesch, J., *Structural plasticity improves stimulus encoding in a working memory model*, Frontiers in Computational Neuroscience. Conference Abstract: Computational and systems neuroscience, February 2010.

Analyzing possible pitfalls of cross-frequency analysis

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

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

One of the central questions in neuroscience is how neural activity is organized across different spatial and temporal scales. As larger populations oscillate and synchronize at lower frequencies and smaller ensembles are active at higher frequencies, a cross-frequency coupling would 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 coupling in LFP, ECoG, EEG and MEG has been tremendous.

In this research project, we evaluate the mathematical foundations of cross frequency analysis and conclude 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.

1) The first conceptual problem is related to isolating physiological frequency components of the recorded signal. The key point is to notice that there are many different mathematical representations for a time series but the physical interpretation we make out of them is dependent on the choice of the components to be analyzed. In particular, when one isolates the components by Fourier-representation based filtering, it is the width of the filtering bands what defines what we consider as our components and how their power or group phase change in time. We will discuss clear cut examples where the interpretation of the existence of CFC depends on the width of the filtering process. *2)* A second problem we investigate deals with the origin of spectral correlations as detected by current cross-frequency analysis. It is known that non-stationarities are associated with spectral correlations in the Fourier space. Therefore, before assigning a functional role to CFC it is necessary to identify and monitor all sources of non-stationarity. *3)* We finally propose that non-linearities are generators of cross frequency interactions. As an example we performed a phase-amplitude coupling analysis of two nonlinearly related signals: atmospheric noise and the square of it (Figure 1) observing an enhancement of phase-amplitude coupling in the second signal while no pattern is observed in the first.
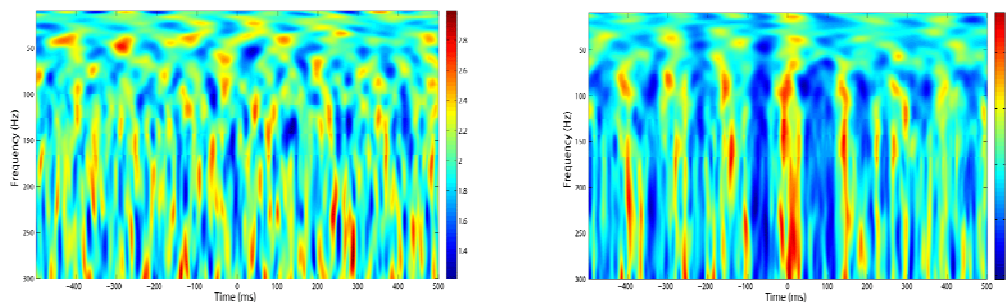
Figure 1. Time-evolution of the amplitudes of high frequency components locked to the trough of a low frequency component (from 4 to 8 Hz) for random noise from an atmospheric source (left) and its square (right).

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

Assessing coupling dynamics from an ensemble of time series

Collaborators: Raul Vicente[1,2], German Gomez-Herrero[3], Wei Wu[4], Kalle Rutanen[5], Miguel C. Soriano[6], G. Pipa[2,7], Michael Wibral[8]

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A fundamental problem that arises in various fields of science is how to detect and characterize interdependencies between simultaneously measured time series. Such coupling analysis is typically the first step for elucidating how the systems underlying the time series interact. For example, in neuroscience, ecology, or econometrics this approach has led to the discovery of new neural codes, better models of population dynamics, and methods to assess the influence of an economic variable, respectively. Tools to unveil interdependencies include linear techniques, such as cross-correlation and coherency analysis, non-linear synchrony measures, and the evaluation of statistical dependencies via mutual information (MI). However, the ultimate aim is often to identify the information flow across time series. Such "causal" dependencies are expected to reflect the effective interactions or coupling between subsystems, and therefore they are arguably the most informative to understand the functioning of a system in mechanistic terms. In this research project we develop a method to reliably estimate the temporal course of coupling interactions, by using several information-theoretic functionals.

The main idea relies in that, fortunately, in several disciplines the experiments lead to multivariate time series which can be systematically repeated. Thus, a typical experimental paradigm renders an ensemble of presumably independent repetitions or trials for each experimental condition. In this project we seek to exploit this multi-trial nature to produce time-resolved estimates for a family of information-theoretic measures that we call entropy combinations. This family includes well-known functional such as MI, TE, and their conditional counterparts: partial mutual information (PMI) and partial transfer entropy (PTE). We use simulations and experimental data to demonstrate that the proposed ensemble estimators of entropy combinations are much more accurate than the simple averaging of individual trial estimates.
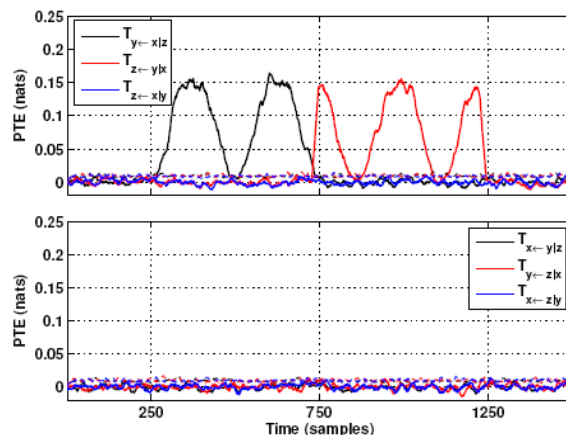
In the Figure we plot the time-variant information flow between three electronic circuits (X->Y->Z) which interact with a coupling strength that follows a sinusoidal variation. The proposed methodology is able to recover both the time course of the interactions and the right directionalities.

Related Publications in 2010:
[1] Vicente R, Wibral M, Lindner M, Pipa G., J Comput Neurosci. 30 (2011) 45-67. Epub 2010 Aug 13.

[2] Wibral M, Rahm B, Rieder M, Lindner M, Vicente R, Kaiser J., Prog Biophys Mol Biol. 105 (2011) 80-97. Epub 2010 Nov 27.

Cortical Gamma Oscillations: Dynamics and Function

Thomas Burwick

In this project, we studied the possible benefit for pattern recognition that may result from using the growing understanding of the functional role of cortical gamma oscillations (30-80 Hz). Studying the applicability of oscillatory neural networks (ONN) for pattern recognition tasks is strongly motivated by the neurophysiological observation that cortical gamma oscillations are involved in several cognitive tasks.

As a result, a new class of ONN models was proposed. These models are obtained by extending earlier models through accompanying each excitatory oscillator with an inhibitory oscillator. We refer to the pairs of excitatory and inhibitory oscillators as columns, emphasizing the intended analogy with cortical columns. Correspondingly, the additional couplings between excitatory and inhibitory oscillators and among inhibitory oscillators are inspired by the cortical analog.

Studying the new class of models, we found that the inhibitory extension allows for novel forms of pattern readout through using the temporal structure that arises with synchronization processes. Remarkably, the resulting readout process - here referred to as "windowing mechanism" - is conceptually close to the mechanism proposed with the communication-through-coherence (CTC) hypothesis, put forward to describe the functionality of cortical gamma oscillations (Fries, 2005).

The mechanisms was studied and illustrated with image recognition examples.
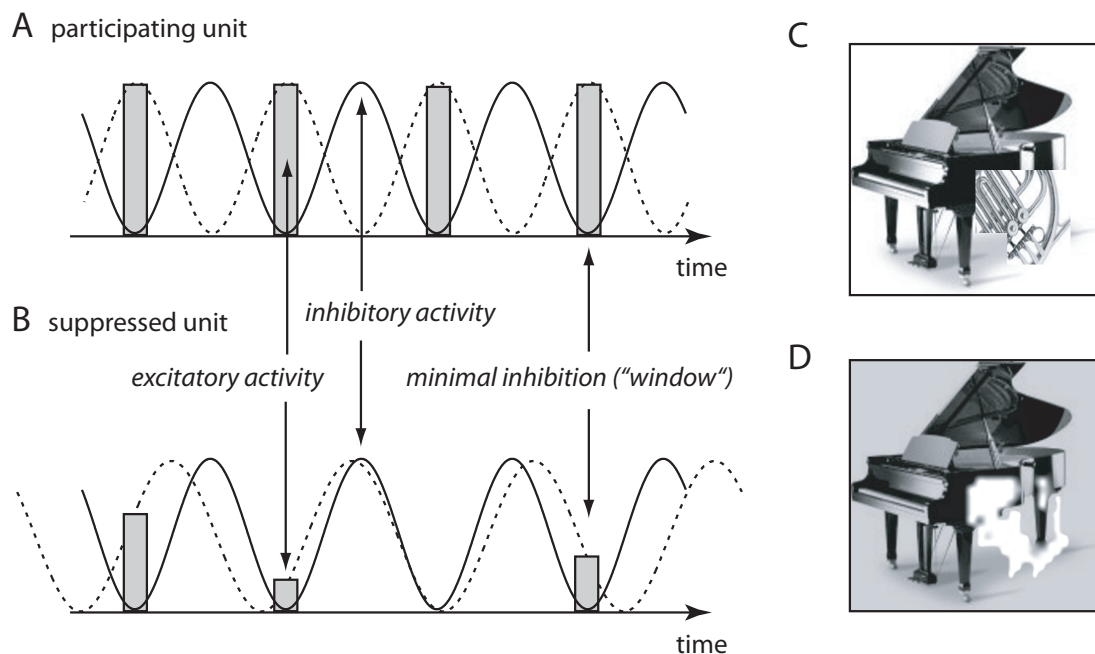
Windowing mechanism: The oscillatory state divides neural units into (A) participating units that escape the inhibitory effect through being active in time windows of low inhibition and (B) suppressed units. (C and D) Example implementation of the windowing mechanism. Several patterns are stored through Hebbian memory. (C) An input image is presented that mixes two of the stored patterns, showing a grand piano and a French horn. (D) The windowing mechanism is able to readout the dominating pattern (grand piano) and selectively inhibit (white region) other activity.

Related publications in 2010:
1) T. Burwick, *Neural oscillations allow for selective inhibition – New perspective on the role of cortical gamma oscillations*, ESANN'2010 proceedings, pages 283 - 288
3) T. Burwick, *Pattern recognition through compatibility of excitatory and inhibitory rhythms*, accepted for publication in Neurocomputing

Unifying procedural memory consolidation and structure learning in motor control

Collaborators: Q. Wang*, C. Rothkopf*, J. Triesch

Humans can improve their performance in procedural movement tasks through practice, but such motor learning has shown puzzling and partly contradictory results with varied training schedules and tasks similarities. 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 interference and facilitation effects have been observed. Furthermore, recent studies have shown that transfer of learning between different tasks is based on abstract structure similarities.

Here we address the question of how these different phenomena can be understood in terms of the shaping of neuronal representations through Spike Time Dependent Plasticity (STDP). We use a sparsely connected recurrent network with stimulus specific input whose connectivity is shaped by STDP. Additionally, this network is connected to a layer of motor neurons mediating the movement sequence through a winner take all mechanism.

We apply this network to a series of experiments on 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 reproduces the difference between blocked training versus interleaved training. The network also shows striking similarity to human performance in tasks with similar training sequences with different training times.

It is shown how psychophysical performance measures are reflective of the underlying neuronal representations in the recurrent network and testable predictions for further experiments are derived. These results are interpreted in terms of the changes in the neuronal representations of the movement sequences. Thus, we show how training schedule and sequence similarity interact to produce a rich set of interference and facilitation effects thereby unifying procedural memory consolidation and structure learning.
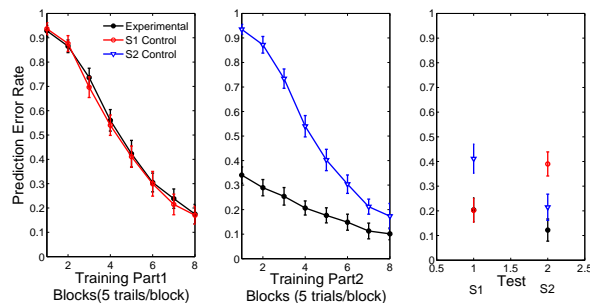
(a) Simulation results for Panzer et al, 2006. showing facilitation for S2 and retroactive interference for S1.
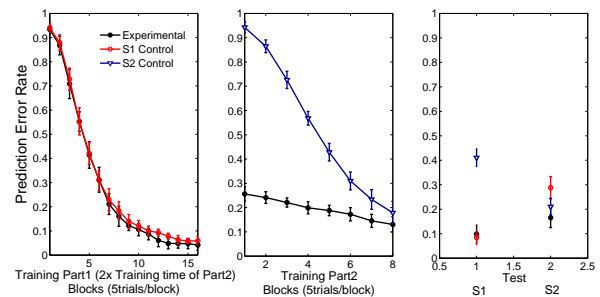
(b) Simulation results for Panzer et al, 2008.Simulation results showing prolonged training on sequence 1 leads to reduced interference. Performance on sequence 1 was better compared with sequence 2 when tested.

Related publications in 2010:

1) Q. Wang, C. Rothkopf, J. Triesch, *Unifying procedural memory consolidation and structure learning in motor control*, Computational and Systems Neuroscience 2011.

* Shared first authorship

Infants in Control: Rapid Learning of Action Outcomes by 6-Month-Olds in a Gaze-Contingent Paradigm

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 Developmental Psychology, Goethe University, Frankfurt, Germany

It has been difficult to study infant learning in the full perception and action cycle, because of the limited motor control abilities of young infants. Here we employ a novel gaze-contingent paradigm to overcome this limitation. We demonstrate that six to eight-month-old infants very quickly learn to selectively take actions to manipulate their environment and learn to anticipate the outcomes of their actions.

All three experiments use a gaze-contingent paradigm. Infants are seated in front of a monitor, which displays images in the central region. Importantly, the display also contains an additional red disc, which allows the infant to change the central image, by directing gaze to it (see Figure below). This red disc therefore has the functionality of a switch. Additionally, when gaze enters the red disc, a sound is played. In the first experiment,the central image is displayed at full contrast for 1.5 seconds and then disappears. The results show that infants direct their gaze to the image area after triggering the switch before the appearance of the new image. This anticipation behavior is observed after only very few trials.

In experiment 2, the red disc again triggers a new image contingent on the infant's gaze. But instead of displaying the central image for 1.5 seconds, each image now fades slowly from full contrast to blank in 17 seconds. In this condition, infants gaze to the red disc well before the central image is faded away and again anticipate appearance of the central image.

In experiment 3, two red discs were shown in the display, one on either side of the central image, which fades as in the second experiment. Only one disc has the function of changing the central image and fixation on the other disc gives neither visual changes on the screen nor any sound. Most infants gaze at the functioning disc significantly more than to the non-functioning disc. Their gaze shows the pattern of first looking at the red disc and then at the central image region.

In conclusion, we demonstrate that the gaze-contingent paradigm can be used in developmental studies with infants as young as 6 month of age. Specifically, these experiments show that 6 to 8-month-old infants are able to learn anticipating their action outcomes and prefer actions that have visual consequences. Overall, infants were much more engaged in the tasks as reflected by the number of trials they carried out compared to passive viewing conditions in comparable habituation paradigms. These results suggest that gaze-contingent paradigms may be used to address a wide variety of classic questions including habituation, joint attention, and object conception in a new way.

Gaze-contingent paradigm where infants can trigger the appearance of a new image by looking at the red disc.

Related publications in 2010:

1) Q. Wang , J. Bolhuis, C. Rothkopf, T. Kolling, M. Knopf, J. Triesch, *Infants in Control: Rapid Learning of Action Outcomes by 6-Month-Olds in a Gaze-Contingent Paradigm*, Society for Research in Child Development, 2011 Biennial Meeting, Paper Symposium

Discounting as task termination, and its implications

Collaborators: Paul Schrater[1], Constantin A. Rothkopf[2]

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

Discounting is a natural part of the formulation of most sequential decisions problems and has been reported to underlie human and animal behavior in numerous empirical studies. Yet, typically discounting is treated as an arbitrary parameter needed to bound the expected future reward, and is treated as a fixed constant for all states. However, rather than an arbitrary parameter, discounting can also be interpreted as the probability of task termination. By assigning individual discount rates to separate states, we show it provides a framework for exploration bonuses, a rational basis for bounded computation and provides a basis for the automatic construction of stochastic options, or macro actions.

Our results capitalize on work by Sonin (2008), who shows a generalization of the Gittins index to a Markov chain that allows for state dependent discount rates. This generalized index shows that the exploratory bonus for an option is the reciprocal of the probability of task termination. Moreover, there is a recursive algorithm to compute the generalized index, which produces an ordering of states in terms of the obtainable reward. Moreover states that are traversed on the way to high-reward states can be eliminated, producing abstract states with new corresponding transition dynamics, and the probability of task-termination on these abstract states. We show how to use this elimination method to construct stochastic options (sub-policies) that find these abstract states, and that the choice between options can be computed via an index function. Using the termination probability formulation, we can derive exploratory incentives for each option and show that the effect of transition uncertainty is to reduce exploration incentive - in particular, incentive is reduced by the uncertainty over the set of next states - effectively a branching factor on the look ahead. This result provides a rational basis for bounding computation in model-based reinforcement learning.

We apply the framework to a well-known reinforcement learning problem that is challenging for exploration - the chain game. Our analysis decomposes the problem into a simple binary choice between two options, given enough experience with the transition probabilities, and we can quantify the difficulty in learning the better option. Humans placed in this environment fell into one of two distinct groups; one group performed enough unrewarded exploratory actions to find the better option while the second group under-explored and found the worst option. In debriefing, subjects in the former group reported finding worse option quickly, but believed that higher rewards were possible and thus continued exploration. Conversely, subjects in the latter group typically reported an initial exploratory phase, but upon finding the worse option believed the rest of the chain wasn't worth exploring. We believe these results provide new insight into the relationship between abstraction, exploration and the overall chance of task termination, and give a computational basis for understanding why exploration should be tied to competence or effectiveness, i.e. the ability to complete the task.

Related publications in 2010:
1) P. Schrater, C. A. Rothkopf: *Discounting as task termination, and its implications*, COSYNE - Computational and Systems Neuroscience, February 25-28, 2010, Salt Lake City, Utah, USA

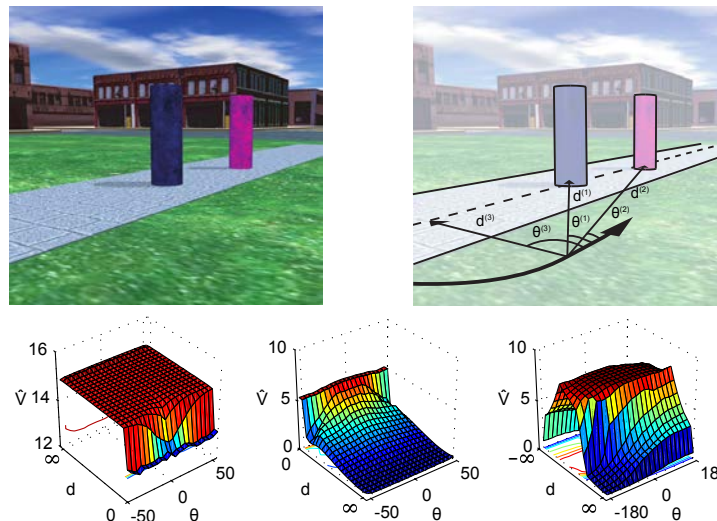# Credit assignment in multiple goal embodied visuomotor behavior

Collaborators: Constantin A. Rothkopf[1], Dana H. Ballard[2]

[1] Frankfurt Institute for Advanced Studies, [2] Department of Computer Science, University of Texas at Austin, USA

The enormous progress in instrumentation for measuring brain states has made it possible to tackle the large issue of an overall model of brain computation. The intrinsic complexity of the brain can lead one to set aside issues related to its relationships with the body, but the field of embodied cognition stresses that understanding of brain function at the system level requires one to address the role of the brain-body interface. While it is obvious that the brain receives all its input through the senses and directs its outputs through the motor system, it has only recently been appreciated that the body interface performs huge amounts of computation that does not have to be repeated by the brain, and thus affords the brain great simplifications in its representations. In effect the brain's abstract states can refer to coded representations of the world created by the body.

But even if the brain can communicate with the world through abstractions, the severe speed limitations in its neural circuitry mean that vast amounts of indexing must be performed during development so that appropriate behavioral responses can be rapidly accessed. One way this could happen would be if the brain used some kind of decomposition whereby behavioral primitives could be quickly accessed and combined. This realization is a tenet of our research program, which studies the capabilities of independent sensorimotor task solvers, which we call modules, in directing behavior. We use virtual environments replete with humanoid avatars to explore the sensitivity of the modular models to the environment. Such settings allow the manipulation of experimental parameters in a systematic way. Our test setting is that of an urban walking environment with an array of rewarded sites.

The issue we focus on in the present paper is how an embodied agent can learn such individual visuomotor modules while pursuing multiple goals. The biologically plausible standard for module programming is that of reinforcement given during exploration of the environment. However this formulation contains a substantial issue when sensorimotor modules are used in combination: The credit for their overall performance must be divided amongst them. We show that this problem can be solved and that carrying out diverse task combinations is beneficial in learning and not a complication, as usually assumed. Our simulations show that fast algorithms are available that allot credit correctly and are insensitive to measurement noise.

Top: Parameterization of navigation task. Bottom: Learned modular value-functions for navigation.

Related publications in 2010:

1) C. A. Rothkopf, D. H. Ballard: *Credit assignment in multiple goal embodied visuomotor behavior*, Frontiers in Psychology, Special Topic: 'Embodied and grounded cognition', 2010

Grasping image statistics

Collaborators: Omid Aladini, Constantin A. Rothkopf, Jochen Triesch

Frankfurt Institute for Advanced Studies

The human ability to parse images and recognize objects therein is still unmatched by artificial system. A wealth of research has demonstrated that many visual tasks can be analyzed by comparing human and animal performance to normative models understanding perception as Bayesian inference of latent causes generating these images. Previously, many visual tasks have been formulated in terms of the statistics of image features conditional on some scene property, including whether an object contour is present or not. This work has shown that indeed such image statistics obtained from natural images can be used to invert the generative model and infer whether a contour is present at an image location.

Almost all of these models have used large collections of labeled images as a means to extract joint statistics of features and image labels such as object category or object contour. Recently, generative models have been proposed, which learn object categories and segmentations in an unsupervised way from collections of images without labels. Contrary to artificial system, humans do have the distinct advantage of being able to obtain tactile information from manual interaction with the environment in addition to visual input. Here we explore only, how such tactile interaction can be used together with visual input in order to learn image statistics without requiring labeled image databases.

A humanoid agent was simulated in a virtual 3d graphics environment. It moves its hand repeatedly on stereotyped trajectories that can be obtained by servoing. The arm moves until it is fully extended or the hand hits a surface. During this process images are captured from the point of view of the agent fixating at a point slightly ahead of its hand. Using this data image features are calculated at the point of fixation including oriented bandpass filter responses at eight orientations and four spatial scales, oriented energy responses with the same set of filters, local luminance gradient direction, and contrast polarity. Furthermore, given that the 3d layout of the scene is fully known, we additionally store whether an object edge was present with each such data item.

The joint statistics of image features and the binary variable coding whether the agent was touching a surface or not can be estimated from the described data set. It is now possible to compute the posterior probability that the hand will intersect a surface at the next time step, given the current observation. We show that this posterior indeed reflects the presence of object edges in the scene, without doing, object segmentation or contour grouping. Thus, the presented work demonstrates that image statistics that can be useful for a large variety of visual tasks may not only be learned from images but benefit from learning in conjunction with tactile interaction within the scene.
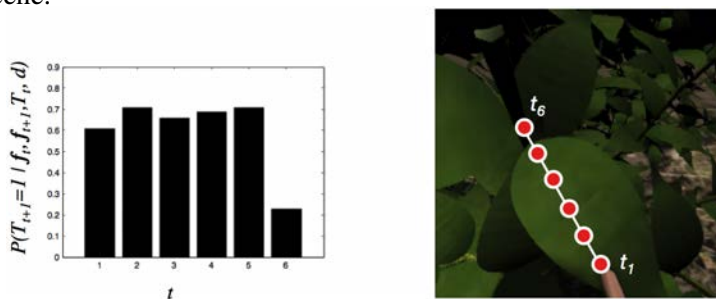

Figure 1: Left: Probability of intersecting an object at the next time step given image features and previous intersections. Right: Corresponding visuo-haptic scene.

Related publications in 2010:

1) O. Aladini, C. A. Rothkopf, J. Triesch: *Grasping image statistics*, COSYNE - Computational and Systems Neuroscience, February 25-28, 2010, Salt Lake City, Utah, USA

Learning hierarchical controllers through reinforcement learning

Collaborators: Hazem Toutounji, Constantin A. Rothkopf, Jochen Triesch

Frankfurt Institute for Advanced Studies

Reinforcement Learning (RL) comprises a set of algorithms for learning to solve the optimal control problem, i.e. carrying out actions in order to maximize collected reward. But it is expensive in storage, computation, and learning time to code every possible dimension relevant for potential tasks. There is nonetheless consistent evidence, including electrophysiological recordings in mammals and fMRI research in humans, that the brain computes with variables present in temporal difference (TD) algorithms of RL, which might suggest the existence of learning algorithms that are capable of reducing the dimensionality of the problem and hence the learning time. For independent action spaces one can learn independent controllers for separate variables describing the full state space. But the question arises how to handle the case in which transition dynamics of multiple controllers are not independent from one another.

