FIAS Frankfurt Institute for Advanced Studies

FIAS Scientific Report 2009

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Preface

Since it took up its operations five years ago, FIAS has been an institute dedicated to fundamental theoretical research in the natural sciences of physics, chemistry, biology, neuroscience, and computer science within a common organizational and intellectual framework. The general research topic embracing a diversity of different research branches is the study of the dynamics, structure formation and self-organization of complex systems in animate and inanimate nature. This theoretical research is pursued in close collaboration with groups having an experimental focus at extramural research institutions, e.g., the Max Planck Institutes for Brain Research and for Biophysics in Frankfurt, and the GSI Helmholtz Center for Heavy Ion Research, Darmstadt. Equally important are the contacts with the departments of Biology, Mathematics and Computer Science, Chemistry, Physics, and Medicine of Goethe University.

In this Annual Report we present some of the ongoing activities of FIAS and of the associated graduate school, the "Frankfurt International Graduate School for Science" (FIGSS) in the year 2009. The main part of the Report consists of a collection of short reports describing the research projects of scientists working at or associated with FIAS.

Important international conferences have been organized by FIAS in the year 2009, both in Frankfurt and abroad. In addition to two Ernst Strüngmann Forum meetings, conferences on subjects as different as Radiation Damage in Biomolecular Systems, Computational Neuroscience, Immunology, Atomic Cluster Collisions, and Nuclear Fragmentations were held.

In the year 2009 FIAS has seen important changes. In July Prof. Christoph von der Malsburg decided to step down as chairman of the Board of Directors of FIAS and to concentrate on his role as coordinator of the Bernstein Focus Neurotechnology. He was succeeded by Prof. Dirk Hermann Rischke, who is also chairman of the physics department of Goethe University. Also the Board of Trustees has seen a change of leadership: Dr. Helmut Maucher, honorary chairman of Nestlé, was followed by the former president of Goethe University, Prof. Rudolf Steinberg.

The scientific staff of FIAS, too, has undergone changes: Three of the six initial Fellows have been offered professorships at other universities. Christian Holm moved to the University of Stuttgart where he became head of the Institute for Computational Physics. Soon afterwards, Robert Berger was appointed professor of organic chemistry at the Technical University of Darmstadt. Finally, at the end of 2009 Michael Meyer-Hermann has been offered professorships in immunology at both the Universities of Braunschweig and Jena. This development proves that the concept of FIAS to provide optimal conditions for young scientists to develop their careers has come to fruition. On the other hand it poses the challenge to find adequate successors and to ensure funding for them.

Intense discussions have been carried out at FIAS concerning the future strategy of the institute. It is important to ensure that the already well-established research areas, in particular theoretical physics and theoretical neuroscience, will maintain their high current level. In addition, efforts have to be made to ensure an ongoing broad diversity of research at FIAS, despite a difficult funding situation. Current needs point towards a strengthening of the areas of biology and chemistry.

Research highlights 2009

Physics
The nuclear and high-energy physics group within FIAS is mainly focused on numerical simulations of the properties of QCD matter and hadron-matter interactions. These activities are centered around the exploration of the QCD phase diagram and the study of elementary matter under extreme conditions. Further research is dedicated to nuclear astrophysics, in particular the properties of compact stars, and to the simulation of heavy-ion irradiation of biological tissue for tumor radiation therapy.
Major breakthroughs in the past year include the development a highly esteemed hybrid model for heavy-ion reactions in the FAIR energy regime (Bleicher), the successful test of a dynamical quasi-particle model for the quark-gluon plasma (Bratkovskaya), the establishment of a link between viscous hydrodynamics and transport theory (Rischke) and the development of models for tumor spheroid growth and radiation treatment (Mishustin, Meyer-Hermann, Bleicher). Very intriguing developments in nuclear structure physics point to the possibility of a significantly changed structure of the neutron drip line of nuclei (Greiner). Here, extremely neutron-rich nuclei might decay via a shower of neutrons.
A central problem for the modeling of strongly interacting matter originates from the very different degrees of freedom at low density and temperature (hadrons) compared to the highly excited state of matter (quarks, gluons). Here substantial progress was achieved formulating a unified approach including quarks and hadrons with a realistic phase transition behavior of the matter (Schramm). This description was applied to heavy-ion physics as well as to calculations of the properties of neutron stars.
The impact of these activities was honored by the successful fundraising within the LOEWE program (HIC for FAIR @ FIAS) and the Beilstein project NanoBIC, where the physics groups lead the FIAS activities. In addition, the activities are strongly supported by the Helmholtz Association (HGF) and GSI with long-term commitments for existing and future positions for scientists on the Fellow and Senior Fellow level. In this respect we are currently envisioning the extension of the FIAS physics activities into the area of lattice-QCD simulations. An important pillar of the nuclear physics program is the collaboration with other groups within the HGF-financed EMMI program, where FIAS is one of the partner institutions.

Neuroscience
Research in the neuroscience group spans a number of different approaches ranging from detailed models of information processing and learning in networks of spiking neurons to more abstract models of visual processing in the brain in the style of biologically inspired computer vision. The most prominent project, the Bernstein Focus for Neurotechnology falls in the latter category. The BMBF funds it with a total of 9.5 Mio. €, not quite half of which goes to FIAS. The project aims at building biologically inspired computer vision systems that closely integrate various visual competences that have so far been treated separately (such as segmentation, stereo vision, motion processing, object recognition, etc.). At the same time, these systems shall learn in an autonomous fashion through interactions with their environment. By now all PhD and post-doc positions have been filled and a robot head was purchased. The recruiting of three new professors (one of them at FIAS) is on its way. Once these positions are filled, Frankfurt will be a rather unique environment for vision research spanning neuroscience and engineering approaches. The neuroscience group has started a number of collaborations within FIAS (Lindenstruth's high performance computing group) and other project partners in the Frankfurt area (Developmental Psychology, Neurophysiology, Computer Science).
Overall, in 2009 the neuroscience group has published a number of papers in prominent journals and prestigeous conferences including PLoS Biology (IF 16), PLoS Computational Biology (IF 6), Neural Computation (IF 3), NIPS (24% acceptance rate) and many others.
In 2009 a new European collaborative project called IM-CLeVeR (Intrinsically Motivated Cumulative Learning Versatile Robots) has been acquired. The project addresses the question of how the brain may learn hierarchial sensori-motor control architectures, how it can do so driven by intrinsic motivations such as curiosity, and how such learning can be mimicked in robots. Furthermore, Jörg Lücke obtained a DFG grant "Non-linear Probabilistic Models for Representational Recognition and Unsupervised Learning in Vision".