Here we consider the case in which actions of one controller affect the transition dynamics of a second controller, as commonly occurs in motor control. As a simple example we consider a 2-dimensional state space, and starting from a random initial condition, a learner is attempting to reach a goal state where the reward is maximal. The reward decays quadratically from the goal state until it reaches a minimum value. At each state the learner can perform any possible 2-dimensional action. The transition dynamics in the horizontal direction depends on the magnitude of the action in the vertical direction since a bigger movement in the vertical direction results in cross-talk, i.e. a bigger overshoot in the horizontal direction.

To solve this task we propose and implement a solution that assumes that each dimension is initially learned with an independent controller. A third controller learns to coordinate these two controllers by performing corrective actions. Importantly, this third controller learns a policy in the horizontal direction for the whole 2-dimensional state space but with a lower resolution. Learning is triggered in all the controllers by a temporal difference error in predicting the reward and uses the SARSA algorithm. The upper controller can start learning either after the lower controllers had already learned a value function or right from the beginning.

In both cases, the multiple controller solution learns significantly faster than the controller using the full joint state space. Furthermore, for very large spaces only the composite controllers are able to find a solution in the allotted time. Also, for the 2-dimensional state spaces of size n^2, storage needed for value functions was reduced from $O(n^4)$ in the full controller case to $O(n^2)$ in the hierarchical case. Thus, we show that a hierarchical system, in which lower level controllers have dependent transition dynamics that are accounted for with an upper low-resolution coordinating controller, is capable of learning a near-optimal solution while saving computation time, storage space, and learning time.
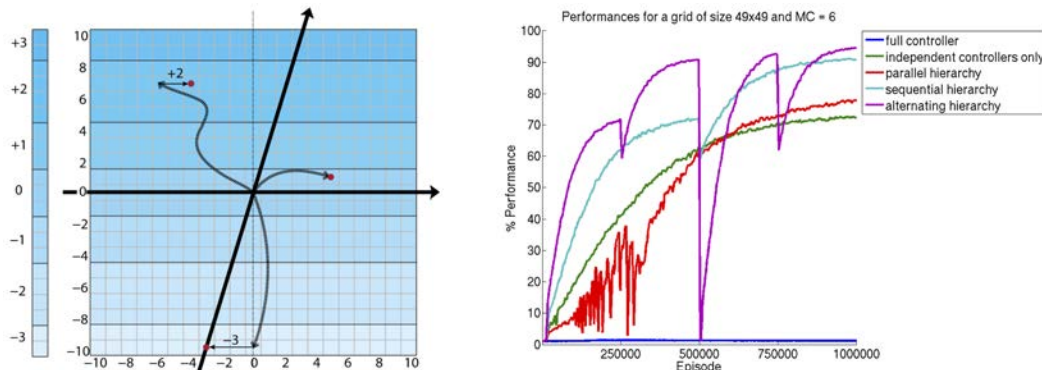
Left: Schematic representation of the weakly interacting task. Right: Performance comparison.

Related publications in 2010:

1) H. Toutounji, C. A. Rothkopf, J. Triesch: *Learning hierarchical controllers through reinforcement learning*, Bernstein Conference on Computational Neuroscience, 27 Sep — 1 Oct, 2010, Berlin, Germany

4.3 Biology, Immunology, Medicine

Breaking down pigeonhole thinking with regard to adaptive and innate immunity by combining in vivo and in silico experiments

Collaborators: M. Meyer-Hermann[1], M. T. Figge[1], A. Garin[2], M. Contie[2], V. Buatois[2], G. Elson[2], M. H. Kosco-Vilbois[2], M. Gunzer[3], K.-M. Toellner[4]

[1] Frankfurt Institute for Advanced Studies, [2] NovImmune SA, Plan les Ouates, Switzerland, [3] Institute for Molecular and Clinical Immunology, Otto-von-Guericke-University, Magdeburg, Germany, [4] MRC Centre for Immune Regulation, University of Birmingham, Birmingham, UK

Adaptive immunity refers to the specific response of the immune system against antigens. In contrast to the fast and unspecific response of innate immunity, the specific response of adaptive immunity is only slowly developed during weeks involving the generation of suitable antibodies towards the encountered antigen.

Germinal centers are specialized microenvironments where the affinity maturation of antibodies takes place. In germinal centers, antigen-activated B cells undergo proliferation, somatic hypermutation, and selection with regard to the antibody affinity. Follicular dendritic cells (FDCs) are key players in driving these events of adaptive immunity via direct interaction with germinal center B cells.

A series of in vivo experiments provide evidence that FDCs express and upregulate Toll-like-receptor (TLR) 4 in situ during germinal center reactions, confirm that FDC maturation is driven by TLR4, and associate the role of FDC-expressed TLR4 with quantitative and qualitative affects of germinal center biology. We demonstrated that TLR4 signaling significantly modulates FDC activation and is required for a proper functioning of the germinal center reaction.

Most interestingly, our data places the common host pattern recognition receptor TLR4 of innate immunity in the heart of adaptive humoral immunity. Thus, innate and adaptive immunity are shown to be closely interwoven and our findings break down the common pigeonhole thinking of two loose concepts as if they would be independent of each other.

The interpretation of these experiments was driven by iterative cycles of predictions from in silico modeling that were subsequently verified by in vivo experiments. The in silico modeling was performed within an agent-based modeling approach that was applied at the level of migrating and interacting cells in the germinal center. Simulating the whole germinal center reaction on the computer allowed predicting new experiments that should be undertaken in order to explain and reconcile observations. From this point of view, our work represents a prime example of modern systems biology where theory and experiment are performed hand-in-hand.
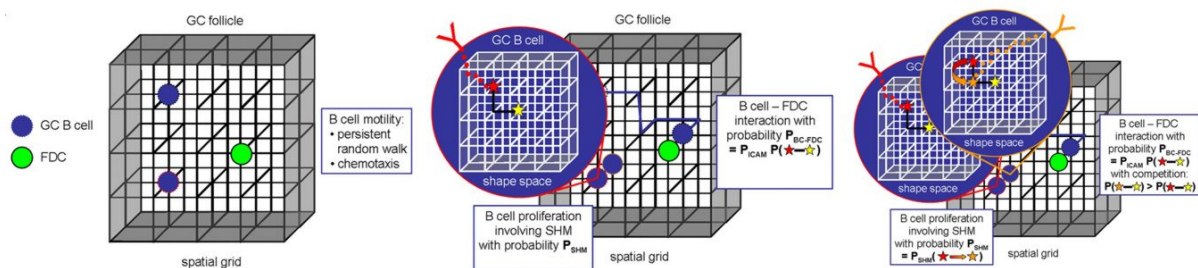
Some aspects of the hybrid agent-based model as applied in the computer simulations of GC reaction

Related publications in 2010:

A. Garin, M. Meyer-Hermann, M. Contie, M.T. Figge, V. Buatois, M. Gunzer, K.-M. Toellner, G. Elson, M.H. Kosco-Vilbois, *Toll-Like Receptor 4 signaling by FDC is pivotal for delivering the consequences of germinal center responses*, Immunity 33, 84-95 (2010)

Magnetoreception mechanisms in birds - towards the discovery of the sixth sense

Collaborators: Ilia A Solov'yov[1,2], Walter Greiner[1] and Klaus Schulten[2,3]

[1]FIAS, Frankfurt; [2]Beckman Institute, University of Illinois at Urbana-Champaign, Urbana, USA; [3]Department of Physics, University of Illinois at Urbana-Champaign, Urbana, USA

The Earth's magnetic field provides an important source of directional information for many living organisms, especially birds, but the sensory receptor responsible for magnetic field detection still has to be identified. Recently, magnetic iron oxide particles were detected in dendritic endings of the ophthalmic nerves in the skin of the upper beak of homing pigeons and were shown to fulfil the special prerequisites of a biological receptor. We studied the proposed receptor theoretically and formulated the criteria for which it becomes operational and can be used for registering the weak magnetic fields as, e.g., the geomagnetic field, by a bird. In another highlight we demonstrated that the magenetic sense of migratory birds may be linked to the protein cryptochrome, found in the retina, the light-sensitive part of the eyes. Cryptochrome's functional capabilities depend on its orientation in an external magnetic field. The product of the reaction in cryptochrome is said to affect the sensitivity of light receptors in the retina of a bird's eye such that a bird literally "sees" the geomagnetic field. However, cryptochrome in the eye most likely is not perfectly aligned with the retina, even if bound to ordered membrane structures found in the outer segments of the eye's light receptors. In our recent report we have shown that birds' vision-based compass is surprisingly insensitive to cryptochrome disorder. We suggested a cloud-like pattern in the visual field that points a bird to the correct orientation.
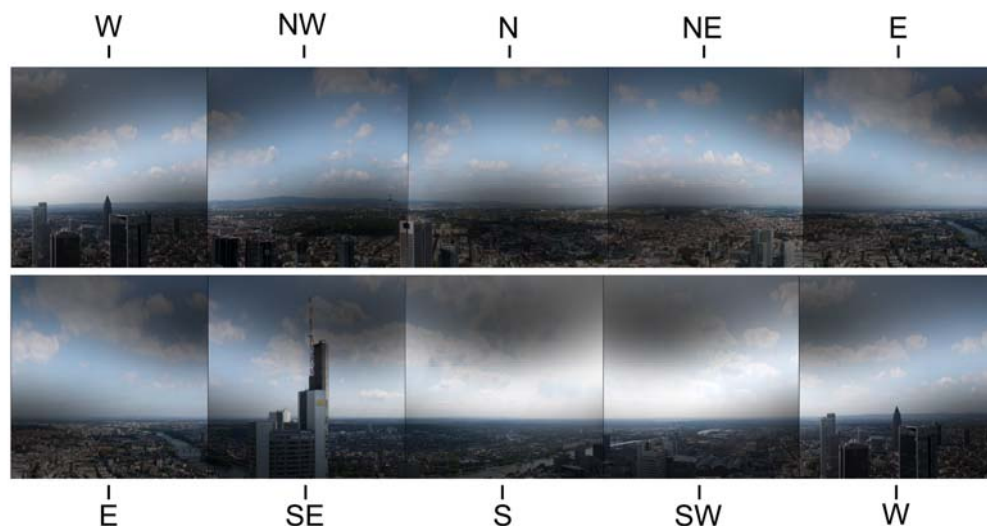
Figure 1: Panoramic view at Frankfurt am Main, Germany. The image shows the landscape perspective recorded from a bird flight altitude of 200 m above the ground with the cardinal directions indicated. The visual field of a bird is modified through the magnetic filter function. The patterns are shown for a bird looking at eight cardinal directions (N, NE, E, SE, S, SW, W, and NW). The geomagnetic field inclination angle is 66°, being a characteristic value for the region.

Related publications in 2010:

1. I.A. Solov'yov, H. Mouritsen and K. Schulten, *Acuity of a Cryptochrome and Vision-Based Magnetoreception System in Birds*, Biophysical Journal, 99, 40-49 (2010).

2. I.A. Solov'yov, K. Schulten and W. Greiner, *Nur dem Schnabel nach?,* Physik Journal, 9, 23-28 (2010);

Effects of X-ray and heavy ion radiation on organotypic slice cultures of liver and pancreas

Mareike Müller[1,2,3,*], Marco Durante[2,3,4], Gisela Taucher-Scholz[2], Franz Rödel[5], Francesco Natale[2], Horst Stöcker[2,3], Horst-Werner Korf[1]

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In this interdisciplinary project, the radiation effects of heavy ions and X-rays on organotypic slice cultures (OSC) of murine liver and pancreas are investigated. In OSC, the native architecture of the tissue, made up of various parenchymal and stromal cells, is preserved. OSC thus represent a more physiological model than cell lines. Moreover, they offer an advantage to whole-animal experiments, as they allow a systematic analysis in a greater number of experimental samples while eliminating the problem of interindividual differences. Liver and pancreas were chosen due to their clinical relevance, as tumors of these organs often have a poor therapeutic prognosis.

OSC were irradiated with X-rays at doses of 2Gy to 50Gy and analyzed for dose-dependent effects of irradiation on cell death and proliferation as well as on circadian rhythmicity of the organs.

All organisms are subjected to circadian rhythms controlled by a certain region in the brain, the suprachiasmatic nuclei. Circadian rhythms persist in peripheral organs such as the liver, even after the organs were removed from the organism. Experiments with transgenic mice, in which luciferase, an enzyme which reacts with luciferin in the medium producing photons, is expressed under the control of the promoter of *Per2*, a rhythmically expressed clock gene, have shown that the liver maintains its circadian rhythm in culture and that irradiation with X-rays at a dose of 50Gy (bottom figure) has pronounced phase-shifting effects at a certain timepoint of the day. This raises the hypothesis that the tissue response to radiation may be dependent on the time of day at which the irradiation is performed. This time-dependent effect should be considered in the future when irradiation therapy is planned for individual patients. Currently, the X-ray experiments are repeated for a significant statistical evaluation. Following this will be heavy ion irradiations at GSI.
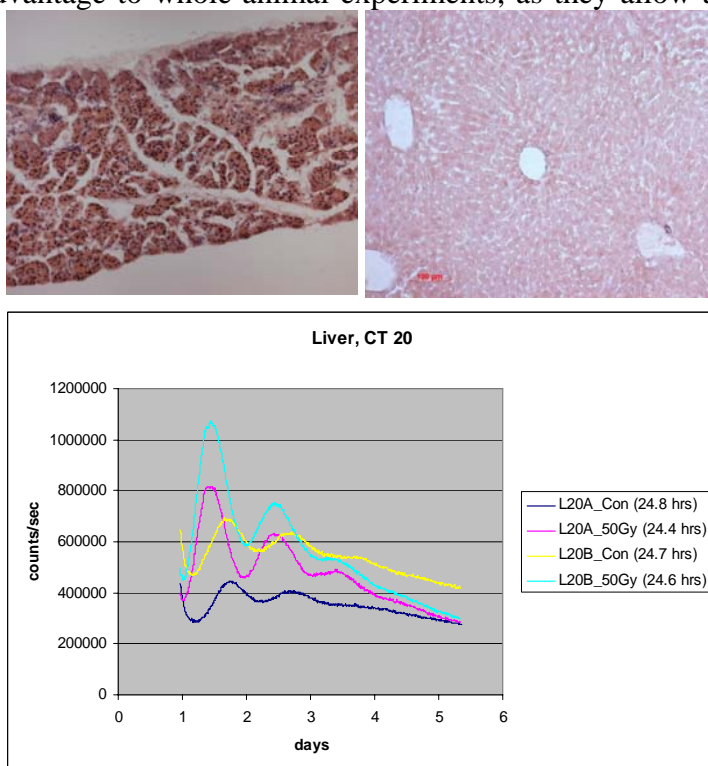
Figure 1 Top left HE-staining of a pancreas section. The exocrine and endocrine part of the tissue are clearly visible as well as the connective tissue. **Top right** HE-staining of a liver section. The central veins and hepatocytes can be identified, indicating that the tissue structure is very well preserved. **Bottom** The number of emitted photons dependent on the rhythmic expression of luciferase is plotted as a function of days in vitro. The tissue maintains its rhythm even after an X-ray dose of 50Gy. Differences in amplitude are due to the different sizes of the OSC, the damping amplitude is caused by the depletion of luciferin in the medium.

Related publications in 2010:

1) F. Merz, M. Müller, G. Taucher-Scholz, F. Rödel, H. Stöcker, K. Schopow, L. Laprell, F- Dehghani, I. Bechmann, *Tissue slice cultures from humans or rodents: a new tool to evaluate biological effects of heavy ions,* Radiat. Environ. Biophys. 49, 457-462 (2010) DOI 101107/s00411-010-0293-1
2) M. Müller, M. Durante, H. Stöcker, F. Merz, I. Bechmann, *Modeling radiation effects at the tissue level*, Eur. Phys. J. D 60, 171-176 (2010)

Optimization of amino acid type-specific ^{13}C and ^{15}N labeling for the backbone assignment of membrane proteins by solution- and solid-state NMR with the UPLABEL algorithm

Collaborators: Frederik Hefke[1,2], Anurag Bagaria[1,2], Sina Reckel[1], Sandra Johanna Ullrich[1], Volker Dötsch[1], Clemens Glaubitz[1] and 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, Goethe University Frankfurt am Main, [3] Graduate School of Science, Tokyo Metropolitan University, Tokyo, Japan

We present a computational method for finding optimal labeling patterns for the backbone assignment of membrane proteins and other large proteins that cannot be assigned by conventional strategies. Following the approach of Kainosho and Tsuji (Biochemistry 21:6273-6279 (1982)), types of amino acids are labeled with ^{13}C or/and ^{15}N such that cross peaks between ^{13}CO(i - 1) and ^{15}NH(i) result only for pairs of sequentially adjacent amino acids of which the first is labeled with ^{13}C and the second with ^{15}N. In this way, unambiguous sequence-specific assignments can be obtained for unique pairs of amino acids that occur exactly once in the sequence of the protein. To be practical, it is crucial to limit the number of differently labeled protein samples that have to be prepared while obtaining an optimal extent of labeled unique amino acid pairs. Our computer algorithm UPLABEL for optimal unique pair labeling, implemented in the program CYANA and in a standalone program, and also available through a web portal, uses combinatorial optimization to find for a given amino acid sequence labeling patterns that maximize the number of unique pair assignments with a minimal number of differently labeled protein samples. Various auxiliary conditions, including labeled amino acid availability and price, previously known partial assignments, and sequence regions of particular interest can be taken into account when determining optimal amino acid type-specific labeling patterns. The method is illustrated for the assignment of the human G-protein coupled receptor bradykinin B2 (B$_2$R) and applied as a starting point for the backbone assignment of the membrane protein proteorhodopsin.
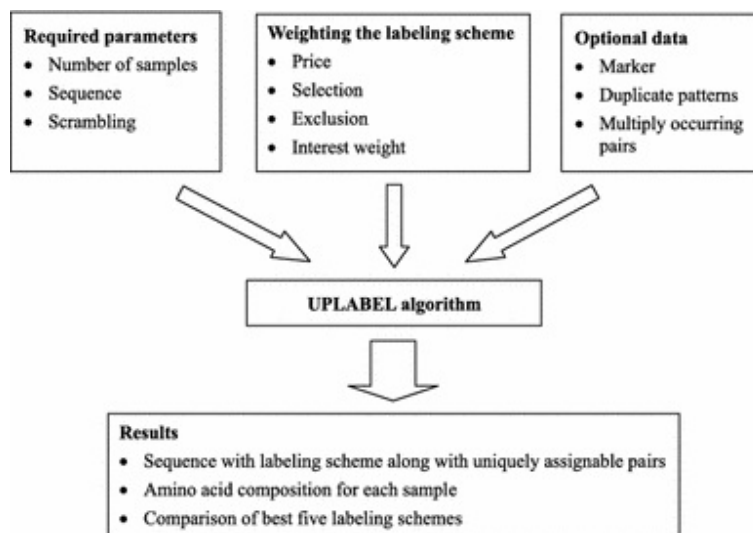
Input and output data of the UPLABEL algorithm

Related publications in 2010:

1) Hefke, F., Bagaria, A., Reckel, S., Ullrich, S. J., Dötsch, V., Glaubitz, C. and Güntert, P. *Optimization of amino acid type- specific 13C and 15N labeling for the backbone assignment of membrane proteins by solution- and solid-state NMR with the UPLABEL algorithm*, J. Biomol. NMR (2010) Published online ahead of print.

Structural insight into the zinc finger CW domain as a histone modification reader

Collaborators: Fahu He[1], Takashi Umehara[1], Kohei Saito[1], Takushi Harada[1], Satoru Watanabe[1], Takashi Yabuki[1], Takanori Kigawa[1,2], Mari Takahashi[1], Kanako Kuwasako[1], Kengo Tsuda[1], Takayoshi Matsuda[1], Masaaki Aoki[1], Eiko Seki[1],Naohiro Kobayashi[1], Peter Güntert[3,4], Shigeyuki Yokoyama[1,5] and Yutaka Muto[1]

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The zinc finger CW (zf-CW) domain is a motif of about 60 residues that is frequently found in proteins involved in epigenetic regulation. Here, we determined the NMR solution structure of the zf-CW domain of the human zf-CW and PWWP domain containing protein 1 (ZCWPW1). The zf-CW domain adopts a new fold in which a zinc ion is coordinated tetrahedrally by four conserved Cys ligand residues. The tertiary structure of the zf-CW domain partially resembles that adopted by the plant homeo domain (PHD) finger bound to the histone tail, suggesting that the zf-CW domain and the PHD finger have similar functions. The solution structure of the complex of the zf-CW domain with the histone H3 tail peptide (1-10) with trimethylated K4 clarified its binding mode. Our structural and biochemical studies have identified the zf-CW domain as a member of the histone modification reader modules for epigenetic regulation.
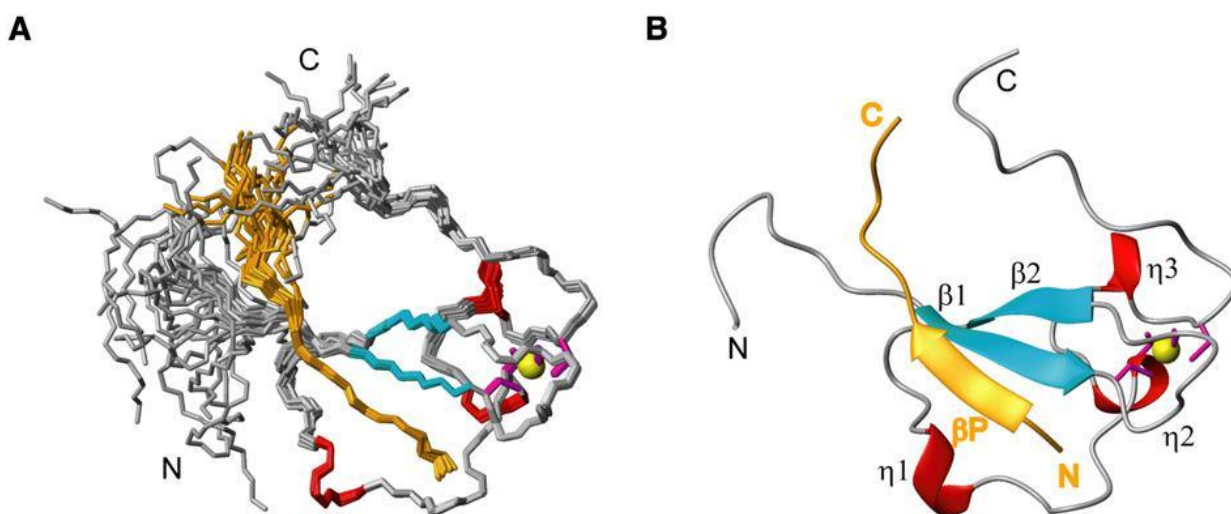
Solution Structure of the Human ZCWPW1 zf-CW-H3$_{(1-10)}$K4me3 Complex

(A) Backbone traces of the 20 conformers of the solution structure (B) Lowest energy structure, in a ribbon representation

Related publications in 2010:

1) He, F., Umehara, T., Saito, K., Harada, T., Watanabe, S., Yobuki, T., Kigawa, T., Takahashi, M., Kuwasako, K., Tsuda, K., Matsuda, T., Aoki, M., Seki, E., Kobayashi, N., Güntert, P., Yokoyama, S. and Muto, Y. *Structural insight into the zinc finger CW domain as a histone modification reader*, Structure 18 (2010) 1127-1139

Determinants of activity in glutaredoxins: an in vitro evolved Grx1-like variant of Escherichia coli Grx3

Collaborators: Tobias H. Elgán[1,2], Anne-Gaëlle Planson[3], Jon Beckwith[3], Peter Güntert[4,5,6,7] and Kurt D. Berndt[1,2]

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The *Escherichia coli* glutaredoxins 1 and 3 (Grx1 and Grx3) are structurally similar (37 % sequence identity), yet have different activities *in vivo*. Unlike Grx3, Grx1 efficiently reduces protein disulfides in proteins such as RR (ribonucleotide reductase), whereas it is poor at reducing S-glutathionylated proteins. An *E. coli* strain lacking genes encoding thioredoxins 1 and 2 and Grx1 is not viable on either rich or minimal medium; however, a M43V mutation in Grx3 restores growth under these conditions and results in a Grx1-like protein [Ortenberg, Gon, Porat and Beckwith (2004) Proc. Natl. Acad. Sci. U.S.A. **101**, 7439-7944]. To uncover the structural basis of this change in activity, we have compared wild-type and mutant Grx3 using CD and NMR spectroscopy. Ligand-induced stability measurements demonstrate that the Grx3(M43V/C65Y) mutant has acquired affinity for RR. Far-UV CD spectra reveal no significant differences, but differences are observed in the near-UV region indicative of tertiary structural changes. NMR ^{1}H-^{15}N HSQC (heteronuclear single quantum coherence) spectra show that approximately half of the 82 residues experience significant ($\Delta\delta > 0.03$ p.p.m.) chemical shift deviations in the mutant, including nine residues experiencing extensive ($\Delta\delta \geq 0.15$ p.p.m.) deviations. To test whether the M43V mutation alters dynamic properties of Grx3, H/D (hydrogen/deuterium) exchange experiments were performed demonstrating that the rate at which backbone amides exchange protons with the solvent is dramatically enhanced in the mutant, particularly in the core of the protein. These data suggest that the Grx1-like activity of the Grx3(M43V/C65Y) mutant may be explained by enhanced intrinsic motion allowing for increased specificity towards larger substrates such as RR.
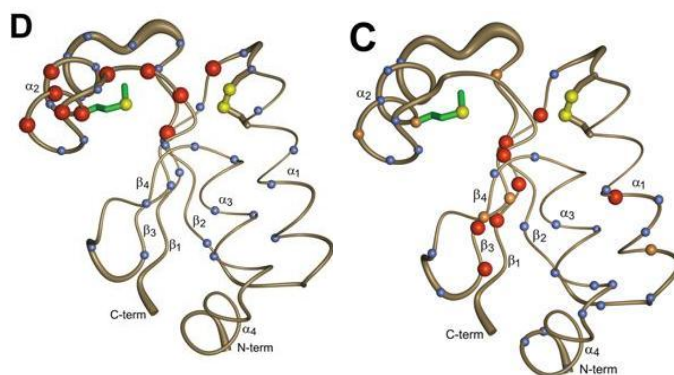
(D)Large (blue balls) and extensive (red balls) chemical shift perturbations mapped on to the oxidized wild-type Grx3 structure (C)the residues representing the slightly faster (blue balls), faster (brown balls), and much faster (red balls) H/D exchange rates have been mapped out on the oxidized wild-type Grx3 structure. The secondary structure of the oxidized wild-type Grx3 is shown above the graphs.