Meso-Bio-Nano-Science

The MBN group as FIAS studies structure formation and dynamics of a variety of systems of different nature on the nanometer scale, ranging from atomic clusters to mesoscopic objects and complex biomolecules.

One research highlight has been the applications of methods from statistical mechanics to describe conformational changes of polypeptides. The relation of the fundamental problem of protein folding to the physics of phase transitions has been demonstrated in detail.

In an effort to contribute to the multidisciplinary project of ion-beam cancer therapy at FIAS, the MBN group has formulated a multiscale approach to the problem. First successful steps in 2009 have been the development of a model for the production of secondary electrons by heavy-ion beams in water and the proposition of the thermal spike model.

The work of the group in the field of nanosystems is focused on understanding the mechanisms of stability, self-organization and growth, as well as the ways of manipulation and control of these systems and their properties. The physics of fullerene clusters (C_{60}) and their interactions has been studied on a broad scale. This includes the growth and structure of fullerene-based nanotubes and polymerization involving nanowires. Using molecular dynamics simulations, phase transitions in nanocarbon structures have been successfully described. Photo-processes (photoabsorption, light scattering, bremsstrahlung) in clusters and endohedral systems (atoms encaged in a fullerene) have been studied using methods from physics and quantum chemistry. Furthermore, the growth of fractals on surfaces has been studied using the deposition, diffusion and aggregation method.

A further research topic of the MBN group related to nanosystems is the study of electromagnetic radiation generated in periodically bent crystals (microundulators). Schemes for the construction of a gamma-laser operating on this principle have been worked out.

Theoretical Biology

In 2009 the Systems Immunology Group at FIAS experienced a break-through on the level of publication and general acceptance of the relevance of mathematical approaches in Immunology.

In the research field of antibody development, important predictions on B-cell selection mechanisms have been published and have been verified in intravital multi-photon experiments in mice lymph nodes (reviewed in Meyer-Hermann et al. Trends Immunol. 30 (2009) 157). The development of new antibody types, in particular, involves the communication between different cell types with immunological synapses. A model for the formation of these synapses has been developed and the necessary set of underlying intracellular mechanisms that allow their formation has been derived (Eur. Phys. J. D51 (2009) 153). This work was newly based on chemical kinetics of receptor-ligand complex binding and dissolution.

A major step in research on rheumatoid arthritis was the development of a first comprehensive model of the interaction of the neuronal, the endocrine and the immune system on a systemic level. The systems immunology group published the first theoretical article in the leading journal for this disease (Meyer-Hermann et al. Arthritis and Rheumatism 60 (2009) 2585). In this article a three-fold improvement of the effect of the treatment of rheumatoid arthritis patients by cortisol by administration of cortisol at specific in-day time points (2a.m.) was predicted. These results impacted on the pharma industry that now developed corresponding drugs that are released with a time delay in order to take advantage of this effect.

The interaction of the neuronal and the immune system (an in-FIAS collaboration between the groups of Triesch and Meyer-Hermann) was demonstrated by the result that the pleiotropic molecule tumor-necrosis-factor-alpha – a main pro-inflammatory cytokine – interferes with synaptic activity in the brain in response to immune stimuli and might induce epileptic seizures (Savin et al. J. Roy. Soc. Interface 6 (2009) 655).

Another a visible success of the group was that it was given the opportunity to organize the reputed Germinal Centre Conference which was held at Frankfurt University. This has strongly promoted the visibility of FIAS in this community and enhanced the role of Theoretical Biology in Immunology research. Last but not least the group activities were acknowledged by three “Rufe” onto positions as full professors.

1. Research Centers

Helmholtz-Gemeinschaft Deutscher Forschungszentren
and
GSI Helmholtzzentrum für Schwerionenforschung GmbH
at FIAS

by Horst Stöcker

The activities of scientists from the diverse sections of the GSI Helmholtzzentrum für Schwerionenforschung at FIAS have been remarkably intensified and reinforced in 2009. This new intensity of cooperation is due to the foundation of the Helmholtz International Center for FAIR (HIC for FAIR), the Helmholtz Alliance ExtreMe Matter Institute (EMMI), and the international Helmholtz Graduate School for Hadron and Ion Research (HGS-HIRe for FAIR). Altogether, more than 100 scientists, financed by the Helmholtz-Gemeinschaft Deutscher Forschungszentren/GSI in 2009, are actively living the idea of this unique cooperation: 1 master student, 65 doctoral students, 28 postdocs, 3 guest professors, 7 guest scientists, 1 Junior Fellow, and 3 Senior Fellows, and 2 EMMI fellows at FIAS. The Senior Fellows are Prof. Peter Braun-Munzinger (Scientific Director of EMMI), Prof. Karlheinz Langanke (Director of Research at GSI), and Prof. Igor Mishustin (FIAS). The scientists come from more than 40 nations and thus reflect the high international reputation of this physics program. Already now, almost 100 publications have resulted from the new strong collaborations between FIAS and GSI or programs of the Helmholtz-Gemeinschaft, respectively, which will contribute to make this fruitful work even more visible.

Helmholtz International Center for FAIR (HIC for FAIR)

by Marcus Bleicher

The Helmholtz International Center for FAIR (HIC for FAIR), created in July 2008, with a substantial financial support by the Helmholtz-Gemeinschaft is a focused think tank that provides exceptional research infrastructure and human resources for the planning of the experimental program and for the design of key components of the FAIR facility. In total HIC for FAIR gathers more than 30 established working groups in the Rhein-Main-Area and is currently establishing more than 30 new working groups at the partner institutions dedicated towards FAIR physics. FIAS hosts two of the seven HIC for FAIR expert groups and provides key contributions in the area of transport theories for FAIR, relativistic dissipative hydrodynamics and dense baryonic matter. The HIC for FAIR partner institution FIAS presently has 3 doctoral students, 3 postdocs and 5 guest scientists financed by HIC for FAIR.

ExtreMe Matter Institute EMMI

The Extreme Matter Institute was founded 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 forms of matter in the Universe. EMMI research is carried out in close collaboration with the 13 international partner institutions; among the German partners are the universities of Darmstadt, Frankfurt, Heidelberg and Münster and the Forschungszentrum Jülich.

The scientific aim of the Alliance is to perform forefront research in the area of matter under extreme conditions. This comprises in particular four key areas of research: 1. Properties of the quark-gluon plasma and the phase structure of strongly interacting matter, 2. Structure and dynamics of dense neutron matter, 3. Electromagnetic plasmas of high energy density, and 4. Ultra-cold quantum gases and extreme states in atomic physics.

FIAS has been a founding member of EMMI and has close ties to the institute. The Scientific Director of EMMI is Prof. Peter Braun-Munzinger, who also is a Senior Fellow of FIAS.

Bernstein-Focus Neurotechnology Frankfurt

Financed under the BMBF Bernstein Program
Period 01.09.2008-31.08.2013
total amount Euro 9.5 Mio, share of FIAS: Euro 5.125.287

Collaborators:

Jörg Bornschein, Pramod Chandrashekhariah, Zhenwen Dai, Marc Henniges, Alexander Heusel, Jenia Jitsev, Manu Punnen John, Christian Keck, Daniel Krieg, Jörg Lücke, Daniela Pamplona, Gervasio Puertas, Wang Quan, Yasuomi Sato, Jochen Triesch, Christoph v. d. Malsburg, Cornelius Weber, Thomas Weisswange, Junmei Zhu

This project (which is coordinated by C. v.d.Malsburg, with the assistance of J. Triesch and R. Mester, Goethe-Uni) has the aim of building a computer-based vision system. There are 15 sub-projects, comprising participants at FIAS, Goethe-Uni, Honda Research Labs Offenbach, Max-Planck-Inst. for Brian Research, and Univ. 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. The project will make optimal use of previous work of the participating groups. 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. Work so far has been concentrated on system definition, establishment of a software and hardware environment and at organizing the conference BCCN2009 (300 participants) for the whole Bernstein Network.

Related publications in 2009:

J. Bornschein, *FPGA coprocessor for simulation of neural networks using compressed matrix storage,* System and Circuit Design for Biologically-Inspired Learning, IGI Global (in review).

J. Lücke, *Receptive Field Self-Organization in a Model of the Fine-Structure in V1 Cortical Columns*, Neural Computation 21 (2009) 2805-2845.

J. Lücke, R. Turner, M. Sahani, and M. Henniges, *Occlusive Components Analysis*, Advances in Neural Information Processing Systems 22, 2009, (in press).

C. Möller, N. Arai, J. Lücke and U. Ziemann, *Hysteresis Effects on the Input-Output Curve of Motor Evoked Potentials*, Clinical Neurophysiology 120 (2009) 1003-1008.

D. Pamplona, C. Weber and J. Triesch, *Foveation with optimized receptive fields*, Frontiers in Computational Neuroscience. Conference Abstract: Bernstein Conference on Computational Neuroscience. doi: 10.3389/conf.neuro.10.2009.14.016

C. A. Rothkopf, Th. Weisswange and J. Triesch, *Computational modeling of multisensory object perception*, in: "Multisensory Object Perception in the Primate Brain", Eds: M.J. Naumer, J. Kaiser, Springer, New York

(in press).

J. Triesch, C. A. Rothkopf and Th. Weisswange, *Coordination in Sensory Integration*, in: “Dynamic Coordination in the Brain”, Strüngmann Forum Reports, Eds: C. v. d. Malsburg, W.A. Phillips, W. Singer, MIT Press, Cambridge (in press).

Demo presented at BCCN 09: G. Tushev, M. Liu, D. Pamplona, J. Bornschein, C. Weber, J. Triesch, *Foveated Vision with FPGA Camera*.

Q. Wang and J. Triesch, *An explanation of the familiarity-to-novelty-shift in infant habituation*, Frontiers in Computational Neuroscience. Conference Abstract: Bernstein Conference on Computational Neuroscience. doi: 10.3389/conf.neuro.10.2009.14.149

C. Weber and J. Triesch, *Goal-Directed Feature Learning*, in Proceedings of the International Joint Conference on Neural Network (IJCNN), Atlanta, 14-19 June 2009, pp. 3319–3326. 2009.

C. Weber and J. Triesch, *Implementations and Implications of Foveated Vision*, Recent Patents on Computer Science 2 (2009).

Th. Weisswange, C. A. Rothkopf, T. Rodemann and J. Triesch, *Can reinforcement learning explain the development of causal inference in multisensory integration?*, in IEEE 8th Intl. Conf. on Development and Learning ICDL2009, Shanghai, 4-7 June 2009. 2009.

T.H. Weisswange, C.A. Rothkopf, T. Rodemann, J. Triesch, *A Reinforcement learning model develops causal inference and cue integration abilities*, Frontiers in Computational Neuroscience. Conference Abstract: Bernstein Conference on Computational Neuroscience. doi: 10.3389/conf.neuro.10.2009.14.151

Project “DAISY”

FP6-2005-015803
Co-PI C. v. d. Malsburg
Period 01.09.2005-31.08.2009
Amount subproject FIAS: Euro 610,000

Collaborators: Jenia Jitsev, Yasuomi Sato, Christoph von der Malsburg

The project is funded under the European program “Bio-inspired Information Technology”. Project DAISY aims at characterizing the architecture of visual cortex in mammals as a model for the information technology of the future. (The term DAISY refers to a connectivity pattern in visual cortex.) The FIAS subproject was aiming at a fully neural implementation of a previously developed and highly successful face recognition system. This implementation was made possible by a hypothetical novel type of neural element (control units), previously introduced by J. Lücke in his PhD thesis in Bochum. The core of the system is a set of circuits by which image segments appearing on the retina in varying position, size and orientation are transformed into an invariant representation in an “invariant window” in infero-temporal cortex. The system achieves face recognition rates that are highly competitive as tested on public benchmarks.

Related publications in 2009:

J. Jitsev and C. v. d. Malsburg, *Experience-driven formation of parts-based representations in a model of layered visual memory*, Frontiers in Computational Neuroscience, Special Issue on “Complex Systems Science and Brain Dynamics”, 2009, 3:15, doi:10.3389/neuro.10.015.2009.

J. Jitsev and C. v. d. Malsburg, *Unsupervised learning of object identities and their parts in a hierarchical visual memory.*, Frontiers in Computational Neuroscience. Conference Abstract: Bernstein Conference on Computational Neuroscience, 2009

J. Jitsev, C. v. d. Malsburg, *Activity-dependent bidirectional plasticity and homeostasis regulation governing structure formation in a model of layered visual memory.* Proc. Eighteenth Annual Computational Neuroscience Meeting, CNS Berlin, Germany. BMC Neuroscience 2009, 10(Suppl 1):P207

Y. Sato, J. Jitsev, P. Wolfrum, and C. v. d. Malsburg, *A correspondence-based neural mechanism for position invariant feature processing.*, Proc. Eighteenth Annual Computational Neuroscience Meeting, CNS Berlin, Germany. BMC Neuroscience 2009, 10(Suppl 1):P366

Y. Sato, J. Jitsev, T. Burwick and C. v. d. Malsburg, *A Global Decision-Making Model via Synchronization in Macrocolumn Units*, in 18th Annual Computational Neuroscience Meeting (CNC’2009), Berlin, 18-23 July 2009. 2009. Accepted for publication.