Related publications in 2010:

1) Elgán, T.H., Planson, A.G., Beckwith, J., Güntert, P. and Berndt, K.D., *Determinants of activity in glutaredoxins: an in vitro evolved Grx1-like variant of Escherichia coli Grx3*, Biochem. J. 430 (2010) 487-495

Solution structure of the catalytic domain of the mitochondrial protein ICT1 that is essential for cell vitality

Collaborators: Yoshihiro Handa[1], Yusuke Hikawa[1], Naoya Tochio[2], Hiroyuki Kogure[1], Makoto Inoue[2], Seizo Koshiba[2], Peter Güntert[3], Yusuke Inoue[1], Takanori Kigawa[2,4], Shigeyuki Yokoyama[2,5] and Nobukazu Nameki[1]

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The ICT1 protein was recently reported to be a component of the human mitoribosome and to have codon-independent peptidyl-tRNA hydrolysis activity via its conserved GGQ motif, although little is known about the detailed mechanism. Here, using NMR spectroscopy, we determined the solution structure of the catalytic domain of the mouse ICT1 protein that lacks an N-terminal mitochondrial targeting signal and an unstructured C-terminal basic-residue-rich extension, and we examined the effect of ICT1 knockdown (mediated by small interfering RNA) on mitochondria in HeLa cells using flow cytometry. The catalytic domain comprising residues 69-162 of the 206-residue full-length protein forms a structure with a β1-β2-α1-β3-α2 topology and a structural framework that resembles the structure of GGQ-containing domain 3 of class 1 release factors (RFs). Half of the structure, including the GGQ-containing loop, has essentially the same sequence and structure as those in RFs, consistent with the peptidyl-tRNA hydrolysis activity of ICT1 on the mitoribosome, which is analogous to RFs. However, the other half of the structure differs in shape from the corresponding part of RF domain 3 in that in ICT1, an α-helix (α1), instead of a β-turn, is inserted between strand β2 and strand β3. A characteristic groove formed between α1 and the three-stranded antiparallel β-sheet was identified as a putative ICT1-specific functional site by a structure-based alignment. In addition, the structured domain that recognizes stop codons in RFs is replaced in ICT1 by a C-terminal basic-residue-rich extension. It appears that these differences are linked to a specific function of ICT1 other than the translation termination mediated by RFs.
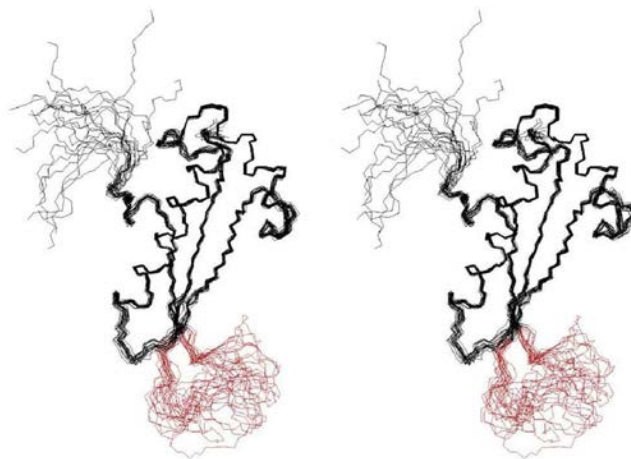
Stereo view of the 20 energy-refined conformers in the solution structure of the catalytic domain (residues 63-162) of the ICT1 protein. The GGQ loop is shown in brown.

Related publications in 2010:

1) Handa, Y., Hikawa, Y., Tochio, N., Kogure, H., Inoue, M., Koshiba, S., Güntert, P., Inoue, Y., Kigawa, T., Yokoyama, S. and Nameki, N. *Solution structure of the mitochondrial protein ICT1 that is essential for cell vitality*, J. Mol. Biol. 404, (2010) 260-273

Structural investigation of the C-terminal catalytic fragment of presenilin 1

Collaborators: Solmaz Sobhanifar[1], Birgit Schneider[1], Frank Löhr[1], Daniel Gottstein[1], Teppei Ikeya[1], Krzysztof Mlynarczyk[2,3], Wojciech Pulawski[2], Umesh Ghoshdastider[2], Michal Kolinski[2], Slawomir Filipek[2,3], Peter Güntert[1,4], Frank Bernhard[1], and Volker Dötsch[1]

[1] Institute of Biophysical Chemistry and Center for Biomolecular Magnetic Resonance and Cluster of Excellence Macromolecular Complexes, Goethe University Frankfurt am Main, [2] Laboratory of Biomodeling, International Institute of Molecular and Cell Biology, Warsaw, Poland, [3] Faculty of Chemistry, University of Warsaw, Warsaw, Poland, [4] Frankfurt Institute for Advances Studies

The γ-secretase complex has a decisive role in the development of Alzheimer's disease, in that it cleaves a precursor to create the amyloid β peptide whose aggregates form the senile plaques encountered in the brains of patients. γ-secretase is a member of the intramembrane-cleaving proteases which process their transmembrane substrates within the bilayer. Many of the mutations encountered in early onset familial Alzheimer's disease are linked to presenilin 1, the catalytic component of γ-secretase, whose active form requires its endoproteolytic cleavage into N-terminal and C-terminal fragments. Although there is general agreement regarding the topology of the N-terminal fragment, studies of the C-terminal fragment have yielded ambiguous and contradictory results that may be difficult to reconcile in the absence of structural information. Here we present the first structure of the C-terminal fragment of human presenilin 1, as obtained from NMR studies in SDS micelles. The structure reveals a topology where the membrane is likely traversed three times in accordance with the more generally accepted nine transmembrane domain model of presenilin 1, but contains unique structural features adapted to accommodate the unusual intramembrane catalysis. These include a putative half-membrane-spanning helix N-terminally harboring the catalytic aspartate, a severely kinked helical structure toward the C terminus as well as a soluble helix in the assumed-to-be unstructured N-terminal loop.
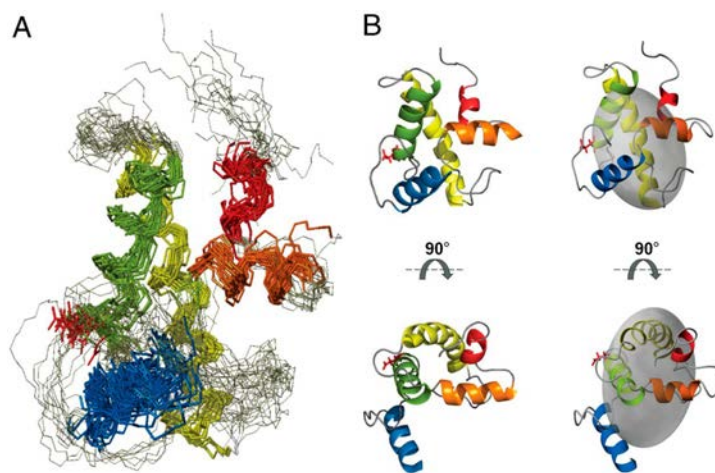
CTF structure. (A) Bundle diagram of the 20 lowest energy CYANA conformers representing the final NMR structure, obtained by superpositioning the backbone atoms of residues E356-L369, L384-A398, I407-F428, F441-T450, and F456-A461. (B) Ribbon diagram of the lowest energy conformer in two different orientations (Left) and its placement within a symmetric shell representing the potential relative position of the micelle (Right). Color scheme: helix β in blue, helix 7 in green, helix 8 in yellow, helix 9a in orange, helix 9b in red, and D385 displayed as ball and stick in red. Structures are shown without the long N-terminal loop for simplicity.

Related publications in 2010:

1) S. Sobhanifar, B. Schneider, F. Löhr, D. Gottstein, T. Ikeya, K. Mlynarczyk, W. Pulawski, U. Ghoshdastider, M. Kolinski, S. Filipek, P. Güntert, F. Bernhard, and V. Dötsch, *Structural investigation of the C-terminal catalytic fragment of presenilin 1*, PNAS 107 (2010) 9644-9649

Solution structure of polytheonamide B, a highly cytotoxic nonribosomal polypeptide from marine sponge

Collaborators: Toshiyuki Hamada[1,2,3], Shigeki Matsunaga[1], Masako Fujiwara[4,5], Kenichi Fujita[4], Hiroshi Hirota[3], Roland Schmucki[6], Peter Güntert[6] and Nobuhiro Fusetani[1,7]

[1] Laboratory of Aquatic Natural Products Chemistry, Graduate School of Agricultural and Life Sciences, The University of Tokyo, Tokyo, Japan, [2] Graduate School of Science and Engineering, Kagoshima University, Kagoshima, Japan, [3] Genomic Sciences Center, RIKEN, Yokohama, Japan, [4] JEOL DATUM LTD, Akishima, Tokyo, Japan, [5] Graduate School of Pharmaceutical Sciences, Tohoku University, Sendai, Japan, [6] Institute of Biophysical Chemistry, Center for Biomolecular Magnetic Resonance, and Frankfurt Institute for AdVanced Studies, Goethe University Frankfurt am Main, [7] Graduate School of Fisheries Sciences, Hokkaido University, Hakodate, Japan

Polytheonamide B (pTB), a highly cytotoxic polypeptide, is one of the most unusual nonribosomal peptides of sponge origin. pTB is a linear 48-residue peptide with alternating D- and L-amino acids and contains a total of eight types of nonproteinogenic amino acids. To investigate the mechanisms underlying its cytotoxic activity, we determined the three-dimensional structure of pTB by NMR spectroscopy, structure calculation, and energy minimization. pTB adopts a single right-handed 6.3-helical structure in a 1:1 mixture of methanol/chloroform with a length of approximately 45Å and a hydrophilic pore of ca. 4Å inner diameter. These features indicate that pTB molecules form transmembrane channels that permeate monovalent cations as gramicidin A channels do. The strong cytotoxicity of pTB can be ascribed to its ability to form single molecule channels through biological membranes.

Structure of polytheonamide B (pTB). (D) Top views of the pTB solution structure from the *N*-terminal side (left) and from the *C*-terminal side (right), showing the hydrophilic core. (F) Schematic representation of pTB inserted in the membrane. In this model, the N-terminal part of pTB penetrates into the cell membrane from the exterior of the cell. The hydrophobic *N*-terminus anchors pTB in the lipophilic interior of the membrane. Although in this model the *C*-terminus sticks out of the membrane, it might be located within the membrane if the membrane is thicker than assumed here.

Related publications in 2010:

1) Hamada, T., Matsunaga, S.,Fujiwara, M., Fujita, K., Hirota, H., Schmucki, R., Güntert, P. and Fusetani, N. *Solution structure of polytheonamide B, a highly cytotoxic nonribosomal polypeptide from marine sponge* J. Am. Chem. Soc. 132, (2010) 12941-12945

NMR protein structure determination in living E. coli cells using nonlinear sampling

Collaborators: T. Ikeya[1,2], A. Sasaki[1,3], D. Sakakibara[1,3], Y. Shigemitsu[1,3], J. Hamatsu[1,3], T. Hanashima[1], M. Mishima[1,3], M. Yoshimasu[4], N. Hayashi[5], T.Mikawa[6,7], D. Nietlispach[8], M. Wälchli[9], B. O. Smith[10], M. Shirakawa[3,11], P. Güntert[1,2,12] and Y. Ito[1,3,6,7]

[1] Department of Chemistry, Tokyo Metropolitan University, Tokyo, Japan, [2] Center for Biomolecular Magnetic Resonance, Institute of Biophysical Chemistry, Goethe University Frankfurt am Main, [3] CREST, Japan Science and Technology Agency, Saitama, Japan, [4] Cellular and Molecular Biology Laboratory, RIKEN, Saitama, Japan, [5] Department of Life Science, Graduate School of Bioscience and Biotechnology, Tokyo Institute of Technology, Yokohama, Japan, [6] Research Group for Bio-Supramolecular Structure-Function, RIKEN, Kanagawa, Japan, [7] Biometal Science Laboratory, RIKEN, Hyogo, Japan, [8] Department of Biochemistry, University of Cambridge, Cambridge, UK, [9] Bruker BioSpin, Yokohama, Kanagawa, Japan, [10] Division of Molecular and Cellular Biology, Faculty of Biomedical and Life Sciences, University of Glasgow, Glasgow, UK, [11] Department of Molecular Engineering, Graduate School of Engineering, Kyoto University, Nishikyo-Ku, Kyoto, Japan, [12] Frankfurt Institute for Advanced Studies

The cell is a crowded environment in which proteins interact specifically with other proteins, nucleic acids, cofactors and ligands. Atomic resolution structural explanation of proteins functioning in this environment is a main goal of biochemical research. Recent improvements to nuclear magnetic resonance (NMR) hardware and methodology allow the measurement of high-resolution heteronuclear multidimensional NMR spectra of macromolecules in living cells (in-cell NMR). In this study, we describe a protocol for the stable isotope (^{1}3C, ^{1}5N and ^{2}H) labeling and structure determination of proteins overexpressed in Escherichia coli cells exclusively on the basis of information obtained in living cells. The protocol combines the preparation of the protein in E. coli cells, the rapid measurement of the three-dimensional (3D) NMR spectra by nonlinear sampling of the indirectly acquired dimensions, structure calculation and structure refinement. Under favorable circumstances, this in-cell NMR approach can provide high-resolution 3D structures of proteins in living environments. The protocol has been used to solve the first 3D structure of a protein in living cells for the putative heavy metal-binding protein TTHA1718 from Thermus thermophilus HB8 overexpressed in E. coli cells. As no protein purification is necessary, a sample for in-cell NMR measurements can be obtained within 2-3 d. With the nonlinear sampling scheme, the duration of each 3D experiment can be reduced to 2-3 h. Once chemical shift assignments and NOESY peak lists have been prepared, structure calculation with the program CYANA and energy refinement can be completed in less than 1 h on a powerful computer system.
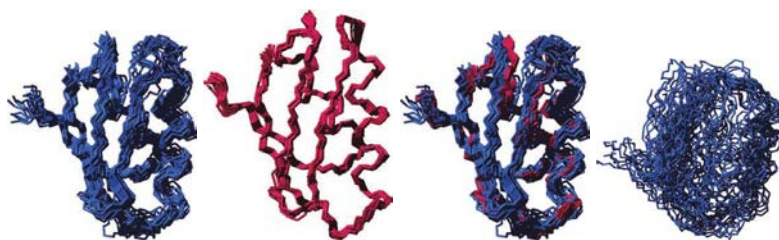
NMR solution structure of TTHA1718 in living E. coli cells. (left) Superposition of the 20 final structures of TTHA1718 in living E. coli cells, showing backbone (N, Cα, C') atoms. (center-left) Superposition of the 20 final structures of purified TTHA1718 in vitro. (center-right) Comparison of TTHA1718 structures in living E. coli cells and in vitro. (right) Superposition of the 20 final structures of TTHA1718 in living E. coli cells calculated without distance restraints derived from NOEs involving methyl groups obtained in methyl-selectively protonated in-cell NMR samples.

Related publications in 2010:

1) T. Ikeya, A. Sasaki, D. Sakakibara, Y. Shigemitsu, J. Hamatsu, T. Hanashima, M. Mishima, M. Yoshimasu, N. Hayashi, T.Mikawa, D. Nietlispach, M. Wälchli, B. O. Smith, M. Shirakawa, P. Güntert and Y. Ito. *NMR protein structure determination in living E. coli cells using nonlinear sampling*, Nature Protocols 5 (2010) 1051-1060

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[2], 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[3], Peter Güntert[1,4,5], Shigeyuki Yokoyama[1,6] and Yutaka Muto[1]

[1] RIKEN Systems and Structural Biology Center, Yokohama, Japan, [2] Protein Design Laboratory, Yokohama City University, Yokohama, Japan, [3] Department of Medical Genome Sciences, Graduate School of Frontier Sciences, The University of Tokyo, Tokyo, Japan, [4] Tatsuo Miyazawa Memorial Program, RIKEN Genomic Sciences Center, Yokohama, Japan, [5] Institute of Biophysical Chemistry, Center for Biomolecular Magnetic Resonance, and Frankfurt Institute for Advanced Studies, Goethe-University Frankfurt am Main, [6] Department of Biophysics and Biochemistry, Graduate School of Sciences, The University of Tokyo, Tokyo, 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 not only has a canonical RRM fold, but also 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.F urther 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.
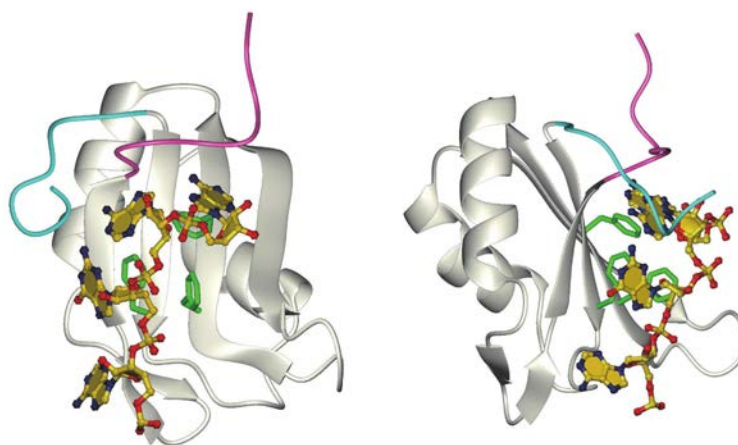
Ribbon representation of the solution structure of the hTra2-β RRM-[5' -(GAAGAA)-3'] complex. The atoms of the RNA molecule are shown in red (oxygen), blue (nitrogen) and gold (other heavy atoms).

Related publications in 2010:

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. and Muto, Y.*Structural basis for the dual RNA-recognition modes of human Tra2-β RRM*, Nucl. Acids Res. (2010) published online ahead of print.

4.4 Atoms, Molecules, Nanosystems

Research projects of Meso-Bio-Nano (MBN) Science Group

group leader: Prof. Andrey Solov'yov,
group web-page: http://fias.uni-frankfurt.de/mbn/index.php/

The research is focused on Bio-Nano Mechanics, i.e. on the structure formation and dynamics of complex MBN systems of different nature. The aggregation of atoms and small molecules into clusters, nanoparticles, micro-droplets is a process in which a wide range of complex bio-, nano- and mesoscopic objects can be created. Some of these systems have been discovered only recently and have become a subject of intensive investigations because of the variety of potentially important applications.

At the current level of technological and computational capabilities, methods and approaches traditionally associated with atomic and molecular physics can now be applied to biomolecular systems. These topics include the elucidation of fundamental physical mechanisms of such biomolecular processes as protein folding, radiation damage of biomolecules, association and dissociation of macromolecular complexes etc. The size of the considered biomolecular systems is usually of the nanometer scale. Therefore, these studies are bundled with the group's activity on the nanoscience front and receive a strong feedback from this interdisciplinary interconnection.

In recent years, numerous nanosystems possessing unique structural, optical, electric and magnetic properties have been discovered. Often, such systems are seen as building blocks for new nanostructured materials with specific tailored properties. The work of the group in this field is focused on theoretical characterization of a variety of selected nanosystems. We try to understand mechanisms of stability, self-organization and growth, as well as the ways of manipulation and control of these systems and their properties. The selection of systems for study is based usually on two criteria. First, the system should possess a certain specific fundamental property controllable during its formation. Second, the system should be important for direct or potential applications in nanotechnology, microelectronics or medicine. Another essential aspect of our activity is an attempt to build up a connection between the analogous processes of growth and self-organization occurring in nanosystems and in biological systems of larger size.

Research directions and sub-directions (the year 2010) include:

1. Structure, structure formation and dynamics of MBN systems:
   - Structure and dynamics of nanosystems.
   - Photo-induced processes in nanostructures.
   - Phase and structural transformations on the nano-scale.
   - Statistical mechanics of polypeptide and protein folding.
   - Dynamics of biomolecules.

2. Exploration of the potential applications of the MBN research:
   - Novel light source: a gamma-laser based on the crystalline undulator.
   - Ion beam cancer therapy.

3. Software development.

4. International collaborations
   - COST Action 'Nano-scale insights into ion-beam cancer therapy' (Nano-IBCT), see
     `fias.uni-frankfurt.de/nano-ibct/`
     `www.cost.esf.org/domains_actions/mpns/Actions/nano-ibct/`
   - Virtual Institute of Nano Films, see `www.vinf.eu/`

1 Research direction: 'Structure and dynamics of nanosystems'

Short description: a study of the structure, structure formation and dynamics of nanosystems as well as their magnetic, thermal and optical properties.
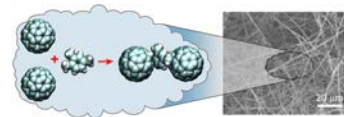
1.1 Research project: 'Fractals on a surface'

MBN Group in collaboration with C. Bréchignac (CNRS, France), I.A. Solov'yov (UIUC, Urbana, USA)
Main results: We developed a theoretical tool for studying of the post-growth processes occurring in nanofractals grown on a surface [1]. A method was developed which accounts for the internal dynamics of particles in a fractal. It was shown that particle diffusion and detachment controls the shape of the emerging stable islands on a surface.
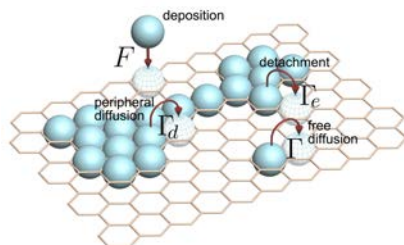
Figure 1: Arrangement of deposited particles on a surface. The important processes which govern pattern formation on a surface are indicated by arrows: F is the particle deposition rate, Γ is the diffusion rate of a free particle, Γ_d is the diffusion rate of a particle along the periphery of an island, and Γ_e is the detachment rate of a particle from the island.
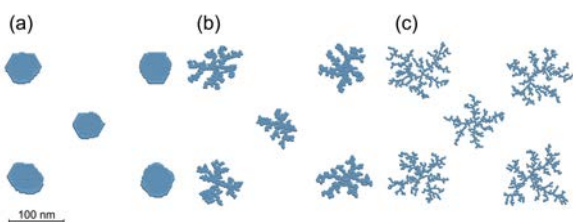
Figure 2: Formation of islands with different morphologies during the particle deposition process: (a) formation of compact islands (low deposition rate); (b) formation of fractals with thick branches (intermediate deposition rate); (c) formation of the fractal structures with thin branches (fast deposition rate) [2].

We demonstrated that the morphology of the islands is governed by the characteristic time for deposited particles to reach the growth region and by the characteristic time for a particle to find an optimum position within an island [2,3]. To deeper understand the self-organization and fragmentation processes on a surface we investigated the influence of essential parameters of the system on 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 [1,3,4].