Y.D. Sato, J. Jitsev, C. von der Malsburg, *A visual object recognition system invariant to scale and rotation*, Neural Network World (ICANN Special Issue), 19(5), 529–544, 2009.

Akihisa Ichiki and Yasuomi D. Sato, *Phase reduction method for stochastic coupled oscillator systems*, Physical Review Letter (to be submitted).

Y. D. Sato, *Temperature-Modulated Synchronization Transition and Spiking Properties of a Pair of Coupled Neural Oscillators*, Physical Review E (to be submitted).

Y. D. Sato, Jenia Jitsev, Thomas Burwick and Christoph v. d. Malsburg, *Synchrony Promotes Global Decision Making in Macrocolumn Units.* Biological Cybernetics (to be submitted).

Yasuomi D. Sato, Effects of Temparture on Synchronization Phenomena in Coupled Spiking Neuron Models. Proceedings of the 2nd International Conference on Cognitive Neurodynamics 2009 (accepted).

Yasuomi D. Sato, Jenia Jitsev, Philipp Wolfrum, Christoph v. d. Malsburg and Takashi Morie, *A Recurrent Network of Macrocolumnar Models for Face Recognition.* In J. Zhu and D. Krieg (Eds.): Proceedings of the Bernstein Conference on Computational Neuroscience 2009, pp. 126-127, (Bernstein Focus Neurotechnology Frankfurt, Frankfurt am Main, 2009).

Yasuomi D. Sato, Jenia Jitsev, Philipp Wolfrum and Christoph v. d. Malsburg, *Introduction: An Invariant Object Recognition System*, Proceedings of the 9th Kyutech-Postech Joint Workshop on Neuroinformatics – Intelligence to Machines, Freedom to Mankind, pp. 5-6, (2009).

Yasuomi D. Sato, Jenia Jitsev, Thomas Burwick and Christoph v. d. Malsburg, *A Global Decision-Making model via Synchronization in Macrocolumn Units,* in the 18th Annual Computational Neuroscience Meeting (CNS’2009), Berlin, 18-23 July 2009. Accepted for publication.

Yasuomi D. Sato, Jenia Jitsev, Philipp Wolfrum and Christoph v. d. Malsburg, *A Correspondence-based Neural*

Mechanism for Position Invariant Feature Processing, in the 18th Annual Computational Neuroscience Meeting (CNS'2009), Berlin, 18-23 July 2009. Accepted for publication.

Y.D. Sato, Y. Tanaka and M. Shiino, Yasuomi D. Sato, Yuji Tanaka and Masatoshi Shiino, *Synchronization Transition in a Pair of Coupled Non-identical Oscillators*, in Proceedings ICONIP 2008, Part I, M. Köppen, ed., vol 5506 of Lecture Notes in Computer Science, pp. 865–872. 2009.

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

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. Essential aspects of this goal have already been demonstrated. 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. First results have been achieved along these lines.

Related publications in 2009:

Urs Bergmann and C. v. d. Malsburg, *Self-Organization of Topographic Bilinear Networks for Invariant Recognition.* Neural Computation (in review), 2009.

J. Zhu and C. v. d. Malsburg, *Steps towards numerical mode analysis of organizing systems,* J. Math. Biol. 59 (2009) 359-376.

Junmei Zhu and Christoph v. d. Malsburg, *The dynamics of a model system for invariant object recognition*, Proceedings "Dynamics Days Europe", pp. 76-77, 2009.

Junmei Zhu and Christoph v. d. Malsburg, *Grouping variables in an underdetermined system for invariant object recognition*, abstract "Computational Neuroscience Meeting (CNS)", 2009.

Project "PLICON": Plasticity and Learning in Cortical Networks

Collaborators: Arthur Franz[1], Prashant Joshi[1], Cristina Savin[1], Constantin Rothkopf[1], Jochen Triesch[1], Giacomo Indiveri[2], Monika Knopf[3], Mary Hayhoe[4], Dana Ballard[4]

[1] FIAS, [2] ETH Zurich, [3] Goethe Universität Frankfurt, [4] University of Texas Austin,

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 studies such interactions through computer simulations and theoretical analysis. For example, an important recent findig 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 try 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 2009:

A. Franz and J. Triesch, *A unified computational model of the development of object unity, object permanence, and occlusion perception*, Infant Behavior and Development. Submitted on 12 August 2009

F. Gerhard, C. Savin, J. Triesch, *A robust biologically plausible implementation of ICA-like learning*, ESANN, April 2009

C. Savin, J. Triesch and M. Meyer-Hermann, *Epileptogenesis due to glia-mediated synaptic scaling*, J. Roy. Soc. Interface 6 (2009) 655-668.

C. Savin and J. Triesch, *Developing a working memory with reward-modulated STDP*, J. Frontiers in Computational Neuroscience. Conference Abstract: Computational and systems neuroscience. doi: 10.3389/conf.neuro.10.2009.03.276

C. Savin and J. Triesch, *A recurrent network acquires working memory properties by reward-dependent STDP*, J. MSRL, June 2009

P. Joshi and J. Triesch, *Optimizing generic neural microcircuits using reward modulated STDP*, In ICANN, 2009: Proceedings of the 19th International Conference on Artificial Neural Networks, volume 5768 of Lecture Notes in Computer Science, pages 239–248, Berlin, Heidelberg, 2009. Springer-Verlag

P. Joshi and J. Triesch, *Rules for information-maximization in spiking neurons using intrinsic plasticity*, Neural Networks, IEEE - INNS - ENNS International Joint Conference on, IJCNN, pages 1456–1461, 2009

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

A. Lazar, G. Pipa and J. Triesch, *SORN: a Self-organizing Recurrent Neural Network*, Front. Comput. Neurosci. 3:23 (2009).

C. A. Rothkopf and D. H. Ballard, *Module activation and credit assignment in reinforcement learning*, (submitted)

C. Savin, P. Joshi, J.Triesch, *Independent Component Analysis in Spiking Neurons*, PLoS Computational Biology, in press

S. Saeb, C. Weber and J. Triesch, *Goal-directed learning of features and forward models*, in International Joint Conference on Neural Networks (IJCNN), Atlanta, 14-19 June 2009, vol. 22 of Neural Networks, pp. 586–592.

2009.

S. Saeb, C. Weber and J. Triesch, *A Neural Model for the Adaptive Control of Saccadic Eye Movements*, in International Joint Conference on Neural Networks (IJCNN), Altanta, 14-19 June 2009.

S. Saeb and C. Weber, *Toward a Goal Directed Construction of State Spaces*, Frontiers in Computational Neuroscience. Conference Abstract: Bernstein Conference on Computational Neuroscience. doi: 10.3389/conf.neuro.10.2009.14.019.

T.H. Weisswange, C.A. Rothkopf, J. Triesch, *A walk through the woods explains the space variant oblique effect*, Frontiers in Systems Neuroscience. Conference Abstract: Computational and systems neuroscience 2009. doi: 10.3389/conf.neuro.06.2009.03.283

2. Graduate Schools

Helmholtz Graduate School for Hadron and Ion Research

by Henner Büsching and Gerhard Burau

Since October 2008 the Helmholtz Graduate School for Hadron and Ion Research (HGS-HIRe) provides a common platform for structured doctoral education in the field of hadron and ion research. The Helmholtz Graduate School is a joint endeavor of the universities at Frankfurt, Darmstadt, Giessen, Heidelberg and Mainz together with FIAS and GSI. More than 130 enthusiastic PhD students from more than 30 nations have been accepted as participants in HGS-HIRe in its first year. Measures for structured doctoral education as lecture weeks, joint colloquia, supportive (soft) skill seminars and individual PhD committees have been established. Furthermore, HGS-HIRe provides and centrally organizes the very successful PhD scholarship programs of GSI (Graduate Program for Hadron and Ion Research - GP-HIR) and HIC for FAIR. Within the first year of existence, the required administrative infrastructure of the school was set up at FIAS. A network between the participating academic and scientific partners has been successfully established to support the PhD students in the realization of their doctoral projects and to enhance significantly the quality of the doctoral education.

Helmholtz Research School for Quark Matter Studies

by Henner Büsching and Gerhard Burau

The Helmholtz Research School for Quark Matter Studies (H-QM) is supported by the Initiative and Networking Fund of the Helmholtz Association. The Research School is a joint endeavor of the Goethe University Frankfurt and FIAS together with GSI. From more than 170 applications 25 PhD students from 13 countries working in the field of theoretical and experimental heavy-ion physics have been selected since the beginning of this program in October 2006. A series of lectures, colloquia, lecture weeks and soft skill seminars supports the PhD students in the development and training of their scientific and professional profiles. On account of the great success of this program, a second group of 25 top PhD students can start the three-year educational program in 2009.

FIGSS

The Frankfurt International Graduate School for Science

by Jochen Triesch

The Frankfurt International Graduate School for Science has continued its growth and now has more than 40 Ph.D. students of which nearly two thirds are international students and about 35% are female. The majority of students work in Physics and in Neuroscience (more than 40% in each group) while the remainder (less than 20%) is attached to Chemistry, Biology, and Computer Science. A number of 21 former FIGSS students already have obtained a Ph.D. degree.

All Ph.D. students associated with FIAS have one advisor at the Institute and one at a department of Goethe University. The duration of Ph.D. 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. Together with the FIAS post-docs, the FIGSS students organize a weekly seminar, where they report their research findings to each other.

The most important innovation in our graduate school this year was the decision to offer a compulsory course on "Methods for the Study of Complex Systems" designed for our first-year PhD students. This course aims to establish a common ground among the diverse group of students and teaches them important tools of the interdisciplinary field of Complex Systems Science. In discussions with all fellows, a set of core methods and techniques was identified and a curriculum for the course was designed. In the current Winter semester, this course is being offered for the first time by Prof. Triesch and his post-doc Dr. John with support by Prof. Bleicher. The course also includes a number of guest lectures by FIAS fellows on applications of the covered methods to their current research. This way, the first year students not only get to know a set of useful techniques and each other but also the Fellows of the Institute and some aspects of the ongoing research.

Courses offered at FIGSS

Summer Semester 2009

A. Solov'yov	Theoretical and computational methods in Meso-Bio-Nano-Science, 2h
E. Bratkovskaya, I. Mishustin	Dynamical models of relativistic heavy-ion collisions, 2h
J. Triesch, C. Rothkopf	Theoretical Neuroscience: Reinforcement Learning, 2+1h
W. Greiner, D. Gridnev	Symmetries in quantum mechanics - Group theory in physics, 2h
M. Meyer-Hermann	Agent-based models of Biological Systems, 2h
J. Reinhardt	Nonlinear Dynamics and Complex Systems, 2+2h
J. Lücke	Probabilistic Unsupervised Learning, 2+1h
R. Berger, A. Dreuw	Introduction to Quantum Chemistry, 2h
R. Berger, A. Dreuw, M. Holthausen	Electronic structure and quantum chemistry, Seminar 2h
S. Schramm	Quantum Theory on the Lattice, 3h
D. Schuch	Nonlinearities and dissipation in classical and quantum physics
E. Engel	Quantum many-particle theory

Winter Semester 2009/10

A. Solov'yov	Theoretical and computational methods in Meso-Bio-Nano-Science, 2h
E. Bratkovskaya, I. Mishustin	Physics of Strongly Interacting Matter 2h
J. Triesch	Methods for the study of complex systems 2+2h
W. Greiner, D. Gridnev	Relativistic wave equations 2h
C. Rothkopf	Recent Advances in Reinforcement Learning: Theory, Agent Modeling, and Human Behavior 2h
S. Schramm	Nuclear and Neutrino Astrophysics 2h
D. Schuch	Riccati and Ermakov Equations and the Quantum-Classical Connection 2h

Regularly held seminars

FIGSS Seminar	– FIAS Fellows
FIAS Colloquium/Seminar	– FIAS Fellows
Seminar on Meso-Bio-Nano-Science	– Solov'yov, Greiner
Current topics in theoretical neuroscience	– Triesch
Selected problems in systems immunology	– Meyer-Hermann
Columns group meeting	– v.d. Malsburg
Nuclear/Heavy ion group meeting	– Mishustin