Related publications in 2010:

1) V.V. Dick, I.A. Solov'yov and A.V. Solov'yov, *Fragmentation pathways of nanofractal structures on a surface*, http://arxiv.org/abs/1001.3992 (2010).
2) I.A. Solov'yov, V.V. Dick, A.V. Solov'yov, *Nanoparticles on a surface: atomistic approach for structure, dynamics and pattern formation*, in Conf. Series 17th Symp. on Atomic, Cluster and Surface Physics (Obergurgl, Austria, January 24-29, 2010), p. 21, ISBN 978-3-902719-52-2, Innsbruck University press (2010).
3) V.V. Dick, I.A. Solov'yov and A.V. Solov'yov, *Nanoparticles dynamics on a surface: fractal pattern formation and fragmentation*, J. Phys.: Conf. Ser. 248, 012025 (2010).
4) V.V. Dick, I.A. Solov'yov, A.V. Solov'yov, *Theoretical study of nanofractal stability on the surface*, in Conf. Series 17th Symposium on Atomic, Cluster and Surface Physics (Obergurgl, Austria, January 24 - 29, 2010), p. 245, ISBN 978-3-902719-52-2, Innsbruck University press (2010).

1.2 Research project: 'Structure and dynamics of clusters and fullerenes'

MBN Group in collaboration with W. Greiner (FIAS), D. Poenaru (Nat. Inst. Phys., Romania), V. Ivanov (St. Petersburg Polytech. Univ., Russia).

Main results:

• For the first time a self-consistent Hartree-Fock calculation of electronic structure of endohedral fullerenes $A@C_{60}$ [1,2]. All atomic electrons together with 240 valence electrons of the fullerene were treated self-consistently. In the case of $Ar@C_{60}$ a strong hybridization of valence shells of the confined atom and some of the fullerene shells is observed. This phenomenon had not been noticed before within the framework of a simpler LDA model (Chakraborty *et al.*, Phys. Rev. A 78, 013201 (2008)). We demonstrate that hybridization appears as a result of an accurate account for the exchange electron-electron interaction.

Figure: HF [1] and LDA (Chakraborty *et al.* (2008)) radial wave function of the $3p$ shell in $Ar@C_{60}$. The atomic $3p$ orbital is also presented.

• In Refs. [3,4] the surface influence on deposited atomic clusters was accounted for as a change in the geometry of the free cluster from spheroidal to semispheroidal (oblate and prolate) shapes. The energy levels for the electrons are calculated using a deformed oscillator quantum well plus squared angular momentum half-cut by an infinite wall located at the surface. The level scheme is used to compute the shell corrections, to which a macroscopic liquid drop energy is added. Clear minima of the total deformation energy are obtained for semispheroids at the same deformation, within a range of atom number from 2 to 100. These minima are interpreted as stable structures of various magic numbers for deposited atomic clusters.

Fig. 7. The total deformation energy of the deposited cluster $E_{cluster} = E_{shell} + E_{macro}$ as a function of the number of atoms N for the three deformations δ (-0.38—oblate, 0—semisphere, 0.67—prolate) with maximum degeneracy as in Fig. 4. The magic numbers are marked.

Related publications in 2010:

1) R.G. Polozkov, V.K. Ivanov, A.V. Verkhovtsev, A.V. Solov'yov, *Self-consistent Hartree-Fock approach to electronic structure of $A@C_{60}$ (A=He,Ne and Ar)*, Science and Technology Bulletin of Saint Petersburg State Polytechnic University, in press (2010) (in Russian).

2) A.V. Verkhovtsev, R.G. Polozkov, V.K. Ivanov, A.V. Korol and A.V. Solov'yov, *Electronic Structure of Endohedral Fullerenes with Noble Gas Atoms*, pp. 83-84, Book of Abstracts of International Conference 'Dynamics of Systems on the Nanoscale (DySoN 2010)' (NRC, Rome, Nov. 16-19, 2010), L. Avaldi, F.A. Gianturco, and A.V. Solov'yov (eds).

3) R.A. Gherghescu, D.N. Poenaru, A.V. Solov'yov, and W. Greiner, *Hemispheroidal atomic clusters on planar surfaces*, Physica E 42, 1555 (2010).

4) R.A. Gherghescu, D.N. Poenaru, A.V. Solov'yov, and W. Greiner, *Spheroidal cap configurations of atomic clusters on planar surfaces*, Eur. Phys. Journ. B 77, 123-132 (2010).

2 Research direction: 'Photo-induced processes in nanostructures'

MBN Group in collaboration with V. Ivanov (St. Petersburg State Polytechnical University, Russia), J.-P. Connerade (Imperial College, UK), A. Müller (Justig-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.
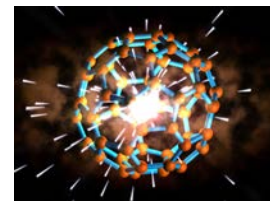
2.1 Research project: 'Photo-processes in clusters'

Main results:

• A consistent many-body theory based on the jellium model is applied for the description of angular resolved photoelectron spectra of metal clusters anions [1,2]. The results of calculations demonstrate the dominant role of the many-body effects in the formation of angular distributions of photoelectrons emitted from sodium clusters and are in a good agreement with recent experimental data of von Issendorff *et al.* (Science 323, 1323 (2009)). The comparison of theory and experiment has been performed for the photoionization of Na^{7-} and Na^{19-}.
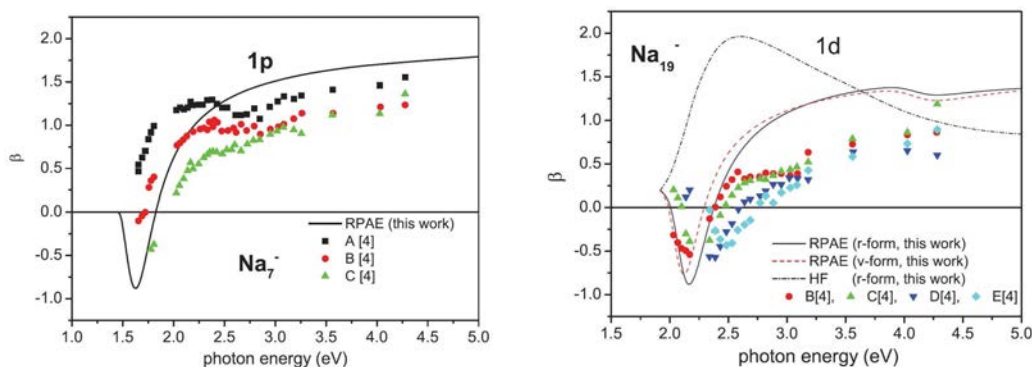
Figure: Angular anisotropy parameter for the partial PI cross section of Na^{7-} and Na^{19-} clusters versus photon energy. Experimental data from von Issendorff *et al.* (2009, 2010).

Related publications in 2010:

1) R.G. Polozkov, V.K. Ivanov, A.V. Solov'yov, *Many-body theory for angular resolved photoelectron spectra of metal clusters*, Phys. Rev. A 81, 021202 (2010).

2) R.G. Polozkov, V.K. Ivanov, A.V. Korol, A.V. Solov'yov, *Theoretical study of the angular distribution of photoelectrons in photoionization of metallic clusters*, Science and Technology Bulletin of Saint Petersburg State Polytechnic University, issue No 1044, pp. 75-80 (2010) (in Russian).

2.2 Research project: 'Photo-processes in fullerenes and endohedral systems'
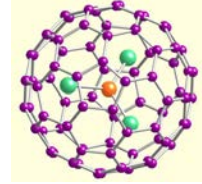
The project aims to study photo-processes (photoabsorption, bremsstrahlung, light scattering) in pristine and endohedral fullerenes. Special attention is paid to the influence of the fullerene on the encaged atom (molecule).

Main results:

• In [1] 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.

The case study, carried out for $Sc^{2+}@C_{80}^{6-}$, 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).
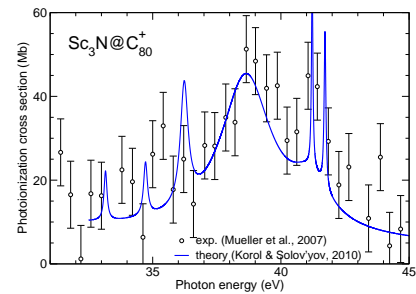
Figure: Photoionization of $Sc_3N@C_{80}$: experiment (Müller *et al.*, 2007) vs theory [1].

• The presence of the fullerene cage leads to so-called confinement resonances (CR) in the photoionization cross section for $A@C_N$. CR appear as a result of interference between a direct wave of the photoelectron escaping and the waves scattered from the cage. The nature of the discrepancy between a number of theoretical predictions on the CR and the experimental results was revealed in [2]. We demonstrated that since in experimental conditions either the direction or the magnitude (or both) of the atomic displacement from the cage center cannot be controlled, proper averaging over the atomic positions must be carried out. The averaging affects the CR structure. Indeed, the CR are due to the interference between the direct and the scattered waves of the photoelectron, both originating from the same source, – the encaged atom. This source is point-like if the atom is at the center. For a non-central position the source acquires a finite size $D \approx 2\langle a \rangle$ ($\langle a \rangle$ is the mean distance from the center). When D exceeds the half-wavelength of photoelectron the CR pattern is destroyed.

• In the PhD thesis [4] a detailed description of the obtained results, the developed theoretical models and numerical methods was given on the he effect of dynamical screening, i.e. the enhancement of the photoabsorption rate by an encapsulated atom due to the change in the electric field as a result of the fullerene polarization.

Related publications in 2010:

1) A.V. Korol, A.V. Solov'yov, *Vacancy decay in endohedral atoms: the role of non-central position of the atom*, J. Phys. B, submitted (2010) (see also arXiv:1011.2053v1).

2) A.V. Korol, A.V. Solov'yov. *Confinement Resonances in Photoionization of Endohedral Atoms: Myth or Reality?* J. Phys. B 43, 201004 (2010) (Fast Track Communication).

3) A.V. Korol, A.V. Solov'yov, *On the photoionization of Endohedral Atoms*, in Conference Series 'XVII Symp. on Atomic, Cluster and Surface Physics 2010', I.Milewski, A. Kendl, P. Scheier (Eds.), Innsbruck University Press, p.193-196, (2010).

4) S. Lo. *Dynamical Screening of an Endohedral Atom*, Dissertation, Goethe-Universität Frankfurt am Main (2010).

3 Research direction: 'Phase and structural transformations on the nano-scale'

Short description: We investigate the transformations of nanoscale systems which can possess the features of phase transitions. We approach this problem both on the molecular dynamics simulations level and by means of statistical mechanics. Particular attention is paid to phase transitions in nano-carbon systems.

3.1 Research project: 'Phase transformations in fullerenes'

MBN Group in collaboration with W. Greiner (FIAS).
Main results:

• We have investigated formation and fragmentation of C_{60} as a general process of phase transition. In order to do this, we have developed a topologically-constrained forcefield and conducted extensive molecular dynamics simulations within the $C_{60} \leftrightarrow C_2$ channel.

• Results of the simulations show that C_{60} experiences a phase transition at 5855 K. At this T the system continuously oscillates between a fullerene cage and a gaseous phase consisting of C_2 and small carbon fragments. These oscillations signify dynamic phase coexistence and correspond to consecutive fragmentation and assembly of the carbon cage. To the best of our knowledge, our work is the first where the processes of fragmentation and formation of a fullerene are observed several times in the course of the simulation.

• We have also constructed a statistical mechanics model that accounted for entropic corrections and the effect of pressure on the phase transition. Assuming local thermodynamic conditions, we correlated our results to generalized temperature and pressure conditions found in arc-discharge experiments and obtained the dependence of the phase transition temperatures on pressure.

Figure 1: Caloric curves and heat capacity plots (inset) for C_{60} (black triangles) and C_{240} (open diamonds).
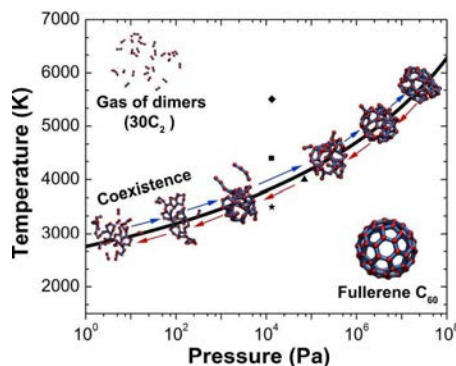
Figure 2: The curve separates the region where the system can be found in either a cage (below the line) or a gaseous state (above it).

• Taking into account in the statistical mechanics model the thermodynamics conditions in experiments, we have obtained for the C_{60} a phase transition temperature of 3800-4200K corresponding to a pressure of 10-100 kPa in good agreement with experimental results. The novelty of the present work is in the fact that it treats the fullerene formation process as a carbon gas - fullerene cage phase transition.

Related publications in 2010:

1) A. Hussien, A.V. Yakubovich, A.V. Solov'yov, *Thermodynamic of carbon Gas-Fullerene Transition*, in Conf. Series 17th Symposium on Atomic, Cluster and Surface Physics (Obergurgl, Austria, January 24 - 29, 2010), pp. 237-240, ISBN 978-3-902719-52-2, Innsbruck University press (2010).

2) A. Hussien, A.V. Yakubovich, A.V. Solov'yov, W. Greiner, *Phase transition, formation and fragmentation of fullerenes*, Europ. Phys. J. D 52, 207-217, (2010).

3) A. Hussien, *Phase Transitions in Carbon-based nanoclusters as seen via molecular dynamics simulations*. Dissertation, FIAS and Goethe-Universität Frankfurt am Main (2010).

3.2 Research project: 'Phase transformations in fullerene-based nanowires'

MBN Group in collaboration with B. Johnson (Cambridge, UK), J. Geng (Bolton, UK), I.A. Solov'yov (UIUC, Urbana, USA)

Main results: Two forms of carbon, fullerenes and carbon nanotubes, are closely related having structural commonality of the sp^2 frameworks. The nanotubes have been widely investigated for the last decade as one-dimensional nanomaterials, but fullerene 1D nanostructures presently only represent laboratory curiosities.
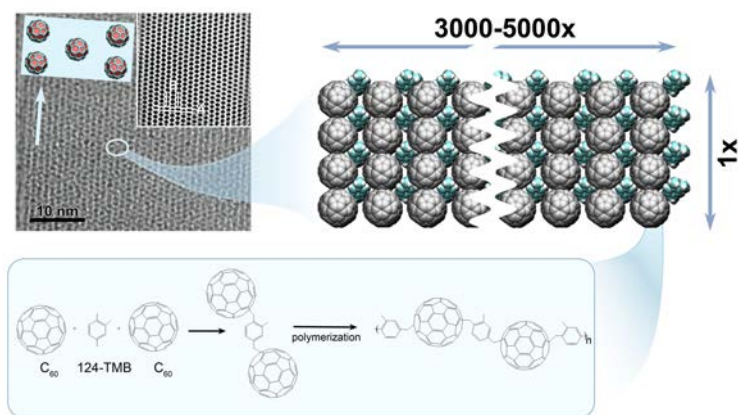
Figure 1. Polymerization transformation in the C_{60}-based nanowire.

We showed the formation of a C_{60}-based nanowire polymer made by first growing the coresponding crystalline nanowire through a solution phase of C_{60} followed by a topochemical polymerization in the solid state. This new material can be potentially important for nanotechnology because of its low dimensionality, high surface area, large length-to-width ratio, crystalline and molecularly cross-linked fullerene-based nanostructure. In comparison with carbon nanotubes, fullerene 1D nanopolymers could be even more attractive in electronic and photonic applications especially for bio-applications as the bio-compatible and totally free from any metal materisl. This clearly contrasts the carbon nanotubes, the growth of which is catalyzed by transition metal nanoparticles, and from which by no means all the metal can be removed by a post-purification process.

We demonstrated that the nanopolymer emerges in a course of a phase transition driven by forming and breaking covalent bond. Because the reactive monomers are preorganized in the crystalline unit cell at a distance commensurate with the repeat distance in the final polymer, the application of thermal or photochemical energies to the nanowires induces polymerization. The studied host (C_{60}) and guest (1,2,4-trimethylbenzene) nature of the polymerization allowed us to suggest a general host-guest route to the synthesis of new types of fullerene-based nanopolymers composed of different organic monomers and fullerenes. In order to understand the polymerization pathway we have employed gas chromatography, mass spectrometry and ^{13}C nuclear magnetic resonance spectroscopy to investigate the nature of the bonds formed during the polymerization process. Theoretical analysis based on detailed calculations of the reaction energetics and structural analysis provided an in-depth understanding of the polymerization pathway.

Related publication in 2010:

1) J. Geng, I.A. Solov'yov, D.G. Reid, P. Skelton, A.E.H. Wheatley, A.V. Solov'yov, B.F.G. Johnson, *Fullerene-based one-dimensional crystalline nanopolymer formed through topochemical transformation of the parent nanowire*, Phys. Rev. B 81, 214114 (2010).

4   Research direction: 'Statistical mechanics of polypeptide and protein folding'

Short description: One of the most challenging questions of contemporary physics and biology is the question of protein folding: the process by which a polypeptide folds into its unique functional 3D structure from a random coil state. The exact mechanism and the principal driving forces of this transition still are not completely understood. Most of the theoretical approaches to the problem are based on the methods of computational biology and on the molecular dynamics simulations. We have been developing an alternative approach for the description of the process based on statistical mechanics.

MBN Group in collaboration with W. Greiner (FIAS), I.A. Solov'yov (UIUC, Urbana, USA)

Main results:

● The method has been elaborated allowing one to construct a partition function and to evaluate, on its basis, all the thermodynamical characteristics of the system of interest [1,2].

● We have demonstrated that basing solely on the formalism of statistical mechanics one can quantitatively describe various features folding-unfolding transition in real proteins such as heat and cold denaturations, increase of the reminiscent heat capacity, temperature range of the transitions, etc [2,3].

Figure: The 3D structure of protein metmyoglobin (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.
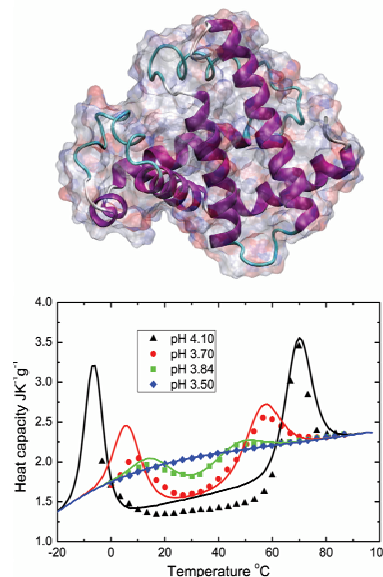
Related publications in 2010:

1) A.V. Yakubovich, A.V. Solov'yov, W. Greiner; *Conformational changes in polypeptides and proteins*, Int. J. Quant. Chem. 110, 257-269 (2010).

2) A.V. Yakubovich, *Theory of phase transitions in polypeptides and proteins*, Dissertation, FIAS and Goethe-Universität Frankfurt am Main (2010).

3) A.V. Yakubovich, A.V. Solov'yov, W. Greiner, *Statistical mechanics of protein folding in water environment*, European Conference on Atoms Molecules and Photons (ECAMP10), (4-9 July 2010, Salamanca, Spain).

5 Research direction: 'Dynamics of biomolecules'

MBN Group in collaboration with S. N. Volkov (Bogolyubov Institute for Theoretical Physics, Ukraine).

5.1 Research project: 'DNA unzipping'

Main results: The process of DNA double helix unzipping is investigated using the algorithm of steered molecular dynamics (SMD). We demonstrate that the base-pairs before complete separation into single-stranded DNA form interlineate stable pre-opened states. These states are realized in the vicinity of unzipping fork and stabilized by the water molecules that incorporate between the complimentary base pair. The existence of such intermediate states was predicted in our previous works on DNA unzipping process. According to the proposed theory, intermediate states of the complementary base pairs are required for realization of the kink-soliton like scenario of DNA unzipping under the action of external force.
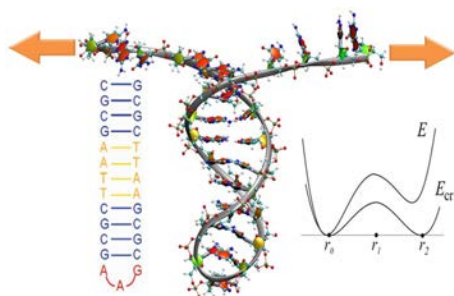
Figure 1. DNA unzipping by an external force.
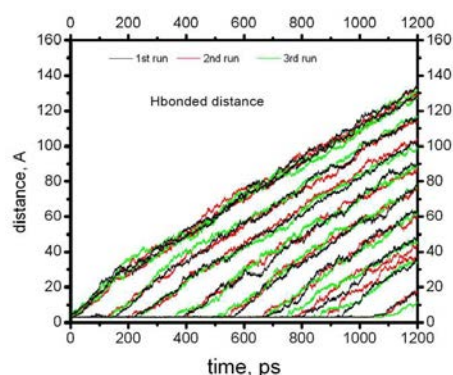
Figure 2. The H-bond distances in base pairs of DNA-hairpin as a function of simulation time.

SMD simulations revealed that each pair under strands separation in DNA duplex takes part in two types of rotations. Before the pair unzipping – in the rotation of the duplex as a whole, and under it's own unzipping – in the rotation in the frame of unzipping fork. The trajectories of strands separation are very similar for the DNA duplex with predominant G·C content and differ substantially for DNA regions with high A·T fraction. This fact allows to support the assumption that process of DNA mechanical unzipping similar in some sense to the thermal double helix separation – the DNA melting.

Related publications in 2010:

1) S.N. Volkov, E. Paramonova, A.V. Yakubovich, and A.V. Solov'yov, *Micromechanics of DNA Unzipping*, pp. 81-82, Book of Abstracts of International Conference 'Dynamics of Systems on the Nanoscale (DySoN 2010)' (NRC, Rome, Nov. 16-19, 2010), L. Avaldi, F.A. Gianturco, and A.V. Solov'yov (eds).

6 Research direction: 'Novel light source: a gamma-laser based on the crystalline undulator'

MBN Group in collaboration with W. Greiner (FIAS), H. Backe & W. Lauth (Mainz Uni., Germany), U. Uggerhoj (Aarhus University, Denmark), S. Connell (Johannesburg University, South Africa), V. Guidi (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 radiation of a free-electron laser type formed by a bunch of ultra-relativistic particles channelling through a periodically bent crystalline-like structure. Potential applications include plasma physics, nuclear physics, solid state physics, molecular biology, medicine and technology.

Main results:

• A scheme of hard x- and gamma-ray laser has been proposed, see Fig. 1. It combines a periodically bent crystal (crystalline undulator) with a conventional undulator. The conventional undulator is fed with a beam of ultrarelativistic charged particles (preferably positrons) with a layered energy distribution (the red curve in Fig.2). The particle beam interacts with the undulator field and an auxiliary radiation wave as it takes place in a conventional free electron laser. This interaction modulates the probability distribution of the particle along the beam axis. Due to the layered energy distribution, the spectrum of the modulation contains a harmonic with a spatial period much smaller than the wavelength of the auxiliary radiation. Due to this harmonic, the radiation process in the crystalline undulator becomes coherent. A patent for the new source of the coherent radiation is submitted [1].

Figure 1. A gamma-laser based on a crystalline undulator.
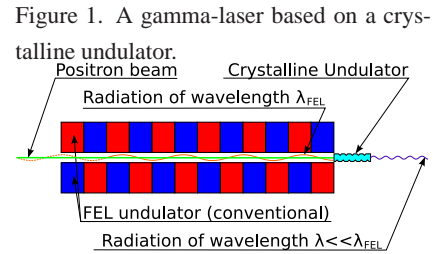
Figure 2. Layered energy disctribution.
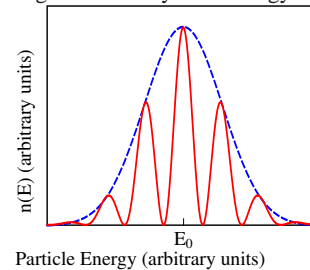
• A simulation of 855 MeV electrons channeling of in Silicon has been performed with a new computer code. The dechanneling lengths for (100), (110) and (111) crystallographic planes have been estimated. The dependence of the intensity of the channeling radiation on the crystal dimension along the beam direction has been calculated. A good agreement of the obtained results 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 an equation of Fokker-Planck type. Approximate analytical solution of the equation is found. 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 finding is of crucial importance for the theory of the crystalline undulator based γ-laser [3,4].

Related publications in 2010:

1) W. Greiner, A. V. Korol, A. Kostyuk, A. V. Solov'yov, *Vorrichtung und Verfahren zur Erzeugung elektromagnetischer Strahlung*, Application for a German patent, June 14, 2010, Ref.: 10 2010 023 632.2.

2) A. Kostyuk, A. Korol, A. Solov'yov and W. Greiner, *Planar Channeling of 855 MeV Electrons in Silicon: Monte-Carlo Simulations*, arXiv:1008.1707 [physics.acc-ph].