Ph.D. degrees received by FIAS/FIGSS students in the year 2009

1	Kai Grass	03.02.2009	Towards realistic modelling of free-solution electrophoresis: a case study on charged macromolecules
2	Veronica Dexheimer	09.06.2009	Chiral symmetry Restoration and Deconfinement in Neutron Stars
3	Mehmet Süzen	03.07.2009	Induced Charge Computation
4	Yun Guo	10.09.2009	Quarkonium States in an Anisotropic Quark-Gluon Plasma
5	Maneesh Mathew	16.10.2009	Modelling Energetics and Stability of Carbon Nanotubes: A Novel Approach
6	Volodymyr Konchakovski (HQM)	23.10.2009	Fluctuations and Correlations in Nucleus-Nucleus Collisions within Transport Approaches
7	Hasnaa Fetehi	29.10.2009	Cell Migration and Organization

3. FIAS Scientific Life

Seminars and Colloquia at FIAS in the year 2009

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. In addition the “FIAS Seminar”, held alternately with the Colloquium, serves as a forum for talks of a somewhat more specialized or local nature. Since 2006 the “FIGSS Student Seminar” has been held, mainly as a platform for Ph.D. students to present their work. All three events are addressing the ‘general public’ at FIAS and bring together the researchers and students from all scientific branches. In addition, various work group seminars are held with a more focussed specialization. Their schedules are not listed in the following.

Interdisciplinary FIAS Colloquium and FIAS Seminar

15.01.2009 **Prof. Dr. Hermann Requardt,** Member of the Managing Board, Siemens AG, Munich
Open Innovation

22.01.2009 **Prof. Dr. Peter Güntert,** Institute of Biophysical Chemistry and FIAS
Automated protein structure analysis from NMR data

29.01.2009 **Prof. Dr. Maneesh Sahani,** Gatsby Computational Neuroscience Unit, University College London
Keeping one's eye on the ball: Inferring dynamical state from ensemble neuronal activity

05.02.2009 **Prof. Dr. Helmut Schwarz,** Institute of Chemistry, Technical University Berlin
Volcanic States: From Coulomb Explosions to Thermochemically Stable Small Polycations

26.02.2009 **Prof. Dr. Thomas Haberer,** Heidelberger Ionenstrahl-Therapiezentrum (HIT)
Rasterscanned Ion Beam Delivery in Tumor Treatments and Monte Carlo Methods

12.03.2009 **Prof. Dr. Raj K. Gupta,** Panjab University, Chandigarh, India
Island of stability for superheavy elements: a new look

30.04.2009 **Prof. Dr. Max Holthausen,** Institute for Inorganic and Analytical Chemistry, Goethe University, Frankfurt
Bioinorganic Models for Dinuclear Copper Proteins: Aliphatic and Aromatic Hydroxylation from a Quantum Chemical Point of View

07.05.2009 **Prof. Dr. Spartak Belyaev,** Kurchatov Institute, Moscow
My Life in Science

14.05.2009 **PD Dr. Axel Pelster,** Institut für Freie Universität Berlin and Universität Duisburg-Essen
Modern Topics of Ultracold Quantum Gases

18.05.2009 **Prof. Dr. Marco Durante,** GSI and TU Darmstadt
Protection from cosmic radiation in space travel

04.06.2009 **Prof. Dr. Sibaji Raha,** Bose Institute, Kolkata, India
Conversion of Neutron Stars to Quark Stars

16.06.2009 **Prof. Dr. Paul Schrater,** University of Minnesota, Minneapolis
Structure Learning in sequential decision making

18.06.2009 **Prof. Dr. Peter Braun-Munzinger,** GSI Darmstadt
The Charmonium Saga

25.06.2009 **Prof. Dr. Thomas Elze,** Dipartamento di Fisica "Enrico Fermi", Universita di Pisa, Italy
Symmetry aspects in emergent quantum mechanics

09.07.2009 **Prof. Dr. Ilya Fabrikant,** University of Nebraska, Lincoln
The theory of electron attachment to clusters and biomolecules

15.10.2009 **Prof. Dr. John Tsotsos,** Dept. of Computer Science, University of Toronto and Centre for Vision Research, York University
A Computational Perspective on Visual Attention

19.10.2009 **Dr. Charles Legendy,** Psychology Department, Columbia University
The role of the stria of Gennari in shape processing

26.10.2009 **Prof. Dr. Klaus Schulten,** University of Illinois at Urbana-Champaign, Beckman Institute for Advanced Science and Technology
Molecular Assembly and Teamwork - Bridge Between Inanimate and Animate Matter

12.11.2009 **Prof. Dr. Tamas Biro,** Central Research Institute for Physics (KFKI), Budapest
Non-extensive Composition Rules and Entropy Formulas

19.11.2009 **Sir Michael Berry,** Professor of Physics, Bristol University
Conical diffraction: imaging Hamilton's diabolical point

26.11.2009 **Prof. Dr. Martin Greiner,** Siemens AG, Munich
Wind power and physics: on turbulence, wind farms and complex networks

3.12.2009 **Dr. Ivan Kisel,** GSI Helmholtzzentrum für Schwerionenforschung, Darmstadt
Event Reconstruction in High Energy Physics Experiments

FIGSS Seminar

12.01.2009 **Dr. Constantin Rothkopf**
Three studies on walking and vision

19.01.2009 ***Dr. Yasuomi Sato***
Visual Object Recognition under Uncertain Conditions, and A Binding Model via Synchronization in Macrocolumn Dynamics

26.01.2009 **Christian Keck**
Correspondence Finding in 2D images

02.02.2009 **Mauricio Martinez**
High-energy dileptons from pre-equilibrated QGP

09.02.2009 **Kai Grass**
Modelling of free-solution electrophoresis

20.04.2009 **Dr. Cornelius Weber**
On Linking Reinforcement Learning with Unsupervised Learning

04.05.2009 **Veronika Dick**
Instability of silver fractals on graphite substrate

18.05.2009 **Dr. Marc Thilo Figge**
Everything you always wanted to know about immune deficiencies

25.05.2009 **Thomas Weisswange**
Can reinforcement learning explain the development of causal inference in multisensory integration?