3) A. Kostyuk, A.V. Korol, A.V. Solov'yov and W. Greiner, *Stable propagation of a modulated positron beam in a bent crystal channel*, J. Phys. B: At. Mol. Opt. Phys. 43, 151001 (2010).

4) A. Kostyuk, A.V. Korol, A.V. Solov'yov and W. Greiner, *Modulated positron beam in a crystal channel*, in "Charged and Neutral Particles Channeling Phenomena - Channeling 2008", S.B. Dabagov and L. Palumbo (Eds.), pp. 438-447 (World Scientific, 2010).

7   Research direction: 'Ion Beam Cancer Therapy' (IBCT)

MBN Group in collaboration with E. Surdutovich (Oakland University, Michigan, USA).

Short description: The multiscale approach to the radiation damage induced by irradiation with ions is aimed to the phenomenological 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 secondaries produced as a result of ionization and excitation of the medium, interaction of secondaries with biological molecules, most important with DNA, the analysis of induced damage, and evaluation of probabilities of subsequent cell survival or death. Evidently, this approach is interdisciplinary, since it is based on physics, chemistry, and biology. Moreover, it spans over several areas within each of these disciplines.

Edited books and journal issues in 2010:

1) I. Baccarelli, F.A. Gianturco, E. Scifoni, A.V. Solov'yov, and E. Surdutovich (editors), Topical issue: *Molecular level assessments of radiation biodamage*, Eur. Phys. J. D 60, 1 (2010).

7.1   Research project: 'Thermo-mechanical pathways of DNA damage'

Main results: In 2010 we have applied the inelastic thermal spike model to high-energy $^{12}C^{6+}$ beams passing through liquid water. The heat transfer has been calculated in the vicinity of the incident-ion track. That analysis suggested that the temperature as well as pressure may be quite high near the track and thus make the environment more hostile to DNA and other biomolecules. However, the initial conditions were not sufficient either for estimating forces or for modeling of thermo-mechanical effects on biomolecules. Therefore we considered a hydrodynamic transport problem on a nanometer scale with these initial conditions [1]. The solved hydrodynamic expansion (a cylindrically symmetric strong explosion) predicted a propagation of a cylindrical shock wave on a nanometer scale, providing dependences of pressure on time and the radius. These dependences give an opportunity to estimate the forces and do further modeling with biomolecules.

The first estimates predict forces of the order of 10 nN. These forces are strong enough to rupture the bonds of DNA, but it acts for a very short time. The future MD simulations should answer the question on whether this thermo-mechanical mechanism is important for DNA damage following irradiation with ion beams.
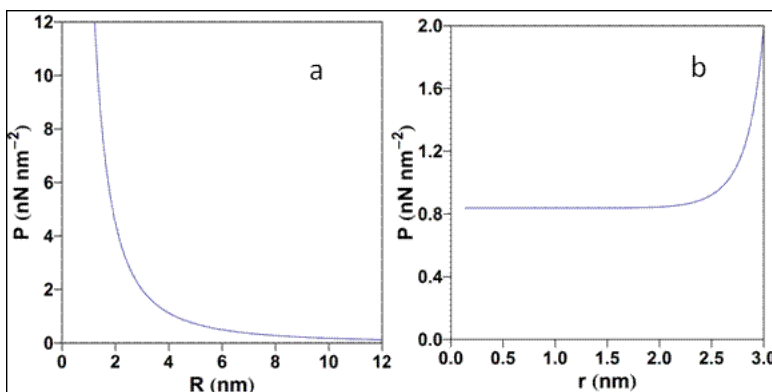
Figure: The dependence of pressure on the wavefront from its radius (a) and the dependence of pressure in the wake of the shock wave (b),[1].

Related publication in 2010:

1) E. Surdutovich and A.V. Solov'yov, *Shock wave initiated by ion passing through liquid water*, Phys. Rev. E 82 051915 (2010).

7.2 Research project: 'Multiscale approach to IBCT'

Main results: A multiscale approach to IBCT to understand the physics related to ion-beam cancer therapy, proposed in 2009, has been further developed. In 2010, we have analyzed the approach to DNA damage complexity which is deemed to be one of the most significant features of high-LET irradiation such as that of 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 nucleus, to fix the complex damage and, as a result, such damage is more lethal than isolated DNA damage. We suggested a way to quantify the complex damage in Ref. [1].

Another significant development was the first study of thermal effect on biomolecules using Molecular Dynamics modeling.
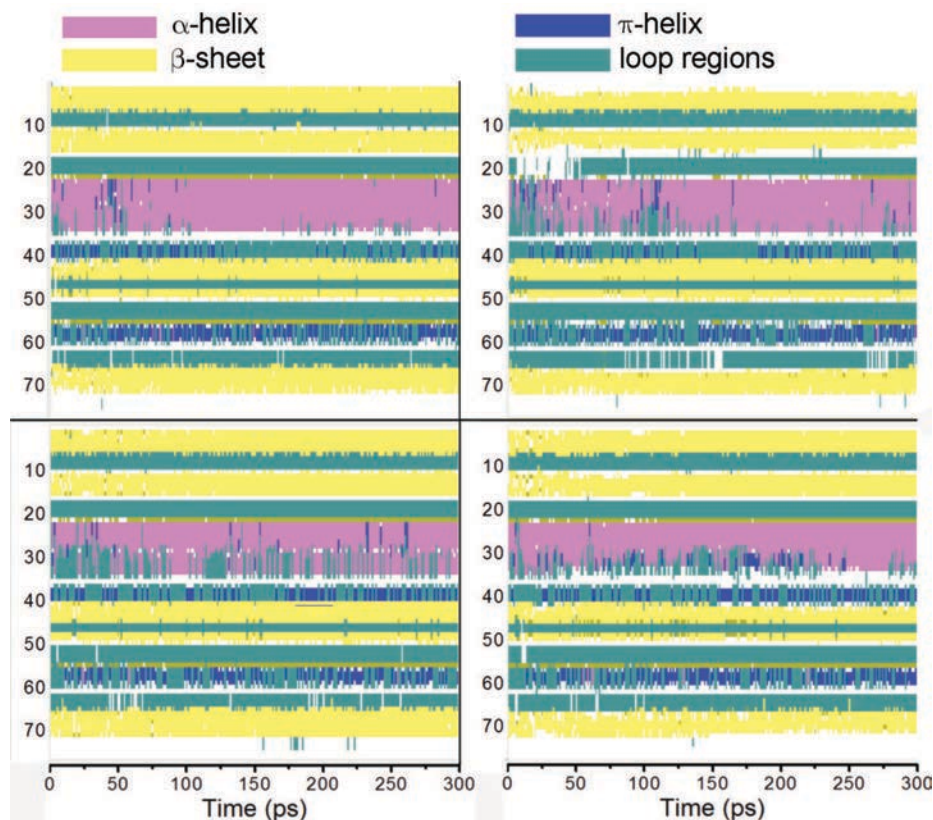
Figure: The dependence of secondary structure of ubiquitin on time in a course of the heating event. The ordinate represents the index of amino acid in the protein. Each color corresponds to different types of secondary structure: purple represents α-helices, yellow represents β-sheets, green represents loop regions and blue represents π-helices. The zero time corresponds to the moment of propagation of the energetic particle.

Related publications in 2010:

1) E. Surdutovich, A. Yakubovich, and A.V. Solov'yov, *Multiscale approach to radiation damage induced by ion beams*, Eur. Phys. J. D 60, 101-108 (2010).

2) E. Surdutovich, E. Scifoni, and A.V. Solov'yov, *Ion-beam cancer therapy: News about a multiscale approach to radiation damage*, Mutat. Res. 704, 206-212 (2010).

7.3 Research project: 'Secondary electrons and radial dose distribution'

Description: This project is an independent subsidiary of the multiscale approach. It stemmed from the study of energy spectra of secondary electrons produced by incident ion. The first goal was to understand how the medium, e.g., liquid water, affects the spectra of secondary electrons. Second was the studying the radial dose distribution in the vicinity of the ion track.

Main results:

• A new parametric model describing the production of secondary electrons at a broad range of energies in liquid water has been developed, [1,2]. For higher electron energies, the dielectric response approach has been applied and compared to the parametric model.
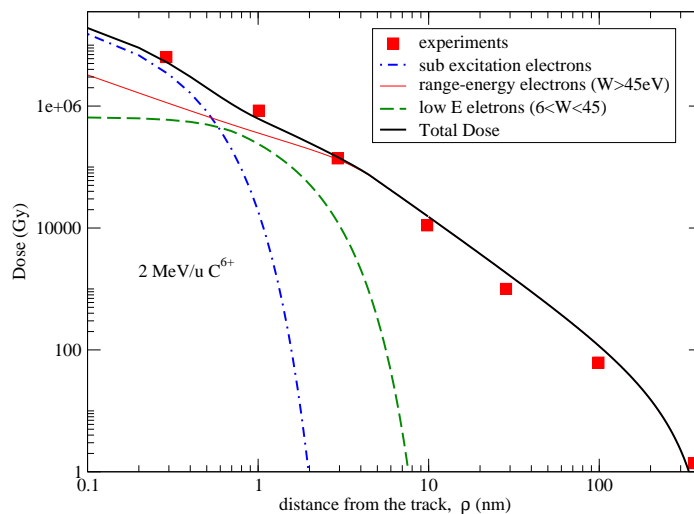
Figure: Linear energy deposition for carbon ions for different initial energies: our model (lines) compared to experiments from GSI (dots)

• The obtained secondary electron spectra were used for calculations of the radial dose deposited along carbon-ion tracks in liquid water using different techniques depending on the energy range of secondary electrons [3]. The models are developed in relation with the experimental data on electron penetration lengths. The results of these models are compared to experimental measurements.

Related publications in 2010:

1) E. Surdutovich, E. Scifoni, and A.V. Solov'yov, *Ion-beam cancer therapy: News about a multiscale approach to radiation damage*, Mutat. Res. 704, 206-212 (2010).

2) E. Scifoni, E. Surdutovich, A. V. Solov'yov, *Spectra of secondary electrons generated in water by energetic ions*, Phys. Rev. E 81, 021903 (2010).

3) E. Scifoni, E. Surdutovich, and A.V. Solov'yov, *Radial dose distribution from carbon ion incident on liquid water*, Eur. Phys. J. D 60, 115-119 (2010).

8 Research direction: 'Software development'

8.1 Research project: 'MBN Explorer'

MBN Group in collaboration with S. Schramm (FIAS), I.A. Solov'yov (UIUC, Urbana, USA).

Main results:

Meso-Bio-Nano Explorer (MBN Explorer) is a software package being developed in the group for the last 6 years. At present it is a powerful tool capable to describe molecular systems at different levels of details. In particular, MBN Explorer is suited to compute the system's energy, to optimize structures, as well as to consider classical and Monte-carlo based dynamics. MBN Explorer allows one 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 a broad range of problems and molecular systems. Most of the existing codes are developed focusing on a particular class of molecular systems, and have severe limitations, while MBN Explorer goes beyond these drawbacks. On demand, MBN Explorer allows to group particles in the system into rigid blocks, thereby significantly reducing the number of degrees of freedom and simplifying the equations of motion. This algorithm is especially useful in studying of molecular dynamics of complex systems, consisting of large interacting building blocks, e.g. proteins or fullerene-based nanowires.
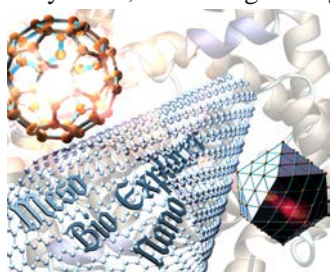
Figure 1: An example of hypothetical Meso-Bio-Nano systems which can be studied using MBN Explorer: a protein hemoglobin, a fullerene, a nanotube and an atomic cluster. The study of structure and properties of these objects individually, as well as together is a typical task for MBN Explorer.

The MBN Explorer code is written in a way that it can be easily extended to treat new types of systems with new potentials. This feature allows one to apply MBN Explorer for a variety of the tasks. The speed of the single-processor calculations using MBN Explorer is compatible with that for other contemporary software packages, e.g. NAMD, CHARMM, GULP or LAMMPS.

High flexibility and universality of the code allowed us to perform calculations of quite different systems, starting from the research of the structure of carbon-based nanowires to the investigation of the diffusion processes of silver clusters on graphite substrates and to the molecular dynamics simulations of the growth of nanotubes on catalyzing particles.

Related publications in 2010:

1) V.V. Dick, I.A. Solov'yov and A.V. Solov'yov, *Nanoparticles dynamics on a surface: fractal pattern formation and fragmentation*, J. Phys.: Conf. Ser. 248, 012025 (2010).

2) V.V. Dick, I.A. Solov'yov and A.V. Solov'yov, *Fragmentation pathways of nanofractal structures on a surface*, http://arxiv.org/abs/1001.3992 (2010).

3) V.V. Dick, I.A. Solov'yov, A.V. Solov'yov, *Theoretical study of nanofractal stability on the surface*. In Conf. Series XVIIth Symposium on Atomic, Cluster and Surface Physics 2010 (Obergurgl, Austria, January 24 - 29, 2010), p. 245, ISBN 978-3-902719-52-2, Innsbruck University press (2010).

4) I.A. Solov'yov, V.V. Dick, A.V. Solov'yov, *Nanoparticles on a surface: atomistic approach for structure, dynamics and pattern formation*. In Conf. Series XVIIth Symposium on Atomic, Cluster and Surface Physics 2010 (Obergurgl, Austria, January 24 - 29, 2010), p. 21, ISBN 978-3-902719-52-2, Innsbruck University press (2010).

8.2 Research project: 'Monte-Carlo code for channeling dynamics and the radiation'

The FORTRAN 95 code is being used for a comprehensive numerical study of the channeling of ultrarelativistic particles and the properties of radiation from 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. The code is being written in FORTRAN 95 which guaranties its high performance and portability.

Presently, the code is able to simulate planar channeling of relativistic electrons and positrons in straight and bent crystals. Examples of the simulated positron 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.
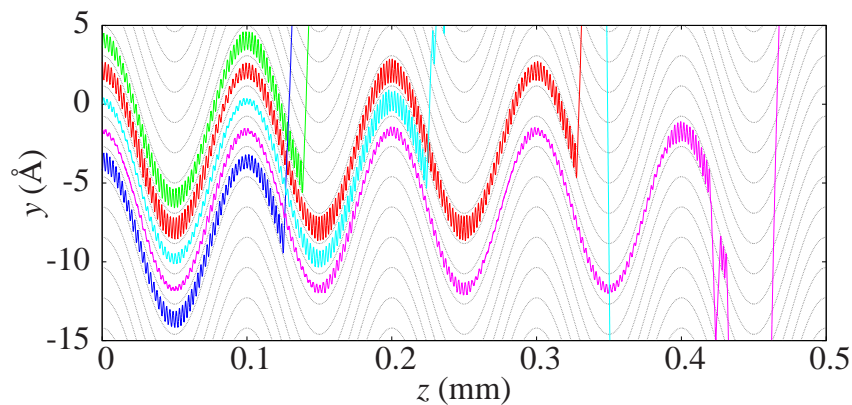
Figure 1: Examples of the simulated trajectories of positrons in a periodically bent crystal.

Related publications in 2010:

1) A. Kostyuk, A. Korol, A. Solov'yov, and W. Greiner, *A new Monte-Carlo Code for Channeling Simulation*, p. 63, Boof of Abstracts of Channeling 2010, 4th International Conference on 'Charged and Neutral Particles Channeling Phenomena', (3-8 October, 2010, Ferrara, Italy).

2) A. Kostyuk, A. Korol, A. Solov'yov, and W. Greiner, *Planar Channeling of Electrons: Numerical Analysis and Theory*, p. 26, Boof of Abstracts of Channeling 2010, 4th International Conference on 'Charged and Neutral Particles Channeling Phenomena', (3-8 October, 2010, Ferrara, Italy).

3) A. Kostyuk, A. Korol, A. Solov'yov and W. Greiner, *Planar Channeling of 855 MeV Electrons in Silicon: Monte-Carlo Simulations*, arXiv:1008.1707 [physics.acc-ph] (2010).

8.3 Research project: 'Development of computer tools for graphical processors (CUDA)'

MBN Group in collaboration with S. Schramm (FIAS).

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

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.
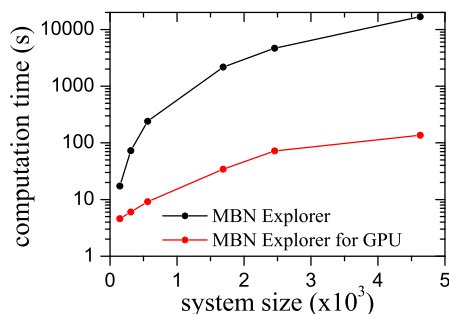
Figure 1. The computational efficiency of the CPU and GPU versions of the MBN Explorer. The computation time, needed to perform 1000 molecular dynamics simulation steps with the Sutton-Chen potential for a variety of Ni-based systems: clusters $Ni_{147}, Ni_{309}, Ni_{561}$, and crystals consist of 1688, 2457, and 4631 particles.

We have extended the software package MBN Explorer that being developed at our group for almost a decade in order to get 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 of the carbon-based materials, metal clusters and carbon-metal systems. With an improved version of MBN Explorer software package we have investigated the structure of a complex consisting of a single-walled carbon nanotube (SWCNT) and a Ni_{309} nanoparticle. We have studied the question of sensitivity of the structure of CWCNT-Ni complex to the parameters of the interparticle interactions. One of the major conclusions of our research is the following. Depending on the strength of the Ni-Ni and Ni-C interactions and temperature different scenarios of system evolution can be realized, from the total collapse and digestion of the nanotube by the Ni particle to the formation of a stable nanotube atop of the Ni cluster.
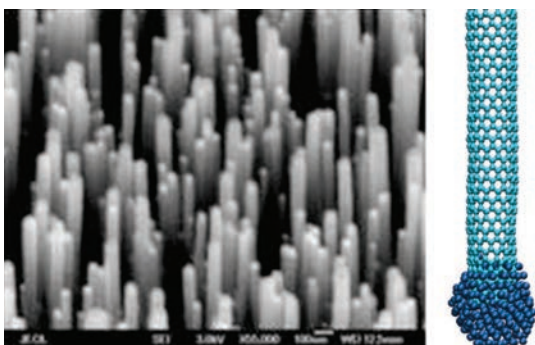
Figure 2: Left: image of the CNT forest grown on a substrate (from southamptonnanofab.com). Right: a CNT attached to a catalytic Ni nanoparticle as seen from molecular dynamics simulations performed on GPU.

8.4 Research project: 'Programs for many-body descriptions of clusters and fullerenes'

MBN Group in collaboration with V. Ivanov (St. Petersburg State Polytechnical Univ., Russia).

Main results:

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 approximation.

The code allows one to compute

(a) electronic wave functions of the ground state, single-electron energy and total energy of the system treating self-consistently all atomic electrons and 240 valence electrons of the fullerene;

(b) discrete and continuum wave fucntions, energy spectrum of discrete excitations and the scattering phase-shifts;

(c) cross sections of photoabsorption and the angular distribution of photoelectrons within single-electron approach as well as within the Random Phase Approximation with Exchange (RPAE) which acocunts for the many-electron correlations.
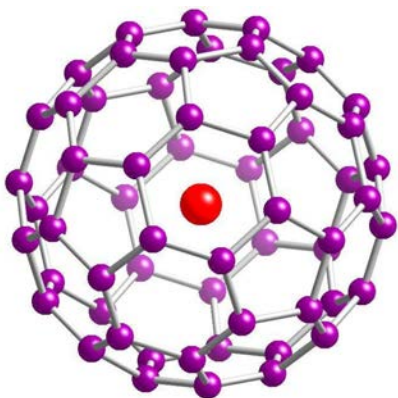
Figure 1: Endohedral system $Ar@C_{60}$. The HF ground and excited states were calculated by self-consistent treatment of all 258 electrons [2].
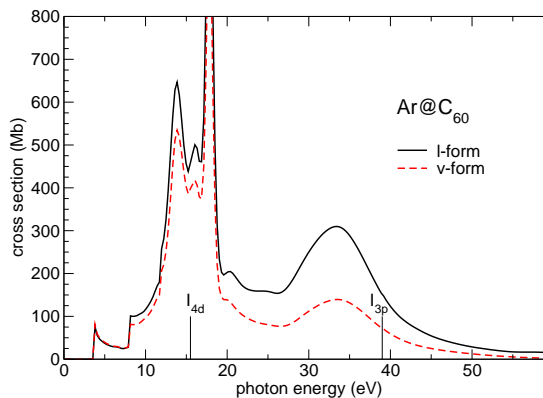
Figure 2: Photoionization cross section for $Ar@C_{60}$ calculated within the HF + RPAE scheme [1].

Related publications in 2010:

1) R.G. Polozkov, A.V. Verkhovtsev,V.K. Ivanov, A.V. Korol and A.V. Solov'yov, *Oscillations in Partial Photoionization Cross Section of Endohedral Noble Gas Fullerenes*, pp. 79-80, Boof of Abstracts of International Conference 'Dynamics of Systems on the Nanoscale (DySoN 2010)' (NRC, Rome, Nov. 16-19, 2010), L. Avaldi, F.A. Gianturco, and A.V. Solov'yov (eds).

2) A.V. Verkhovtsev, R.G. Polozkov, V.K. Ivanov, A.V. Korol and A.V. Solov'yov, *Electronic Structure of Endohedral Fullerenes with Noble Gas Atoms*, pp. 83-84, Boof of Abstracts of International Conference 'Dynamics of Systems on the Nanoscale (DySoN 2010)' (NRC, Rome, Nov. 16-19, 2010), L. Avaldi, F.A. Gianturco, and A.V. Solov'yov (eds).

Quantum correlations in the two–photon decay of heavy helium–like ions

Collaborators: F. Fratini[1,2], A. Surzhykov[1,2], T. Jahrsetz[1,2], M. Tichy[3], A. Buchleitner[3], S. Fritzsche[2,4]

[1] Universität Heidelberg [2] GSI, Darmstadt [3] Universität Freiburg [4] Frankfurt Institute for Advanced Studies

Studies on the two-photon transitions in atomic systems have a long tradition, going back to the 1930's. Originally focused on the decay of light atoms and ions, the interest in these investigations has recently shifted towards the high-Z domain. For instance, a series of experiments were performed recently at the GSI storage ring in order to explore the two-photon decay of helium-like uranium U^{90+} ions [1]. Until now these experiments were restricted to the total and energy-differential rates. Owing to the recent advances in x-ray detector technologies, however, the photon-photon angular and *polarization* correlations are also likely to be observed in the future. Analysis of these correlations will reveal important information on the relativistic, many-body and parity non-conservation phenomena in heavy atomic systems [2].

In this work, we have performed a theoretical analysis of the quantum correlations between the polarization states of two photons emitted in the decay of helium-like ions. Based on the relativistic, second-order perturbation and density matrix theory, detailed calculations have been performed for the degree of *entanglement* (given by the concurrence measure $\mathscr{C}$) for the $1s2s\,^1S_0 \to 1s^2\,^1S_0$ and $1s2p\,^3P_0 \to 1s^2\,^1S_0$ two-photon transitions. For these two transitions in helium–like uranium U^{90+} we display in Fig. 1 the concurrence measure as a function of the opening angle between the photons. The predictions have been obtained for the *energy sharing* parameter $y = E_{\gamma_1}/(E_{\gamma_1} + E_{\gamma_2}) = 1/4$. As seen from the figure, the (degree of) quantum correlations is very sensitive to the decay geometry. In particular, our calculations show that the concurrence of two photons emitted in the $1s2s\,^1S_0 \to 1s^2\,^1S_0$ decay vanishes at the opening angle $\theta = \pi/2$, while it is maximal for the parallel ($\theta = 0$) and back–to–back ($\theta = \pi$) photon emission. This behaviour can be well understood from the conservation of the projection of the total angular momentum of the overall system "ion + two photons". For $\theta = 0$ and π, for example, such a conservation law immediately implies maximally entangled Bell (linear polarization) states $|\Psi_{\theta=0}> = |yy> + |xx>$ and $|\Psi_{\theta=\pi}> = |yy> - |xx>$ and, hence, maximal degree of entanglement, $\mathscr{C} = 1$.

A qualitatively similar behaviour of the concurrence measure can be observed for the $1s2p\,^3P_0 \to 1s^2\,^1S_0$ two-photon transition. However, in contrast to the decay of $^1S_0$ state, the degree of entanglement is not symmetric anymore with respect to the opening angle $\theta = \pi/2$ as caused by the interference between the possible decay channels (see right panel of Fig. 1).
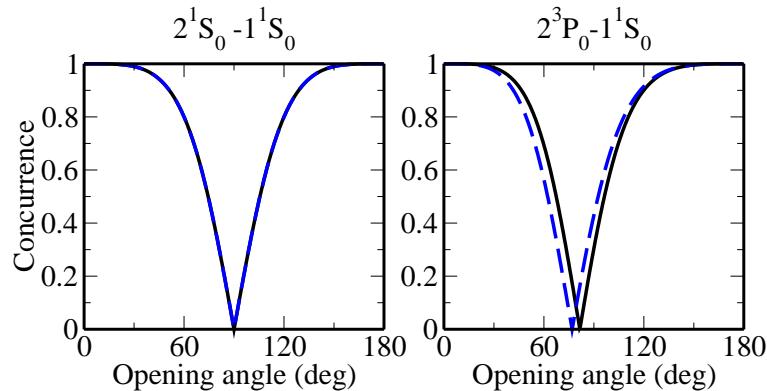
Concurrence of two photons in full relativistic theory (black) and dipole approximation (blue).

Related publications in 2010:
1) S. Trotsenko *et al.*, *Spectral shape of the two-photon decay of the $2\,^1S_0$ state in He-like tin*, Phys. Rev. Lett. 104 (2010) 033001
2) A. Surzhykov, A. Volotka, F. Fratini, J. P. Santos, P. Indelicato, G. Plunien, Th. Stöhlker, S. Fritzsch, *Angular correlations in the two-photon decay of heliumlike heavy ions*, Phys. Rev. A 81 (2010) 042510

Angular correlations in the sequential two-photon double ionisation of noble gases

Collaborators: S. Fritzsche[1,2], A. N. Grum-Grzhimailo[3], E. V. Gryzlova[3], N. M. Kabachnik[3,4]

[1] Frankfurt Institute for Advanced Studies [2] GSI, Darmstadt [3] Moscow State University, Russia [4] Universität Hamburg

Recent experiments with intense ultraviolet (XUV) radiation sources, such as high harmonics or free electrons lasers, opened a new route for studying non-linear processes with atoms and molecules in the XUV regime. Among these processes, the two-photon double ionization (TPDI) has attracted much recent interest since it enables one to explore the transition from a *sequential* towards the *direct* emission of two electrons. While the energies of the emitted electrons are 'sharp' for a sequential photoionization, due to the formation of an intermediate state of the single-ionized atom, the two electrons 'share' continuously the total energy of both photons in the non-sequential or simultaneous TPDI.

Typically, the sequential TPDI remains the *dominant* process at all moderate photon intensities, if the photon energy is larger than the ionization threshold of the singly-charged ion. In order to analyze the angular emission from noble gases, we applied the density matrix and statistical tensor formalism. In particular, expressions were derived for the angular distribution of the first and second photoelectron as measured in non-coincidence experiments. For the second electron, for example, the anisotropy coefficient,

$$\beta_2 = [\beta^{(2)} + \mathscr{A}_{20}(J_i)a_2][1 + \mathscr{A}_{20}(J_i)a_0]^{-1},$$

is different from that for free (i.e. unpolarized) ions, $\beta^{(2)}$, because of the alignment $\mathscr{A}_{20}(J_i)$ of the singly-charged ion that arises after the emission of the first electron. Moreover, since the angular momentum of two photons is absorbed, a second anisotropy parameter β_4 typically occurs that vanishes only for zero alignment of the intermediate state.

A series of Multiconfiguration Hartree- and Dirac-Fock computations have been performed for neon, argon and krypton on the angular distribution and correlation function of the emitted electrons. These angular correlations can be studied experimentally by detecting the angle-resolved electrons in coincidence. In order to separate the effect of true angular correlation from the angular dependence of two consecutive independent photoemissions, we have introduced, calculated and analysed the *true* angular correlation function which arises from the alignment and orientation of the intermediate ionic states [cf. Figure 1 for an example].
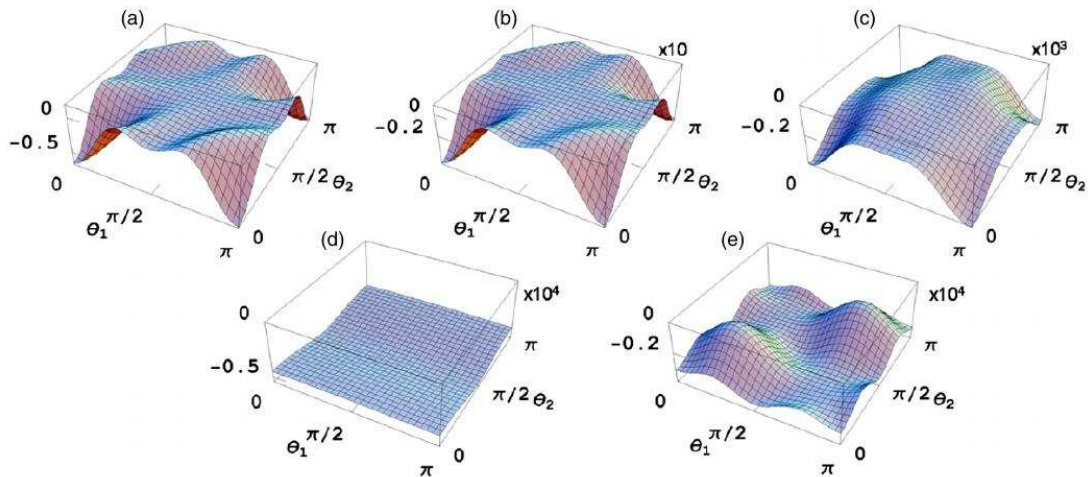
True angular correlations for the sequential TPDI of Kr through the intermediate state ^2P of Kr^+.

Related publications in 2010:

1) E. V. Gryzlova, A. N. Grum-Grzhimailo, S. Fritzsche and N. M. Kabachnik, *Angular correlations between two electrons emitted in the sequential two-photon double ionization of atoms*, J. Phys. B43 (2010) 225602.
2) M. Meyer *et al.*, *Two-photon excitation and relaxation of the $3d - 4d$ resonance in atomic Kr*, Phys. Rev. Lett. 104 (2010) 213001.

4.5 Scientific Computing, Information Technology

The ALICE High Level Trigger - Heavy-Ions and Hardware Acceleration

Collaborators: T. Alt, S. Gorbunov, S.Kalcher, M. Kretz, V. Lindenstruth, A. Masoodi, D. Ram, D. Rohr, O. Smørholm, T. Steinbeck

Recently the new particle accelerator Large Hadron Collider (LHC) has started operation at the European Center for Particle Physics CERN. Initially bunches of protons have been collided followed by lead ions in November 2010. One of the experiments records and analyses data from these collisions is ALICE. Although it also works with proton collisions, it's primary focus is on the research of heavy-ion collisions, in particular the search for a state of matter predicted to have existed shortly after the big-bang, the Quark-Gluon-Plasma. During the collisions large amounts of data are produced by the experiment. Heavy-ion collisions, for example, are expected to be up to 80 MB large at a rate of up to 8 kHz. For these data rates it is not feasible to read out every single collision for storage and analysis. Instead an online selection of the physically most interesting collisions is done and only those are stored. This selection takes place in a hierarchical trigger system, with increasing discrimination of what is considered interesting. The High Level Trigger (HLT) is the last trigger stage and the first system processing the complete data from a collision. From this data the trajectory of every detectable particle passing through the experiment is reconstructed and a decision is made whether the data is to be stored or discarded. In order to process its input data rates of up to 25 GB/s, the HLT consists of a large farm of multi-processor computers. It receives data from the experiment via ca. 250 optical links ending in special interface cards that autonomously copy the data into their host computer's memory. Once inside a computer, a software framework takes over the transport of the data, which is processed and merged successively in a processing pipeline. The HLT has analysed and processed ALICE collision data since the first LHC collisions at the end of 2009 and been in operation throughout 2010. At the end of 2010 also heavy-ions collisions were successfully processed. Here the HLT was the only feasible method of using a live online display for viewing reconstructed collisions in the ALICE main control room and the first heavy-ion collisions have been presented there in fractions of a second after having taken place. A screenshot of one of these reconstructed collisions from the HLT is shown below. During heavy-ion running two special kinds of hardware accelerators have been used succesfully. A co-processor on the interface cards performs the first reconstruction step even before data enters the host computer. In addition, the trajectory determination for the largest detector has been done using normal consumer graphics cards. Both accelerators have shown that they work well with the requirements of such an online system. The HLT itself has shown in 2010 that it is capable of running continuously and of meeting the demands presented by the processing of data from proton and heavy-ion collisions.
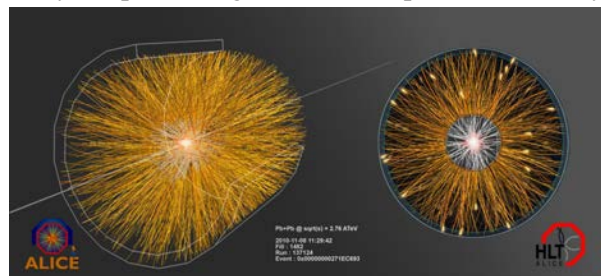
Display of a heavy-ion collision in ALICE.

Related publications in 2010:

1) K.Aamodt et al., *First proton–proton collisions at the LHC as observed with the ALICE detector: measurement of the charged particle pseudorapidity density at sqrt(s) = 900 GeV*, European Physical Journal C - Particles and Fields, Volume 65, Numbers 1-2

2) Kalliopi Kanaki for the ALICE HLT collaboration, *Results from the first p+p runs of the ALICE High Level Trigger at LHC* , Proceedings of the CHEP 2010, Taipeh

3) C. Lara, et al., *Autonomous System Management for the ALICE High-Level-Trigger Cluster using the SysMES Framework*, Proceedings of the CHEP 2010, Taipeh

4) V. Lindenstruth, *Gafikkarten für die Datenflut*, Physik-Journal, Januar 2011

First Collisions with the ALICE TRD Global Tracking Unit

Collaborators: S. Kirsch[1,2], F. Rettig[1], D. Hutter[3], V. Lindenstruth[1]

[1] Frankfurt Institute for Advanced Studies, Frankfurt, Germany

[2] CERN, Geneva, Switzerland

[3] Kirchhoff Institute for Physics, Heidelberg, Germany

Throughout the past year, the Large Hadron Collider at CERN continuously delivered proton-proton and first heavy-ion collisions towards the end of the year. As central component in the ALICE Transition Radiation Detectors (TRD) read-out and trigger system, the Global Tracking Unit (GTU) provided highly reliable read-out operation with the TRD supermodules installed at the experiment. During these collision phases a total of $1.2 \cdot 10^9$ events were recorded yielding more than 130 TBytes of data.

The TRD is designed to provide fast triggers based on the online reconstruction of charged particle tracks within approximately $6.5\,\mu$s after the collision. A total of 1.2 million analog channels are processed by more than 65 500 multi-chip modules to find and parameterize short track segments of particles traversing the TRDs drift chambers. The GTU, a systolic trigger processor of 109 FPGAs arranged in a three-level hierarchy, receives these track segments as well as detector raw data at an aggregate net bandwidth of about 250 GByte/s. In the lowest processing layer the GTU performs a full, three-dimensional online reconstruction of charged particle tracks with transverse momentum $p_t \geq 2\,$GeV in less than $1.6\,\mu$s. Trigger algorithms for various signatures are then applied at the two higher layers.

Starting in mid-2010, the GTU provided online track reconstruction and track-based trigger algorithms for various signatures, like high-p_t e^-, e^-/e^+-pairs as well as jets and cosmic particles (Fig. 1a, 1b).

Besides the developments related to fast triggering, one focus was to improve the highly reliable data transport and implement control logic capable of administering the buffering of multiple events. The approach chosen features a hardware/software co-design with dedicated hardware entities to generate the required control signals. Simultaneously, one of the embedded CPUs supervises the operation of GTU segment and can interact to resolve abnormal, erroneous situations.

(a) Jet event   (b) Triggered cosmic event with tracklets
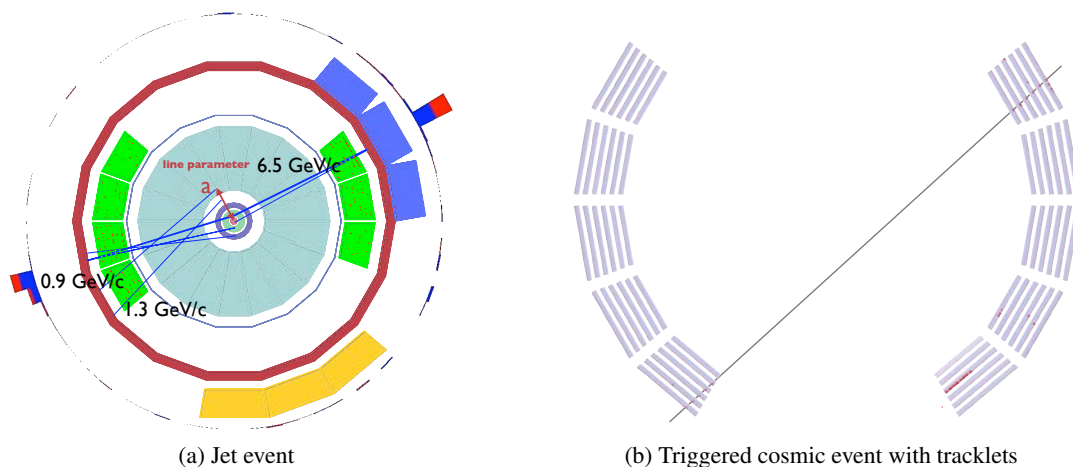
Figure 1: Recorded events, found by the GTU using track-based trigger algorithms. Online calculation of the line parameter a allows for a fast momentum estimation with only 50 ns latency.

Related publications in 2010:

1) S. Kirsch, et al., *An FPGA-based high-speed, low-latency processing system for high-energy physics*, IEEE Proc. Intl. Conf. on Field Programmable Logic and Applications (FPL), Milano, 08-2010 (2010)

2) D. Hutter, *Multi-Event Buffering und HDL-Simulationsframework für die Global Tracking Unit des ALICE-Übergangsstrahlungsdetektors*, Diploma thesis, (2010) 93

SCALUS - SCALing by means of Ubiquitous Storage

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

[1] Frankfurt Institute for Advanced Studies,

For large research facilities such as FAIR scalable mass storage systems are of great significance. The FAIR Tier-0 center alone will be required to handle more than 30 Petabytes of data. Therefore, based on the tremendous need for storage capacity and I/O performance, storage research increasingly gains importance. Over the past years, several trends have considerably changed the design of storage systems, starting from new storage media over the widespread use of storage area networks, up to grid and cloud storage concepts. Furthermore, to achieve cost efficiency, storage systems are increasingly assembled from commodity components. Thus, we are in the middle of an evolution towards a new storage architecture made of many decentralized commodity components with increased processing and communication capabilities, which requires the introduction of new concepts to benefit from the resulting architectural opportunities.

In late 2010 the consortium of the Marie Curie Initial Training Network (MCITN) "SCALing by means of Ubiquitous Storage (SCALUS)" began its research program. SCALUS is an EU funded research project with 11 full partners and further associated partners from 6 european countries. It consists of top European institutes and companies in storage and cluster technology (see below), building a demanding but rewarding interdisciplinary environment for young researchers. The vision of this MCITN is to deliver the foundation for ubiquitous storage systems, which can be scaled in arbitrary directions (capacity, performance, distance, security). It aims at elevating education, research, and development inside the area of storage system research with a focus on cluster, grid, and cloud storage.

Enhanced reliability and fault tolerance, as well as security, are key requirements of new storage architectures. The network partners at the Frankfurt Institute for Advanced Studies aim to advance the utilization of elaborate coding and encryption techniques in distributed storage systems. The main obstacle here is the additional computational overhead that can adversely affect the system's overall performance. To cope with this several approaches are envisioned, including the use of custom field programmable gate arrays (FPGAs), general purpose computing on graphics processing units (GPGPU), upcoming general purpose HPC application coprocessors, and the exploitation of upcoming extensions to the vector instructions set of modern commodity CPUs. The goal is to provide encoding and encryption techniques in a generalized way to several layers of an I/O stack with as little impact on performance as possible through the use of state of the art acceleration methods.

SCALUS Partners:
Frankfurt Institute for Advances Studies (Goethe Universität Frankfurt), Paderborn Center for Parallel Computing, Universität Hamburg, Barcelona Supercomputing Center, University of Durham, INRIA (Institut National de Recherche en Informatique et en Automatique), Foundation for Research and Technology - Hellas Institute of Computer Science, Universidad Politecnica De Madrid, ARMINES - Ecole des Mines de Nantes, XLAB, Fujitsu Technology Solutions GmbH, CERN, Microsoft Research, NEC, SUN.

http://www.scalus.eu/

Research projects by Christos Dimitrakakis

1. Context models on sequences of covers

Collaborators: C. Dimitrakakis[1]

[1] Frankfurt Institute for Advanced Studies

An interesting class of hierarchical statistical models allowing closed form Bayesian inference in a variety of applications are context models. Via a simple construction based on a conditional random walk, we then obtain enables exact, incremental, non-parametric, polynomial-time inference of (conditional) measures. I demonstrate the approach on problems of conditional density estimation, sequence prediction and reinforcement learning in partially observable and continuous spaces.

Related publications in 2010:

1) C. Dimitrakakis, *Context model inference for large or partially observable MDPs*, ICML Workshop on reinforcement learning and search in very large spaces.

2) C. Dimitrakakis, *Context models on sequences of covers*, arXiv:1005.2263, submitted to AAAI 2011.

3) C. Dimitrakakis, *Bayesian variable order Markov models*, In Proceedings of the 13th International Conference on Artificial Intelligence and Statistics (AISTATS), volume 9 of JMLR: W.CP, Chia Laguna Resort, Sardinia, Italy, 2010

2. Preference and prior elicitation and inverse reinforcement learning

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

[1] Frankfurt Institute for Advanced Studies

Preference elicitation is a well-known problem in statistical decision theory. The goal is to determine, whether a given decision maker prefers some events to other events, and if so by how much. Similarly, prior elicitation is the problem of determining prior beliefs of decision maers. They are of relevance to behavioural psychology, where a proper procedure allows more robust experimental conclusions. Rather than examining wether humans are "Bayesian" or not (a non-falsifiable hypothesis) we can instead make conclusions about how reasonable their priors and preferences are.

There are also direct practical applications, such as determining customer preferences. Finally, there are applications in apprenticeship learning and inverse reinforcement learning: By analysing the apparent preferences of an expert while performing a particular task, we may be able to discover behaviours that match or even surpass the performance of the expert in the very same task.

Related publications:

1) A. Rothkopf, C. Dimitrakakis, *Preference elicitation and inverse reinforcement learning* , submitted to AAAI 2011.

2) C. Dimitrakakis, *Falsifying the Bayesian behavioural hypothesis*, submitted to COSYNE 2011.

3. Expected loss analysis of thresholded authentication protocols in noisy conditions

Collaborators: C. Dimitrakakis[1], A. Mitrokotsa[2], S. Vaudenay[2]

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

A number of authentication protocols have been proposed recently, where at least some part of the authentication is performed during a phase, lasting *n* rounds, with no error correction. This requires assigning an acceptable threshold for the number of detected errors. This paper describes a framework enabling an expected

loss analysis for all the protocols in this family. Furthermore, computationally simple methods to obtain nearly optimal value of the threshold, as well as for the number of rounds is suggested. Finally, a method to adaptively select both the number of rounds and the threshold is proposed.

Related publications in 2010:
1) C. Dimitrakakis, A. Mitrokotsa, S. Vaudenay, *Expected loss analysis of thresholded authentication protocols in noisy conditions*, submitted to IEEE Transactions on Information Theory

4. Phoneme and Sentence-Level Ensembles for Speech Recognition

Collaborators: C. Dimitrakakis[1], S. Bengio[2]

[1] Frankfurt Institute for Advanced Studies, [2] Google Inc.

We address the question of whether and how boosting and bagging can be used for speech recognition. In order to do this, we compare two different boosting schemes, one at the phoneme level, and one at the utterance level, with a phoneme level bagging scheme. We control for many parameters and other choices, such as the state inference scheme used. In an unbiased experiment, we clearly show that the gain of boosting methods compared to a single hidden Markov model is in all cases only marginal, while bagging significantly outperforms all other methods. We thus conclude that bagging methods, which have so far been overlooked in favour of boosting, should be examined more closely as a potentially useful ensemble learning technique for speech recognition.

Related publications in 2010:
1) C. Dimitrakakis, S. Bengio, *EURASIP Journal on Audio, Speech and Music Processing*, to appear

e-NMR gLite grid enabled infrastructure

Collaborators: Nuno Loureiro-Ferreira1[1], Tsjerk A. Wassenaar[1], Sjoerd J. de Vries[1], Marc van Dijk[1], Gijs van der Schot[1], Johan van der Zwan[1], Rolf Boelens[1] , Andrea Giachetti[2], Dario Carotenuto[2], Antonio Rosato[2], Ivano Bertini[2], Torsten Herrmann[3], Anurag Bagaria[4,5], Victor Zharavin[4,5], Hendrik R. A. Jonker[4], Peter Güntert[4,5], Harald Schwalbe[4], Wim F. Vranken[6], Stefano Dal Pra[7], Mirco Mazzucato[7], Eric Frizziero[7], Sergio Traldi[7], Marco Verlato[7], Alexandre M. J. J. Bonvin[1]

[1] Bijvoet Center for Biomolecular Research, Faculty of Science, Utrecht University, Utrecht, The Netherlands, [2] Magnetic Resonance Center, University of Florence, Sesto Fiorentino, Italy, [3] University of Lyon, Centre de RMN à Trés Hauts Champs, Villeurbanne, France, [4] Institute of Organic Chemistry and Chemical Biology and Biomolecular Magnetic Resonance Center, Goethe University Frankfurt am Main, [5] Frankfurt Institute for Advanced Studies, [6] European Bioinformatics Institute, Hinxton, Cambridge, United Kingdom, [7] Istituto Nazionale di Fisica Nucleare, Sez. di Padova, Padova, Italy

The e-NMR project is an European e-infrastructure that aims at providing the bio-NMR community with a software platform integrating and streamlining computational approaches necessary for NMR data analysis. The infrastructure is grid enabled with fifteen gLite based partners sharing computational resources. A main focus of the consortium is to provide protocoled services through easy-to-use web interfaces, while retaining sufficient flexibility to handle specific requests by expert users. Various programs relevant for structural biology scientists are grid ported and already available through the e-NMR web portal, including HADDOCK, XPLOR-NIH, CYANA and CS-ROSETTA among others. A general overview of the project current status toward EGEE/EGI integration, as well as brief guidelines on how to become an e-NMR site/user will be considered. With more than 170 registered users, enmr.eu is currently the second largest vir- tual organization in the life sciences. The state of the project can be found on the web page http://www.enmr.eu.
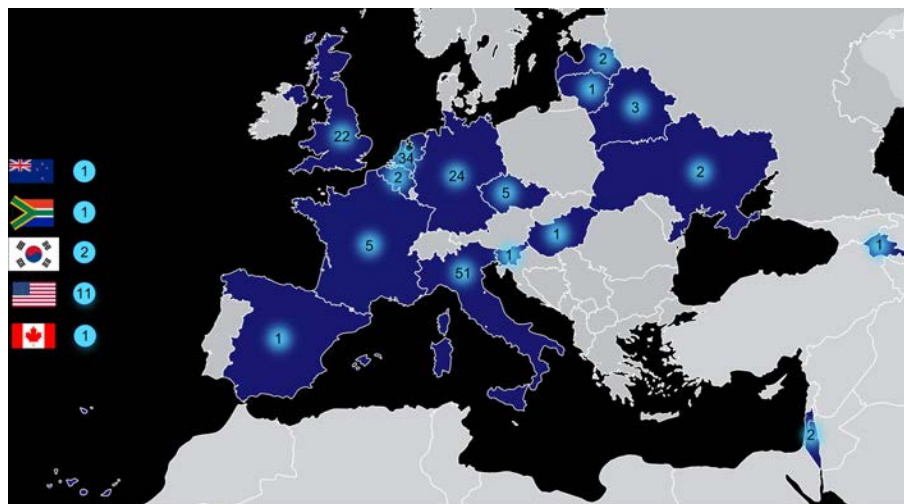
Geographical view of e-NMR users distribution

Related publications in 2010:

1) Loureiro-Ferreira, N., Wassenaar, T. A., de Vries, S. J., van Dijk, M., van der Schot, G., van der Zwan, J., Boelens, R., Giachetti, A., Carotenuto, D., Rosato, A., Bertini, I., Herrmann, T., Bagaria, A., Zharavin, V., Jonker, H. R. A., Güntert, P., Schwalbe, H., Vranken, W. F., Dal Pra, S., Mazzucato, M., Frizziero, E., Traldi, S., Verlato, M. Bonvin, A. M. J. J. *e-NMR gLite grid enabled infrastructure* In IBERGRID 4th Iberian Grid Infrastructure Conference Proceedings (Eds. A. Proença, A. Pina, J. García Tobío and L. Ribeiro), Netbiblo, La Coruña, Spain, (2010) pp. 360-382

5. Talks and Publications

Conference and Seminar Talks by FIAS Members 2010

Victor Begun

– International Workshop 'Statistical Particle Production', Bad Liebenzell, Germany, Apr. 25-28, 2010: *Pion number fluctuations and correlations in the statistical system with fixed isospin*