08.06.2009 **Dominik Smith**
The thermodynamics of a not-so-hot Gluon Gas

15.06.2009 **Prof. Dr. Michael Strickland,** Gettysburg College
A Parallel Algorithm for Solving the 3d Schrödinger Equation

22.06.2009 **Dr. Yasuomi Sato**
Introduction of Integrated Visual Recognition - Synchronization, Spiking neurons to Visual recognition

06.07.2009 **Dr. Tomoi Koide**
Shear viscosity, bulk viscosity and heat conductivity in relativistic non-Newtonian fluid

Conferences and meetings (co)organized by FIAS in the year 2009

▹ **PECU, Meeting of the collaborative research project *"Photon emission in crystalline undulators",*** Frankfurt, Jan. 16, 2009

▹ ***"The Social Brain",*** 11. Meeting of the Junior Research Group "Philosophy of Mind", Berlin, May 20–22, 2009
www.ici-berlin.org/event/2009-05-20-the-social-brain

▹ **RADAM2009, *"VIth conference on Radiation Damage in Biomolecular Systems",*** Frankfurt, July 1–4, 2009
fias.uni-frankfurt.de/radam2009/

▹ **Germinal Centre Conference: *"16th International Conference on Lymphatic Tissues and Germinal Centres in Immune Reactions",*** Frankfurt, July 5–9, 2009
www.gcc16.org/

▹ **ISACC2009, *"Atomic cluster Collisions: Structure and Dynamics from the Nuclear to the Biological Scale",*** Ann Arbor, July 14–18, 2009
fias.uni-frankfurt.de/isacc2009/

▹ **Ernst Strüngmann Forum, *"Dynamic Coordination in the Brain: From Neurons to Mind",*** Frankfurt, August 16–21, 2009
fias.uni-frankfurt.de/esforum/forums/esf05_coordination.html

▹ **NUFRA2009, *"Second International Conference on Nuclear Fragmentation",*** Kemer/Turkey, Sept. 27 – Oct. 4, 2009
fias.uni-frankfurt.de/nufra2009

▹ **BCCN2009, *"Bernstein Conference on Computational Neuroscience",*** Frankfurt, Sept. 30 – Oct. 2, 2009
bccn2009.org

▹ **Ernst Strüngmann Forum, *"Better Doctors, Better Patients, Better Decisions: Envisioning Healthcare 2020",*** Frankfurt, October 25–30, 2009
fias.uni-frankfurt.de/esforum/forums/esf06_healthcare2020.html

4.1 Nuclear Physics, Particle Physics, Astrophysics

Group Report: Prof. Igor Mishustin, FIAS Senior Fellow

Main research fields: Physics of strongly interacting matter (equation of state, effective models motivated by QCD); Nuclear 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 supernova matter); medical applications (modeling heavy-ion energy deposition in extended media, radiation damage of biomolecules and cells).

Group members: Dr. Alexey Larionov (postdoc), Dr. Giorgio Torrieri (postdoc), Dr. Igor Pshenichnov (long-term visitor), Dr. (Hab.) Leonid Satarov (long-term visitor), Dr. Alexander Botvina (long-term visitor), Johan Bjerrum-Bohr (PhD student), Claudio Ebel (graduate student), Daniel Yueker (Diploma student).

Short-term visitors: Prof. Laszlo Csernai (Bergen University), Dr. (Hab.) Yuri Ivanov (Kurchatov Institute, Moscow), Dr. Abhijit Bhattacharyya (Calcutta University), Andrey Merdeev and Maxim Dmitriev (PhD students, Kurchatov Institute, Moscow).

Collaborations a) inside FIAS: Prof. W. Greiner, Prof. H. Stoecker, Prof. Andrey Solov'yov, Dr. M. Meyer-Herrmann; b) in ITP, Goethe University: Prof. D. Rischke, Prof. M. Bleicher, Prof. S. Schramm, Dr. T. Koide, G. Denicol; at GSI (Darmstadt): Prof. W. Trautmann, Prof. M. Durante, Dr. D. Schardt; at Heidelberg University: Prof. J. Schaffner-Bielich, M. Hempel; at Niels Bohr Institute (Copenhagen): Prof. J. Bondorf, Prof. Jens Joergen Gaardhoje, Dr. Th. Dossing; also Prof. J. Kapusta (University of Minnesota), Dr. J. Randrup (LBNL, Berkeley), Prof. J. Pochodzalla (Mainz University), Prof. L. Bravina (Oslo University), Prof. B. Tomasik (Univerzita Mateja Bela), Riza Ogul (Selcuk University, Turkey).

Conferences organized in 2009

International Conference on Nuclear Fragmentation (NUFRA2009): From Basic Research to Applications (Kemer, Turkey, September 27- October 4, 2009), about 40 talks and 80 participants, detailed see on http://fias.uni-frankfurt.de/nufra2009/

Conference talks presented in 2009

1. Igor Mishustin, *Hydrodynamic modeling of phase transitions in rapidly expanding systems*, 5th International Workshop on Critical Point and Onset of Deconfinement (CPOD2009), Brookhaven National Laboratory, June 8-12, 2009.

2. I.N. Mishustin, *Modelling heavy-ion energy deposition in extended media,* VIth conference on Radiation Damage in Biomolecular Systems RADAM2009 (Frankfurt, Germany, July 1-4, 2009).

3. Igor Mishustin, *Hydrodynamical modeling of deconfinement phase transition in relativistic nuclear collisons*, Round Table Workshop on NICA Physics (Dubna, Russia, 9-12 September, 2009).

4. Igor Mishustin, *Modeling of supernova matter*, International Conference on Nuclear Fragmentation, NUFRA2009 (Kemer, Turkei, Sep. 27-Oct. 4, 2009).

5. Alexander Botvina, *Formation of hypernuclei in high energy nuclear reactions*, International Conference on Nuclear Fragmentation, NUFRA2009 (Kemer, Turkei, Sep. 27-Oct. 4, 2009).

6. I.A. Pshenichnov, *Beams of light and heavy nuclei in extended media: a challenge of nuclear fragmentation*, NUFRA2009 (Kemer, Turkey, Sept. 27-)ct. 4, 2009)

7. I.A. Pshenichnov, *Nuclear beams in extended media: issues of nuclear fragmentation,* 14th Geant4 Users Workshop (Catania, Italy, October 25-29, 2009).

8. I.A. Pshenichnov, *Beams of light and heavy nuclei in tissue-like media,* Workshop on Nuclear Models for use in Hadron Therapy (Juelich, Germany, October 10-11, 2009).

9. A.B. Larionov, *Transport calculations of antiproton-nucleus interactions*, XXXI Mazurian Lakes Conference on Physics NUCLEAR PHYSICS and the Road to FAIR (Piaski, Poland, Aug, 30-Sept. 06, 2009).

Papers published or submitted in 2009

1. Barbara Betz, Jorge Noronha, Giorgio Torrieri, Miklos Gyulassy, Igor Mishustin, Dirk H. Rischke, Universality of the Diffusion Wake from Stopped and Punch-Through Jets in Heavy-Ion Collisions, Phys. Rev. C79 (2009) 034902; arXiv:0812.4401 [nucl-th]

2. Pratik Agnihotri, Juergen Schaffner-Bielich, Igor N. Mishustin, Boson stars with repulsive self-interactions, Phys. Rev. D79 (2009) 084033; arXiv:0812.2770 [astro-ph].