– International Workshop 'Statistical Particle Production', Bad Liebenzell, Germany, Apr. 25-28, 2010: *Statistical fluctuations and correlations in hadron-resonance gas*

– International Workshop 'Statistical Particle Production', Bad Liebenzell, Germany, Apr. 25-28, 2010: *Modified bag models for the quark gluon plasma equation of state*

– Sixth Workshop on Particle Correlations and Femtoscopy (WPCF2010), Kiev, Ukraine, Sept. 14-18, 2010: *Fluctuations and correlations in pion system with fixed isospin*

Marcus Bleicher

– Symposium on proton-proton interactions, Frankfurt am Main, Feb. 2010: *The UrQMD model*

– International Workshop on High Density Nuclear Matter, Cape Town, South Africa, April 2010: *Hybrid approaches to heavy ion collisions and future perspectives*

– International Workshop on Hot and Cold Baryonic Matter, Budapest, Hungary, Aug. 2010: *Hybrid approaches to heavy ion collisions and future perspectives*

– Critical point and onset of deconfinement, Dubna, Russia, Aug. 2010: *Perspectives in dynamical models of heavy ion reactions*

– Dileptons in Matter, Trento, Italy, Sept. 2010: *Hybrid approaches to heavy ion collisions and future perspectives*

– TORIC Workshop, Villasimius, Italy, Sept. 2010: *Hybrid approaches to heavy ion collisions and future perspectives*

– Public outreach: Two public lectures at the 'Weltmaschine' exhibition, Frankfurt, Jan. 24, 2010: *CERN, Illuminati und Antimaterie*

Alexander Botvina

– Joint SPHERE (Strange Particles in Hadronic Environment Research in Europe) and JSPSMeeting, Prague, Czech Republic, Sept. 4-6, 2010: *Production of hyper-nuclei in reactions induced by relativistic hadrons and heavy-ions*

– Seminar at the Physics Department, Liège University, Belgium, June 4, 2010; *Multifragmentation of nuclei and stellar matter in supernova explosions*

Elena Bratkovskaya

– International Symposium on 'Advances in Nuclear Physics in Our Time', Goa, India, 28 Nov. - 2 Dec., 2010: *Signatures of the strongly interacting QGP in relativistic heavy-ion collisions*

– The 4th International Conference on 'Hard and Electromagnetic Probes of High Energy Nuclear Collisions (Hard Probes 2010)', Eilat, Israel, Oct. 10-15, 2010: *Theoretical view of SPS and RHIC dilepton measurements*

– International Workshop on 'Electromagnetic Probes of Strongly Interacting Matter', ECT Trento, Sept. 13-17, 2010: *Dileptons from off-shell transport*

– 6th International Workshop on 'Critical Point and Onset of Deconfinement' (CPOD), JINR, Dubna, Russia, Aug. 23-29, 2010: *Dynamics of hot and dense nuclear and partonic matter*

– International Advanced School of Theoretical Physics 'Dense QCD phases in Heavy-Ion Collisions' (DM2010), Dubna, Russia, Aug. 21 - Sept. 4, 2010: *Observables of the deconfinement transition*

– International Workshop on 'High Density Nuclear Matter', Cape Town, South Africa, Apr. 6-9, 2010: *Signatures of the strongly interacting QGP in relativistic heavy-ion collisions*

– (Mini-)Symposium on proton-proton interactions, Frankfurt am Main, Germany, Feb. 15-16, 2010: *The (common and unique) characteristics of particle production and nucleon stopping in HSD*

– 26th Winter Workshop on 'Nuclear Dynamics', Ochto Rios, Jamaica, Jan. 2-9, 2010: *'Dileptons from the nonequilibrium Quark-Gluon Plasma'*

– Seminar at University of Münster, June 7, 2010: *Dynamics of hot and dense nuclear and partonic matter*,

Veronika Dick

– European Conference on Nano Films (ECNF 2010) Liège, Belgium, March 22-25, 2010: *Stability of a nanofractal on surface*

Christos Dimitrakakis

– Talk at IDSIA, Lugano, Switzerland, June 2010: *Context MDPs*

– ICML 2010 Workshop reinforcement learning and search in very large spaces, Haifa, Israel, 25 June, 2010: *Context model inference for large or partially observable MDPs*,

Stephan Fritzsche

– Colloqium at Jyväskylä University, Jyväskylä, Finnland, Jan. 22, 2010: *Coherence transfer in the excitation and decay of atoms*

– Seminar at Oulu University, Electron Spectroscopy Group, Oulu, Finnland, Feb. 17, 2010: *Capturing the continuum: Description of 'free electrons' in relativistic calculations*

– Atomic Physics Seminar, Universität Kiel, Jun 22, 2010: *Atomic multi-photon processes in intense FEL radiation*

– Seminar of the Physics Institute, Northwest University Lanzhou, P.R. China, Sep. 13, 2010: *Atomic multi-photon processes in intense FEL radiation*

– Frühjahrstagung der DPG, Atomphysik u.a., Hannover, Mar. 10, 2010: *Sequential two-photon double ionization of atoms in intense FEL radiation*

– Kick-Off Workshop 'Atomic, Molecular and Plasma Physics within PNI', Hamburg, Apr. 16, 2010: *Multi-photon dynamics of atoms and ions in strong fields*

– Symposium on Trends in Experimental Physics: Multi-Particle Coincidence Spectroscopy of Atoms and Molecules, Uppsala, Sweden, May 28, 2010: *Direct and sequential double ionization in intense FEL radiation*

– EMMI Workshop on Physics Prospects at the ESR and HITRAP, Eisenach, June 28, 2010: *Relativistic dynamics of (slow) highly-charged ions*

– 463. WE-Heraeus-Seminar on the Ultra-fast Atomic Physics – Towards the Zeptosecond Regime, Bad Honnef, Aug. 22, 2010: *Relativistic dynamics of high-Z ions in fast ion-electron and ion-atom collisions*

– 15. International Conference on the Physics of Highly Charged Ions (HCI 2010), Shanghai, P.R. China, Sept. 3, 2010: *Relativistic effects in electron-ion and ion-ion collisions*

Peter Güntert

— eNMR: Extend-NMR Workshop on NMR structure calculation - GRID applications and integrated tools, Vilnius, Lithuania, October 4-8, 2010: *CYANA*

— eNMR: Extend-NMR Workshop on NMR structure calculation - GRID applications and integrated tools, Vilnius, Lithuania, October 4-8, 2010: *Automated NOE assignment and structure calculation*

— ICMRBS 2010 Satellite Meeting: Protein Structure Calculation Workshop, Brisbane, Australia, August 30-31, 2010: *Automated NMR protein structure determination with CYANA*

— XXIIIrd International Conference on Magnetic Resonance in Biological Systems (ICMRBS), Cairns, Australia, August 22-27, 2010: *New developments in automated protein structure analysis with CYANA*

— Talk at Intervet Innovation GmbH, Schwabenheim, Germany, August 4, 2010: *Automated NMR protein structure determination*

— Joint EUROMAR 2010 and 17th ISMAR Conference, Florence, Italy, July 4-9, 2010: *Blind-test evaluation of automated protein structure determination by NMR and new developments in CYANA*

— eNMR Extend-NMR Workshop on NMR structure calculation - GRID applications and integrated tools, Vilnius, Lithuania, June 7-11, 2010: *CYANA*

— eNMR: Extend-NMR Workshop on NMR structure calculation - GRID applications and integrated tools, Vilnius, Lithuania, June 7-11, 2010: *Automated NOE assignment and structure calculation*

— Colloquium of the Department of Chemistry, Tokyo Metropolitan University, Tokyo, Japan, May 31, 2010: *New developments in automated protein structure analysis with CYANA*

Vladimir Konchakovski

— International Strong and Electroweak Matter Conference, Montreal, Canada, June 2010: *Dijet attenuation at RHIC with HSD Transport*

— 24th International Nuclear Physics Conference, British Columbia, Vancouver, Canada, 4-9, 2010: *Di-Jet Correlations in Heavy-Ion Collisions at RHIC Energies with the Microscopic HSC Transport Approach*

— 6th International Workshop on Critical Point and Onset of Deconfinement, JINR, Dubna, Russia, Aug. 23-29, 2010: *Dijet attenuation at RHIC with HSD Transport*

— Workshop on Particle Correlations and Femtoscopy, Kiev, Ukraine, Sept. 2010: *Fluctuations and Correlations in the HSD Transport Approach*

Andrey Korol

— Seminar at Institut für Atom- und Molekülphysik, Justig-Liebig-Universität Giessen, Jan. 21, 2010: *On the Photoionization processes of endohedral atoms.*

— Mini-Workshop on Crystalline Undulator and Related Phenomena, Frankfurt am Main, Germany, Feb. 25, 2010: *Polarizational bremsstrahlung*

— XV International Symposium on Small Particles and Inorganic Clusters (ISSPIC XV), Oaxaca City, Mexico, Sept. 19-24, 2010: *Photo-induced processes in fullerenes*

— International Conference 'Dynamics of Systems on the Nanoscale (DySoN 2010)' Rome, Italy, Nov. 16-19, 2010: *Photo-induced processes in fullerenes*

Andriy Kostyuk

— Mini-Workshop on Crystalline Undulator and Related Phenomena Frankfurt am Main, Germany, Feb. 25, 2010: *Monte-Carlo simulations of particles motion in crystalline undulators*

— 4th International Conference on Charged and Neutral Particles Channeling Phenomena Ferrara, Italy, Oct. 3-8, 2010: *Planar channeling of electrons: numerical analysis and theory*

— International Conference 'Dynamics of Systems on the Nanoscale (DySoN 2010)', Rome, Italy, Nov. 16-19, 2010: *Crystalline undulator as a source of coherent radiation*

Olena Linnyk

— Collaboration meeting for the STAR (Solenoidal Tracker at RHIC) experiment at Brookhaven National Laboratory, Upton, USA, Nov. 12-18, 2010: *Dileptons as signals of quark gluon plasma*

— 4th International Conference on Hard and Electromagnetic Probes of High Energy Nuclear Collisions (Hard Probes 2010), Eilat, Israel, Oct. 10-15, 2010: *Dilepton production in the strongly interacting Quark-Gluon-Plasma (sQGP)*

— International workshop Electromagnetic Probes of Strongly Interacting Matter: Status and Future of Low-Mass Lepton-Pair Spectroscopy, Trento, Italy, Sept. 13-17, 2010: *Dileptons from the Quark-Gluon Plasma*

— International Nuclear Physics Conference (INPC 2010), University of British Columbia, Vancouver, Canada, Jul. 4-9, 2010: *Properties of hot quark matter probed by dileptons produced in relativistic heavy-ion collisions*

— International Conference on Strong and Electro-Weak Matter (SEWM 2010), McGill University, Canada, June 29 - July 2, 2010: *Probing QCD matter with dileptons*

— Seminar at Texas A&M University, USA, Nov. 23, 2010: *Dilepton production at SPS and RHIC energies*

Igor Mishustin

— DISCOVERY colloquium at Niels Bohr Institute, Copenhagen, March 24, 2010: *Nuclear fragmentation reactions in basic research and medical applications*

— ALICE group seminar, Niels Bohr Institute, Copenhagen, March 23, 2010: *Hydrodynamic modeling of relativistic heavy-ion collisions*

— ADS Working group meeting, Jülich Forschungszentrum, Sept. 23, 2010: *Optimization of neutron flux and energy deposition in spallation targets*

— ADS Working group meeting, Jülich Forschungszentrum, Sept. 23, 2010: *Non-equilibrium phase transitions in relativistic heavy-ion collisions*

— International Workshop 'Critical Point and Onset of Deconfinement' CPOD 2010, Dubna, Russia, Aug. 22-27, 2010: *Hydrodynamic modeling of deconfinement phase transition in nuclear collisions*

— International Workshop 'Strangeness in nuclei', ECT* Trento, Italy, Oct. 3-7, 2010: *Production of hypernuclei in relativistic heavy-ion collisions,*

— International Conference 'Dynamics of Systems on the Nanoscale' DySoN 2010, NRC, Rome, Italy, Nov. 16-19, 2010: *Monte Carlo simulations of ion-beam cancer therapy: from nuclear fragmentation to microdosimetry*

— International Symposium 'Advances in Nuclear Physics in Our Time', Goa, India, Nov. 28 - Dec. 2, 2010: *Production of heavy and superheavy nuclei in explosive processes*

Rodrigo Negreiros

— COMPstar EOS Workshop, GSI, Darmstadt, Germany: *Invited talk*

— EMMI workshop: Neutron Matter in Astrophysics: From Neutron Stars to the r-Process: *Invited talk*

- Thermal Evolution of Hybrid Stars modeled with an SU(3) non-linear Sigma Model, GSI, Darmstadt, Germany: *Invited talk*

- MODE-SNR-PWN Workshop 'Properties of bare strange stars associated with surface electric fields', Bordeaux, France: *Invited talk*

- Joint Bonn-Munich Pulsar Meeting 'Probing the Inner Composition of Compact Stars', Garching, Germany: *Invited talk*

Piero Nicolini

- COST Action MP0905 'Black holes in a violent universe' – 1st group meeting, Bonn, Germany, 2010: *Black holes in the presence of a minimal length*

- Seminar at the University of Sussex, United Kingdom, Nov. 2010: *Evaporating black holes in the presence of a minimal length*

- Seminar at the University of Waterloo, Math. Dept. Canada, Sept. 2010: *Evaporating black holes in the presence of a minimal length*

- Seminar at the Rochester Astrophysics Institute, USA, Sept. 2010: *Evaporating black holes in the presence of a minimal length*

- Seminar at the University of Waterloo, Phys. Dept., Canada, March 2010: *Evaporating black holes in the presence of a minimal length*

- Seminar at Technische Universität Dortmund, Germany, Feb. 2010: *Evaporating black holes in the presence of a minimal length*

Harri Niemi

- Seminar at the University of Jyväkylä, Jan. 2010: *Precision tests of Israel-Stewart hydrodynamics*

- Hydro Group Meeting, J. W. Goethe University, Apr. 2010: *Viscous hydro vs. transport: shear and diffusion*

- Seminar at the University of Jyväskylä, Oct. 2010: *Heat flow and shear viscosity in ultrarelativistic gases*

- Hydro Group Meeting, J. W. Goethe University, Nov. 2010: *Effects of temperature dependent η/s in heavy-ion collisions*

Dorin Poenaru

- THEORY-1: Scientific Workshop on Nuclear Fission Dynamics and the Emission of Prompt Neutrons and Gamma Rays, Sinaia, Romania, 27-29 Sept. 2010: *Extension of nuclear fission theory to the Coulomb explosion of metallic cluster*

Paul Romatschke

- Seminar at University of Rome, June 2010: *A new look at cold quark matter in compact stars*

- Colloquium at Goethe University Frankfurt, July 2010: *Looking inside Neutron Stars: Microscopic Calculations Confront Observations*

- SEMW 2010, Montreal, Canada, July 2010: *Compact star observations and implications on equation of state*

- TORIC Workshop 2010, Villasimius, Sardinia, Italy, Sept. 26-30, 2010: *Hydro for HIC*

- GSI EMMI day, Nov. 2010: *Theory of relativistic heavy-ion collisions: Achievements and challenges*

- Seminar at TU Vienna, Dec. 2010: *First heavy-ion collisions at the LHC: a 'better than perfect' fluid?*

Constantin Rothkopf

— Gordon Conference on Sensory Coding and the Natural Environment, Bates College, Lewiston, ME, USA, July 25-30, 2010: *Visuomotor behavior in naturalistic virtual environments: from receptive fields to value functions*

— Invited talk with the Vision Group, Psychology department at the University of Minnesota, Minneapolis, USA, April 19, 2010

— Invited talk in the Colloquium series of the psychology department at the University of Giessen, Giessen, Germany, Jan. 20, 2010

Chihiro Sasaki

— Excited QCD, Tatra National Park, Slovakia, Jan. 31-Feb. 6, 2010: *The phase structure of dense QCD from chiral models* (invited talk)

— New Frontiers in QCD 2010 'Exotic Hadron Systems and Dense Matter', YITP Kyoto, Japan, March 9, 2010; *The phase structure of dense QCD from chiral models*

— CBM Workshop on on hot and dense nuclear matter, GSI Darmstadt, April 14, 2010: *Thermodynamics of dense baryonic matter in effective field theories* (invited talk)

— International Workshop on 'Extreme QCD 2010', Physikzentrum Bad Honnef, Germany, June 21-23, 2010: *Thermodynamics of dense hadronic matter in chiral models* (invited talk)

— ECT*-EMMI International Workshop on 'Chiral Symmetry and Confinement in Cold, Dense Quark Matter', European Centre for Theoretical Studies in Nuclear and Related Areas (ECT*), Trento, Italy, July 19 - 23, 2010: *Thermodynamics of dense hadronic matter in chiral models* (invited talk)

— 6th International Workshop on Critical Point and Onset of Deconfinement, Dubna, Russia, Aug. 23-29, 2010; *Thermodynamics of dense hadronic matter in a parity doublet model* (plenary talk)

— The first heavy ion collisions at the LHC, CERN, Aug. 30 - Sep. 4, 2010: *Trace anomaly, chiral symmetry breaking and parity doubled nucleons*

— 3rd Asian Triangle Heavy-Ion Conference (ATHIC), Wuhan, China, Oct. 17-20, 2010: *Problems and challenges in hadron physics - from the perspective of chiral approaches* (invited lecture).

— Seminar at Johann Wolfgang Goethe-Universität, Frankfurt, May 19, 2010; *Phases of dense QCD from chiral thermodynamics*

— Seminar at Seoul National University, Seoul, Korea, July 30, 2010: *Problems and challenges in hadron physics*

— Seminar at Hanyang University, Korea, Oct. 28, 2010 *Selected issues on parity doubled nucleons*

— Seminar at Nagoya University, Japan, Nov. 2, 2010: *Selected issues on parity doubled nucleons*

— Seminar at Chiba University, Chiba, Japan, Dec. 1, 2010: *Problems and challenges in hadron physics*

Christian Schmidt

— Workshop on 'Strong Interactions in the 21st Century', Tata Institute of Fundamental Research, Mumbai, India, Feb. 10-12, 2010: *Generalized hadronic susceptibilities and critical behavior of QCD at zero and nonzero density*

— Workshop on 'New Frontiers in QCD', Kyoto, Japan, March 1-19, 2010: *Critical behavior of baryon number fluctuations at zero and nonzero density*

— CBM Physics Workshop, GSI, Darmstadt, Germany, Apr. 14, 2010: *Recent lattice results on QCD thermodynamics*

- 'Lattice 2010', Villasimius, Italy, June 14-19, 2010: *On the universal O(N) scaling behavior of (2+1)-flavor QCD*

- INT Program 10-2a: 'Quantifying the Properties of Hot QCD Matter', Seattle, WA, USA, May 24-July 16, 2010: *Lattice QCD at nonzero density*

- International conference on 'Quark confinement and the hadron spectrum IX', Universidad Complutense de Madrid, Spain, Sept. 3, 2010: *Chiral and deconfining aspects of the QCD transition*

- Workshop on 'Lattice QCD confronts experiments', Japanese-German Seminar 2010, Mishima, Japan, November 4-6, 2010: *Hadronic fluctuations at freeze-out*

- Workshop on 'Nonperturbative Aspects of QCD at Finite Temperature and Density', Tsukuba, Japan, November 8-9, 2010: *Hadronic fluctuations at freeze-out*

Stefan Schramm

- XLVIII International Winter Meeting on Nuclear Physics, Bormio 2010: *Phase structure of strongly interacting matter and results for heavy-ion collisions and neutron stars*

- Modeling of the Parton-Hadron Phase Transition, Villasimius 2010: *Hot and dense matter and the phase transition in quark-hadron approaches*

- Symposium on Advances in Nuclear Physics in Our Time, Goa 2010: *Nuclear matter, nuclei, and neutron stars in hadron and quark-hadron models*

- 6th International Conference on Physics and Astrophysics of Quark Gluon Plasma, Goa 2010: *Hot and dense matter in quark-hadron models*

Emanuele Scifoni

- International Conference 'Dynamics of Systems on the Nanoscale (DySoN 2010)' Rome, Italy, Nov. 16-19, 2010: *Radial dose distribution around an ion beam track on the nanoscale.*

Andrey Solov'yov

- Talk at INF Initiative III: Building up the Israel Community on Nanofilms, Technion, Haifa, Israel, May 2010: *Virtual Institute of Nano Films*

- Talk at VINF Training school, Technion, Haifa, Israel, May 2010: *Formation and fragmentation of fractals on a surface*

- Talk at COST Office, COST Domain Committee, Brussels, Belgium, Feb. 20, 2010: *Nano-scale insights into Ion Beam Cancer Therapy*

- XVII Symposium on Atomic, Cluster and Surface Physics, Obergurgl, Austria, Jan. 24-29, 2010: *Nanoparticles on a surface: atomistic Approach for structure, dynamics and pattern formation*

- Mini-Workshop on Crystalline Undulator and Related Phenomena, Frankfurt am Main, Germany, Feb. 25, 2010: *Gamma-Laser.*

- Theory of Atomic and Molecular Clusters (TAMC VI), Mexico City, Mexico, June 13-17, 2010: *Nanoparticles dynamics on surface: fractal pattern formation and fragmentation*

- 7th International Conference on 'Radiation Damage in Biomolecular Systems (RADAM 2010)', Madrid, Spain, June 30 - July 4, 2010, *Multiscale approach to radiation damage induced by ion beams: current status and perspectives*

- International Conference 'Dubna-Nano2010', Dubna, Russia, July 5-10 July, 2010: *Nanoparticles dynamics on a surface: fractal pattern formation and fragmentation*

- 7th Int. Conference on Atomic a Molecular Data and Their Applications, Vilnus, Lithuania, Sept. 21-24, 2010: *Atomic data needs for radiation damage modelling underlying radiotherapy*

- 4th International Conference on Charged and Neutral Particles Channeling Phenomena, Ferrara, Italy, Oct. 3-8, 2010 *Crystalline undulator based laser: Recent theoretical advances*

- International Conference 'Dynamics of Systems on the Nanoscale (DySoN 2010)', Rome, Italy, Nov. 16-19, 2010: *Opening DySoN 2010.*

- International Symposium 'Advances in Nuclear Physics in our time', Goa, India, Nov. 2010

Ilya Solov'yov

- International Conference 'Dynamics of Systems on the Nanoscale (DySoN 2010)' Rome, Italy, Nov. 16-19, 2010. *Nanoparticles Dynamics on a Surface: Fractal Pattern Formation and Fragmentation*

- European Conference on Nano Films (ECNF 2010), Liège, Belgium, 22-25 March 2010, *Uncovering a preferential growth of C_{60}-based nanowires and carbon nanotubes*

Giorgio Torrieri

- Summer school 'Dense QCD phases in heavy ion collisions', Dubna, Russia, Aug. 21 - Sept. 4: *Course on hydrodynamics*

- CPOD 2010 - Critical Point and the Onset of Deconfinement, Dubna, Russia, Aug. 23-29, 2010: *Invited talk*

- EMMI Workshop 'Quarkonium and deconfined matter in the LHC era', Martina Franca, Italy, June 16-18, 2010: *Invited talk*

- International Workshop on Hot and Cold Baryonic Matter HCBM2010, Budapest, Hungary, Aug. 15-20, 2010: *Invited talk*

- BEACH 2010 - IX International Conference on Hyperons, Charm and Beauty Hadrons, Perugia, June 21-26, 2010: *Plenary talk*

- International Workshop 'Statistical Particle Production', Bad Liebenzell, Germany, Apr. 25-28, 2010: *Statistical particle production: Beyond the first moment* (Invited talk)

- Quantifying the properties of hot QCD matter, INT summer institute, Seattle, Washington: *Invited tal*

- Seminar, Nuclear physics group, Iowa State University, April 23, 2010

- Seminar, Particle theory group, University of Connecticut, Storrs, April 19, 2010

- Seminar, Theory group, Brookhaven National Laboratory, April 9, 2010

- Seminar, Pontificia Universidad Catlica de Chile, Santiago, Chile, January 12, 2010

Jochen Triesch

- Seminar at Münster University, Germany, Jan. 12, 2010: *How is Working Memory Working?*

- Seminar at Bielefeld University, Germany, Jan. 27, 2010: *How is Working Memory Working?*

- International Workshop 'Computational and Systems Neuroscience' COSYNE2010, Snowbird, Utah, USA, March 1 - 2, 2010: *Unsupervised Learning in Recurrent Networks*

- Workshop 'Heidelberger Bildverarbeitungssymposium' Frankfurt, Germany, March 9, 2010: *Einführung und Vorstellung des Bernstein Fokus: Neurotechnologie*

- International Workshop 'Working Memory and Executive Control' Weizmann Institute, Rehovot, Israel, March 23 - 24, 2010: *Towards Developing a Working Memory with Reward-Modulated STDP*

- Public evening lecture at the FIAS Forum, Frankfurt, April 15, 2010: *Knnen wir unseren Augen trauen? Was uns Wahrnehmungsfehler ber das Gehirn verraten*

– Workshop 'Ringberg Symposium' Castle Ringberg, Tegernsee, Germany, June 6 - 9, 2010: *Unsupervised Learning in Recurrent Networks*

– Popular science talk for law firm 'Luther', June 10, 2010: *Können wir unseren Augen trauen? Was uns Wahrnehmungsfehler über das Gehirn verraten*

– Popular science talk at local high school 'Ernst Reuter Schule' August 26, 2010: *Können wir unseren Augen trauen? Wie unser Gehirn die Wirklichkeit sieht*

– International Workshop of EU-project 'IM-CLeVeR' Univ. of Ulster, UK, November 9 - 11, 2010: *Some Thoughts on Novelty Detection*

– International Workshop of EU-project 'IM-CLeVeR' Univ. of Ulster, UK, November 9 - 11, 2010: *Visual Processing at FIAS*

– Seminar at Max-Planck Institute for Mathematics in the Sciences, Leipzig, Germany, November 8, 2010: *Learning in the brain: more than meets the synapse*

Thomas Weisswange

– Talk at Honda Research Institute Europe, Offenbach, Germany. Aug. 26, 2010: *Bayesian cue integration as a developmental outcome of reward mediated learning*

Alexander Yakubovich

– European Conference on Nano Films (ECNF 2010), Liège, Belgium, March 22-25, 2010: *On phase transitions in finite systems*

– International Conference 'Dynamics of Systems on the Nanoscale (DySoN 2010)' Rome, Italy, Nov. 16-19, 2010: *Temperature Driven Nanoscale Conformational Transitions in Biomolecular Systemse*

FIAS Conference Abstracts and Posters 2010

Bernstein Conference on Computational Neuroscience

27 Sep. - 1 Oct. 2010, Berlin, Germany

- J. Bornschein, M. Henniges, G. Puertas, J. Eggert, and J. Lücke, *Binary Hidden Variables and Sparse Sensory Coding*, Front. Comput. Neurosci. Conference Abstract, doi:10.3389/conf.fncom.2010.51.00114

- Z. Dai and J. Lücke, *A Probabilistic Generative Approach to Invariant Visual Inference and Learning*, Front. Comput. Neurosci. Conference Abstract, doi:10.3389/conf.fncom.2010.51.00121

- F. Gerhard, G. Pipa, and W. Gerstner, *Estimating small-world topology of neural networks from multi-electrode recordings*, Front. Comput. Neurosci. Conference Abstract, doi:10.3389/conf.fncom.2010.51.00088

- J. Jitsev and C. von der Malsburg, *Self-generated off-line reprocessing in a recurrent hierarchical memory network and its functional consequences*, doi:10.3389/conf.fncom.2010.51.00097

- Daniel Krieg, Africa Perianez, and Jochen Triesch, *An objective function for STDP: increasing the separability in self-organized recurrent neural networks*, doi:10.3389/conf.fncom.2010.51.00010

- S. Saeb, C. Weber, and J. Triesch, *Learning coordinated eye and head movements: unifying principles and architectures*, Front. Comput. Neurosci. Conference Abstract, doi:10.3389/conf.fncom.2010.51.00065

- H. Toutounji, C. A. Rothkopf, and J. Triesch, *Learning hierarchical controllers through reinforcement learning*, Front. Comput. Neurosci. Conference Abstract, doi:10.3389/conf.fncom.2010.51.00017

Computational and Systems Neuroscience (COSYNE2010)

25 - 28 Feb. 2010, Salt Lake City, Utah, USA

- O. Aladini, C. A. Rothkopf, and J. Triesch, *Grasping image statistics*, Front. Neurosci. Conference Abstract, doi:10.3389/conf.fnins.2010.03.00049

- A. Lazar, G. Pipa, and J. Triesch, *Spontaneous Activity in a Self-Organizing Recurrent Network Reflects Prior Learning*, Front. Neurosci. Conference Abstract, doi:10.3389/conf.fnins.2010.03.00336

- C. Savin and J. Triesch, *Structural plasticity improves stimulus encoding in a working memory model*, Front. Neurosci. Conference Abstract, doi:10.3389/conf.fnins.2010.03.00231

- P. Schrater and C. A. Rothkopf, *Discounting as task termination, and its implications*, Front. Comput. Neurosci. Conference Abstract, doi:10.3389/conf.fnins.2010.03.00135

- Thomas H. Weisswange, Constantin Rothkopf, Tobias Rodemann, and Jochen Triesch, *Model averaging as a developmental outcome of reinforcement learning*, Front. Neurosci. Conference Abstract, doi:10.3389/conf.fnins.2010.03.00245

NIPS 2010 Workshop on Learning on Cores, Clusters and Clouds LCCC

11 Dec. 2010, Whistler, British Columbia, Canada

- J. Bornschein, Z. Dai, and J. Lücke, *Approximate EM Learning on Large Computer Clusters*

NIPS 2010 Workshop on Learning and Planning from Batch Time Series Data

11 Dec. 2010, Whistler, British Columbia, Canada

– J. A. Shelton, M. B. Blaschko, A. Gretton, J. Müller, E. Fischer, and A. Bartels, *Similarities in resting state and feature-driven activity: Non-parametric evaluation of human fMRI*

NIPS 2010 Workshop 'Women in Machine Learning WiML 2010'

6 Dec. 2010, Vancouver, Canada

– J. A. Shelton, M. B. Blaschko, and A. Bartels, *Augmentation of fMRI Data Analysis using Resting State Activity and Semi-supervised Canonical Correlation Analysis*

Nineteenth Annual Computational Neuroscience Meeting: CNS*2010

24 - 30 July 2010, San Antonio, Texas, USA.

– Felipe Gerhard, Robert Haslinger, and Gordon Pipa, *Goodness-of-fit tests for neural population models: the multivariate time-rescaling theorem*, BMC Neuroscience 11 (Suppl. 1) (2010) 46

Society for Neuroscience 40th annual meeting (SfN2010

13 - 17 Nov. 2010, San Diego, CA, USA

– O. F. Jurjut, D. Nikolić, W. Singer, C. Weber, and R. C. Muresan, *Quantifying the stimulus-specificity and time-locking of spatiotemporal spike patterns*, Poster:505.4/LLL16

– A. Lazar, G. Pipa, J. Triesch, *Learning Bayesian priors in a recurrent network with STDP*

– Raul Vicente, Belén Sancristóbal, Jordi Garcia-Ojalvo, and Gordon Pipa, *Neuronal oscillations improve the performance of reservoir computing in memory tasks*

Computations, Decisions and Movement

19 - 22 May 2010, Rauischholzhausen, Germany

– Constantin Rothkopf and Paul Schrater, *Discounting as probability of task termination in sequential decision problems*, Front. Comput. Neurosci. Conference Abstract, doi:10.3389/conf.fnins.2010.01.00019

XVIIth Biennial International Conference on Infant Studies

10 - 14 March 2010, Baltimore, Maryland, USA

– Q. Wang and J. Triesch, *A Model of the Familiarity-to-Novelty-Shift in Infant Habituation*

– A. Franz and J. Triesch, *A Computational Model of the Development of Visual Expectation in Infancy*

Visual Neuroscience – from Spikes to Awareness

29 Aug. - 10 Sept. 2010, Rauischholzhausen, Germany.

– L. Scocchia, G. M. Cicchini, and J. Triesch, *Orientation discrimination under memory and perceptual loads: the effect of task difficulty and similarity*

10th annual meeting of the Vision Science Society

7 - 12 May 2010, Naples, Florida, USA

− B. Sullivan, C. Rothkopf, M. M. Hayhoe, and D. H. Ballard *Modeling gaze priorities in driving*, Front. Neurosci.

Rhine-Main Neuroscience Network 1st Biennial Meeting

24 - 26 Nov. 2010, Oberwesel, Germany

− T. H. Weisswange,C. A. Rothkopf, T. Rodemann, and J.Triesch, *Model averaging as a developmental outcome of reinforcement learning*

− A. Perianez, *Separability Increased in Self-Organized Recurrent Neural Networks*

− C. A. Rothkopf, T. H. Weisswange, and J. Triesch, *A Walk through the Woods Explains the Space Variant Oblique Effect*

− C. Keck, J. Bouecke, and J. Lücke, *Learning of Lateral Connections for Representational Invariant Recognition*

− D. Krieg, *An Objective Function for STDP: Increasing the Separability in Self-Organized Recurrent Neural Networks*

− M. Henniges, G. Puertas, J. Bornschein, J. Eggert, and J. Lücke, *Binary Sparse Code*

33rd European Conference on Visual Perception ECVP'10

22 - 26 Aug. 2010, Lausanne, Switzerland

− L. Scocchia, G. M. Cicchini, and J. Triesch, *What's up? Orientation discrimination while holding orientations in memory*, Perception 39, ECVP Abstract Supplement, p. 38

2nd Biennial Schizophrenia International Research Conference

10 - 14 April 2010, Florence, Italy

− Sharmili Sritharan, Christine Grützner, Anna Rotarska-Jagiela, Wolf Singer, and Peter J. Uhlhaas, *Cortical thickness deficits and gamma band oscilations in schizophrenia*, Schizophrenia Research 117 (2010) 367

− P. Uhlhaas, C. Grützner, M. Wibral, M. Leweke, and W. Singer, *High-frequency gamma-band oscillations during perceptual organisation in chronic and first-episode schizophrenia patients*, Schizophrenia Research 117 (2010) 481

HRI European Graduate Network Symposium 2010

20 - 22 Sept. 2010, Offenbach, Germany

− T. H. Weisswange, C. A. Rothkopf, T. Rodemann, and J. Triesch, *Model averaging as a developmental outcome of reinforcement learning*

13th International Conference on Artificial Intelligence and Statistics (AISTATS)

13 - 15 May 2010, Chia Laguna Resort, Sardinia, Italy

− A. Lazar, *Bayesian variable order Markov models*

Neuroinformatics 2010, 3rd INCF Congress of Neuroinformatics

10 Aug. - 1 Sept. 2010, Kobe, Japan

– Gordon Pipa, Marta Castellano, Raul Vicente, and Bertram Scheller, *Temporal Structure of Incoming Spike Trains Modulate Structure Formation by STDP*, Poster P28

Semiconductor Lasers and Laser Dynamics IV

12 - 16 April 2010, Brussels, Belgium

– O. D'Huys, R. Vicente, and J. Danckaert, *Synchronization and symmetry breaking of delay-coupled oscillators: on the role of phase and amplitude instabilities*, Proc. SPIE 7720, 772023 (2010)

International Conference Dynamics of Systems on the Nanoscale (DySoN 2010)

16 - 19 Nov. 2010, Rome, Italy

– V. V. Dick, I. A. Solov'yov, P. V. Nikolaev, and A. V. Solov'yov, *Towards Understanding the Mechanisms of Silver Nanoparticles Diffusion of Graphene*, Book of Abstracts p. 77

– A. V. Korol and A. V. Solov'yov, *Photo-Induced Processes in Fullerenes*, Book of Abstracts p. 54

– A. Kostyuk, A. Korol, A. Solov'yov, and W. Greiner, *Planar Channeling of Electrons: Numerical Analysis and Theory*, Book of Abstracts p. 26

– A. Kostyuk, A. V. Korol, A. Solov'yov, and W. Greiner, *Crystalline undulator as a Source of Coherent Radiation*, Book of Abstracts p. 60

– A. Kostyuk, A. Korol, A. Solov'yov, and W. Greiner, *A new Monte-Carlo Code for Channeling Simulation*, Book of Abstracts p. 63

– R. G. Polozkov, A. V. Verkhovtsev, V. K. Ivanov, A. V. Korol, and A. V. Solov'yov, *Oscillations in Partial Photoionization Cross Section of Endohedral Noble Gas Fullerenes*, Book of Abstracts p 79

– R. G. Polozkov, V. K. Ivanov, A. V. Korol, and A. V. Solov'yov, *Metal Cluster Anions: Photoionization Cross Section and Photoelectron Angular Distribution*, Book of Abstracts p. 52

– E. Scifoni, E. Surdutovich, and A. V. Solov'yov, *Radial Dose Distribution around an Ion Beam Track on the Nanoscale*, Book of Abstracts p. 43

– I. A. Solov'yov, V. V. Dick, and A. V. Solov'yov, *Criteria of Nanoscale Surface Pattern Formation*, Book of Abstracs p. 75,

– I. A. Solov'yov, V. V. Dick, and A. V. Solov'yov, *Nanoparticles on a Surface: Atomistic Approach for Structure, Dynamics and Pattern Formation*, Book of Abstracs p. 50

– I. A. Solov'yov, P. V. Nikolaev, A. V. Yakubovich, V. V. Dick, and A. V. Solov'yov, *MBN Explorer – a Flexible Program for Simulating Molecular and Nanostructured Materials*, Book of Abstracs p. 85

– E. Surdutovich and A. V. Solov'yov, *Nanoscale Transport Phenomena and Radiation Damage Induced by Ions*, Book of Abstracs p. 42

– A. V. Verkhovtsev, R. G. Polozkov, V. K. Ivanov, A. V. Korol, and A. V. Solov'yov, *Electronic structure of endohedral fullerenes with noble gas atoms*, Book of Abstracts p. 83

– S. N. Volkov, E. Paramonova, A. V. Yakubovich, and A. V. Solov'yov, *Micromechanics of DNA Unzipping*, Book of Abstracs p. 81

– A. Yakubovich, E. Surdutovich, W. Greiner, and A. V. Solov'yov, *Temperature Driven Nanoscale Conformational Transitions in Biomolecular Systems*, Book of Abstracs p. 45

European Conference on Nano Films (ECNF 2010)

22 - 25 March 2010, Liège, Belgium

− V. V. Dick, I. A. Solov'yov, and A. V. Solov'yov, *Stability of a nanofractal on surface*, Book of Abstracts p. 113

− A. V. Solov'yov, *Nanoparticles on a surface: Atomistic approach for structure, dynamics and pattern formation*, Book of Abstracts p. 120

− I. A. Solov'yov, J. Geng, A. V. Solov'yov, and B. F. G. Johnson, *Uncovering a preferential growth C_{60}−based nanowires and of carbon nanotubes*, Book of Abstracts p. 121

− A. V. Yakubovich, A. Hussien, A. V. Solov'yov, and W. Greiner, *On phase transitions in finite systems*, Book of Abstracts p. 123

XVIIth Symposium on Atomic, Cluster and Surface Physics

24 - 29 January 2010, Obergurgl, Austria

− V. V. Dick, I. A. Solov'yov, and A. V. Solov'yov, *Theoretical study of nanofractal stability on the surface*

− A. Hussien, A. V. Yakubovich, A. V. Solov'yov, and W. Greiner, *Thermodynamics of the Carbon Gas-Fullerene Transition*

− A. V. Korol and A. V. Solov'yov, *Confinement Resonances in the Photoionization of Endohedral Atoms: Myth or Reality*

− I. A. Solov'yov, J. Geng, A. V. Solov'yov, and B. F. G. Johnson, *Understanding of the Formation Process of Exceptionally Long Fullerene-Based Nanowires*

European Conference on Atoms Molecules and Photons (ECAMP10)

4 - 9 July 2010, Salamanca, Spain

− V. V. Dick, I. A. Solov'yov, and A. V. Solov'yov, *Theoretical study of nanofractal stability on the surface*

− A. Kostyuk, A. Korol, A. Solov'yov, and W. Greiner, *Crystalline Undulator as a Source of Coherent Radiation*

− P. V. Nikolaev, I. A. Solov'yov, V. V. Dick, A. V. Yakubovich, and A. V. Solov'yov, *MBN Explorer – a flexible program for simulating molecular and nanostructured materials*

− E. Scifoni, A. V. Solov'yov, and E. Surdutovich, *Electron production and radial dose distribution from energetic ions in liquid water*

− I. A. Solov'yov, J. Geng, A. V. Solov'yov, and B. F. G. Johnson, *Uncovering a Solvent-Controlled Preferential Growth of Buckminsterfullerene (C_{60}) Nanowires*

− A. V. Yakubovich, A. V. Solov'yov, and W. Greiner, *Statistical mechanics of protein folding in water environment*

7th International Conference on Radiation Damage in Biomolecular Systems (RADAM 2010)

30 June - 4 July 2010, Madrid, Spain.

− E. Scifoni, E. Surdutovich, and A. V. Solov'yov, *Radial dose distribution for energetic carbon ions in liquid water*, Book of Abstracts p. 90

− A. V. Solov'yov and E. Surdutovich, *Multiscale approach to radiation damage induced by ion beams: current status and perspectives*, Book of Abstracts p. 16

− E. Surdutovich and A. V. Solov'yov, *Investigations of DNA damage by ion beams*, Book of Abstracts p. 96

XVth International Symposium on Small Particles and Inorganic Clusters (ISSPIC XV)

19 - 24 Sept. 2010, Oaxaca City, Mexico

− V. V. Dick, I. A. Solov'yov, and A. V. Solov'yov, *Formation and fragmentation of fractals on surface*

− A. Korol, A. V. Solov'yov, R. G. Polozkov, and V. K. Ivanov, *Photo-induced Processes in Metallic Clusters and Fullerenes*, Book of Abstracts p. 15

− P. V. Nikolaev, I. A. Solov'yov, V. V. Dick, and A. V. Solov'yov, *A universal computer tool for simulating molecular and nanostructured materials*

International Conference on Theoretical Physics DUBNA-NANO2010

5 - 10 July 2010, Dubna, Russia

− Veronika V. Dick, Ilia A. Solov'yov, and Andrey V. Solov'yov, *Nanoparticles dynamics on a surface: Fractal pattern formation and fragmentation*, Book of Abstracts p. 149

4th International Conference on Charged and Neutral Particles Channeling Phenomena

3 - 8 October 2010, Ferrara, Italy

− A. Korol, A. Kostyuk, A. Solov'yov, and W. Greiner, *Computer Modeling of MAMI Experiment: Radiation Spectra*, Book of Abstracts p. 66

− A. Kostyuk, A. Korol, A. Solov'yov, and W. Greiner, *A new Monte-Carlo Code for Channeling Simulation* Book of Abstracts p. 63

− A. Kostyuk, A. Korol, A. Solov'yov, and W. Greiner, *Crystalline Undulator as a Source of Coherent Radiation*, Book of Abstracts p. 64

− A. Kostyuk, A. Korol, A. Solov'yov, and W. Greiner, *Planar Channeling of Electrons: Numerical Analysis and Theory*, Book of Abstracts p. 26

− A. Solov'yov, A. Kostyuk, A. Korol, and W. Greiner, *Crystalline Undulator Based Laser: Recent Theoretical Advances*, Book of Abstracts p. 32

International Conference on Atomic and Molecular Data and their Applications ICAMDATA 7

21 - 24 Sept. 2010, Vilnius, Lithuania

− A. V. Solov'yov and E. Surdutovich, *Atomic and molecular data needs for radiation damage modeling underlying radiotherapy*

Zakopane Conference on Nuclear Physics 'Extremes of the Nuclear Landscape"

30 Aug. - 5 Sept. 2010, Zakopane, Poland

− N. Buyukcizmeci, F. Bulut, M. Erdogan, H. Imal, and R. Ogul, A. S. Botvina, I. N. Mishustin, W. Trautmann, *Investigating the isotopic effects in nuclear fragmentation*, Acta Physica Polonica B3 (2011) 697

International Conference on 'Hard and Electromagnetic, Probes of High Energy Nuclear Collisions

10 - 15 Oct. 2010, Eilat, Israel

– V.P. Konchakovski, *Jets correlations in heavy-ion collisions at RHIC energies within the microscopic HSD transport approach*

Experimental signatures for Quantum Gravity

Stockholm, Sweden

– B. Niedner, M. Sprenger, P. Nicolini, M. Bleicher, and L. Modesto, *Fractal dimensions and modified neutrino oscillations from a minimal length*

International Workshop 'Hot & Cold Baryonic Matter 2010'

15-20 Aug. 2010, Budapest, Hungary

– Vitalii Ozvenchuk, *Dynamical equilibration of the strongly interacting parton-hadron matter*

Critical Point and Onset of Deconfinement

23 - 29 Aug. 2010, Dubna, Russia

– Vitalii Ozvenchuk, *Dynamical equilibration of the strongly interacting parton-hadron matter*

461. Wilhelm and Else Heraeus Seminar "Extreme QCD 2010"

21 - 23 June 2010, Bad Honnef, Germany

– Veronica Dexheimer, *A novel approach to modeling hybrid stars*
– Nan Su, *Reorganizing the Yang-Mills thermodynamics at intermediate coupling*

Workshop for Future Challenges in Tracking and Trigger Concepts

7 - 11 June 2010, GSI, Darmstadt, Germany

– Matthias Bach *SIMT Kalman Filter High throughput track fitting*
– David Rohr *ALICE TPC Online Tracking on GPU*

Cumulative listing of journal articles and conference proceedings published in the year 2010 with at least one author quoting the FIAS affiliation. The listing also displays papers which have not (yet) been published in print, but are publicly available on a preprint server. Conference abstracts or posters are not included.

FIAS Publications 2010

[1] K. Aamodt and others (ALICE collaboration), "Alignment of the ALICE Inner Tracking System with cosmic-ray tracks," *J. Instrum.* **5** (2010) P03003, `arXiv:1001.0502` `[physics.ins-det]`.

[2] 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." 2010. `arXiv:1012.1657 [nucl-ex]`.

[3] K. Aamodt and others (ALICE collaboration), "Charged-particle multiplicity measurement in proton-proton collisions at $\sqrt{s} = 0.9$ and 2.36 TeV with ALICE at LHC," *Eur. Phys. Journ.* **C68** (2010) 89–108, `arXiv:1004.3034 [hep-ex]`.

[4] K. Aamodt and others (ALICE collaboration), "Charged-particle multiplicity measurement in proton-proton collisions at $\sqrt{s} = 7$ TeV with ALICE at LHC," *Eur. Phys. Journ.* **C68** (2010) 345–354, `arXiv:1004.3514 [hep-ex]`.

[5] K. Aamodt and others (ALICE collaboration), "Elliptic Flow of Charged Particles in Pb-Pb Collisions at $\sqrt{s_{NN}} = 2.76$ TeV," *Phys. Rev. Lett.* **105** (2010) 252302, `arXiv:1001.0502` `[physics.ins-det]`.

[6] K. Aamodt and others (ALICE collaboration), "First proton-proton collisions at the LHC as observed with the ALICE detector: measurement of the charged-particle pseudorapidity density at $\sqrt{s} = 900$ GeV," *Eur. Phys. Journ.* **C65** (2010) 111–125, `arXiv:0911.5430 [hep-ex]`.

[7] K. Aamodt and others (ALICE collaboration), "Midrapidity antiproton-to-proton ratio in pp collisions at $\sqrt{s} = 0.9$ and 7 TeV measured by the ALICE experiment," *Phys. Rev. Lett.* **105** (2010) 072002, `arXiv:1006.5432 [hep-ex]`.

[8] K. Aamodt and others (ALICE collaboration), "Charged-Particle Multiplicity Density at Midrapidity in Central Pb-Pb Collisions at $\sqrt{s_{NN}}$=2.76 TeV," *Phys. Rev. Lett.* **105** (2010) 072001, `arXiv:1011.3916 [nucl-ex]`.

[9] K. Aamodt and others (ALICE collaboration), "Transverse momentum spectra of charged particles in proton-proton collisions at $\sqrt{s} = 900$ GeV with ALICE at the LHC," *Phys. Lett.* **B693** (2010) 53–68, `arXiv:1007.0719 [hep-ex]`.

[10] K. Aamodt and others (ALICE collaboration), "Two-pion Bose-Einstein correlations in pp collisions at $\sqrt{s} = 900$ GeV," *Phys. Rev.* **D82** (2010) 052001, `arXiv:1007.0516 [hep-ex]`.

[11] K. Aamodt and others (ALICE collaboration), "Two-pion Bose-Einstein correlations in central Pb-Pb collisions at $\sqrt{s_{NN}} = 2.76$ TeV." 2010. `arXiv:1012.4035 [nucl-ex]`.

[12] R. Abir, C. Greiner, M. Martinez, and M. G. Mustafa, "Generalisation of Gunion-Bertsch Formula for Soft Gluon Emission." 2010. `arXiv:1011.4638 [nucl-th]`.

[13] E. G. Adelberger *et al.*, "Solar fusion cross sections II: the pp chain and CNO cycles." 2010. `arXiv:1004.2318 [nucl-ex]`.

[14] S. V. Akkelin, P. Braun-Munzinger, and Y. M. Sinyukov, "Thermal nature of charmonium transverse momentum spectra from Au-Au collisions at the highest energies available at the BNL Relativistic Heavy Ion Collider (RHIC)," *Phys. Rev.* **C81** (2010) 034912, `arXiv:0906.3712 [nucl-th]`.

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