3. L.M. Satarov, M.N. Dmitriev, I.N. Mishustin, Equation of state of hadron resonance gas and the phase diagram of strongly interacting matter, Phys. Atom. Nucl. 72 (2009) 1390-1415; arXiv:0901.1430 [hep-ph].

4. Giorgio Torrieri, Igor Mishustin, Boris Tomasik, Bulk viscosity-driven freeze-out in heavy ion collisions, talk given at the International School of Nuclear Physics, 30th Course: Heavy-Ion Collisions from the Coulomb Barrier to the Quark-Gluon Plasma, (Erice-Sicily, 16 - 24 September 2008), to be published in proceedings; arXiv:0901.0226 [nucl-th].

5. Andrey V. Solov'yov, Eugene Surdutovich, Emanuele Scifoni, Igor Mishustin, Walter Grainer, Physics of ion beam cancer therapy: a multi-scale approach, Phys. Rev. E79 (2009) 011909; arXiv:0811.0988 [physics.bio-ph].

6. A.B. Larionov, I.A. Pshenichnov, I.N. Mishustin and W. Greiner, Antiproton-nucleus collisions simulation within a kinetic model with relativistic mean fields, Phys. Rev. C80 (2009) 021601; arXiv:0903.2152 [nucl-th].

7. Abhijit Bhattacharyya, Igor N. Mishustin, Walter Greiner, Deconfinement phase transition in compact stars: Maxwell vs. Gibbs construction of the mixed phase, submitted for publication in J. Phys. G: Nucl. Part. Phys.; arXiv:0905.0352 [nucl-th].

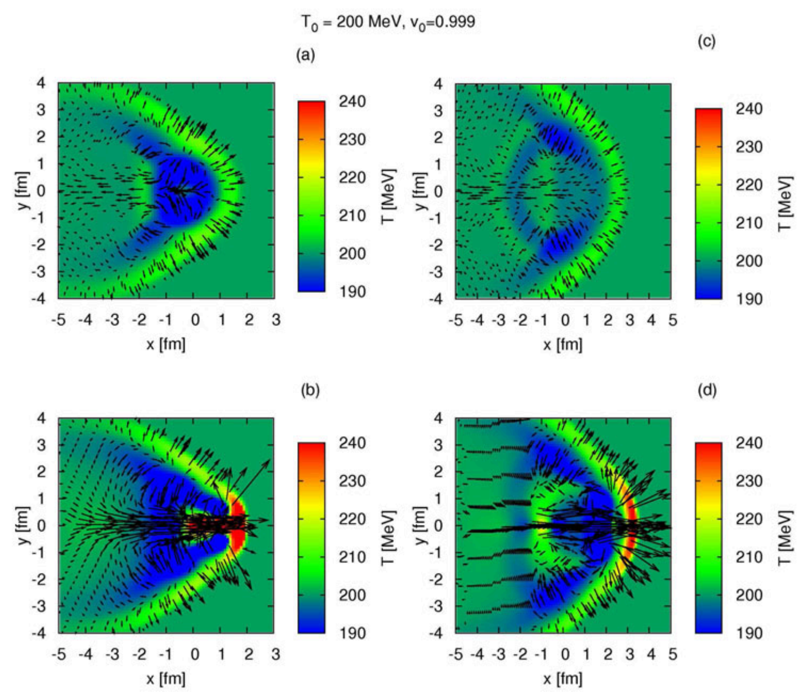
8. Yu.B. Ivanov, I.N. Mishustin, V.N. Russkikh, and L.M. Satarov, Elliptic flow and dissipation at AGS-SPS energies, submitted for publication in Phys. Rev. C; arXiv:0907.4140 [nucl-th].

9. R Ogul, U Atav, F Bulut, N Buyukcizmeci, M Erdogan, H Imal, A S Botvina and I N Mishustin, Surface and symmetry energies in isoscaling for multifragmentation reactions, J. Phys. G: Nucl. Part. Phys. 36 (2009) 115106.

Jet energy loss and Mach cones in a hydrodynamic medium

Collaborators: Giorgio Torrieri, Igor Mishustin, Barbara Betz, Miklos Gyulassy, Jorge Noronha, Dirk Rischke, Horst Stöcker

The observation of jet suppression at RHIC has opened the still unresolved question of what happens with the missing jet energy. The fluid-like behavior observed at RHIC suggests the possibility that this energy is thermalized and "encoded" in the collective flow pattern, perhaps via phenomenon such as "Mach cone". The observation of this phenomenon would be a further confirmation of collective behavior and would allow us to constrain the equation of state and transport properties of the system created in heavy ion collisions. We have used a 3D relativistic hydrodynamics code to study different scenatios of jet energy deposition into the medium, and to link jet energy deposition properties to experimentally observable particle abundances and kinematic two-particle correlations [1,2]. The Figure shows a sample of such calculations, the temperature (color) and flow(arrows) for a jet before (left panel) and after (right panel) it stops. A wide variety of sources (including ansatze put in "by hand", as well as sources motivated by theoretical calculations such as AdS/CFT and pQCD) and hydrodynamic solutions (static and flowing) was surveyed this way, and the signal systematics was put together and compared to experimental data. It was found that, even in an ideal fluid, the diffusion wake and thermal smearing kill the conical signal in azimuthal correlations of the particles (right panel) even if this signal is visible in the hydrodynamic evolution. It was furthermore found that a diffusion wake can appear as a conical signal in the hydrodynamic flow. This signal, however, is "fake", because it does not obey Mach's law for the opening angle. In the future calculations will be extended for the case of an expanding background.



Hydrodynamic solutions to the Mach cone problem. Four panels show results for different assumptions abour the jet energy loss. The diffusion wake is clearly seen behind the cone head in all cases.

Related publications:

1) B. Betz, J. Noronha, G. Torrieri, M. Gyulassy, I. Mishustin and D. H. Rischke, *Universality of the Diffusion Wake from Stopped and Punch-Through Jets in Heavy-Ion Collisions*, Phys. Rev. C79 (2009) 034902

2) B. Betz, M. Gyulassy, D. H. Rischke, H. Stöcker and G. Torrieri, *Jet Propagation and Mach Cones in (3+1)d Ideal Hydrodynamics*, J. Phys. G 35 (2008)104106

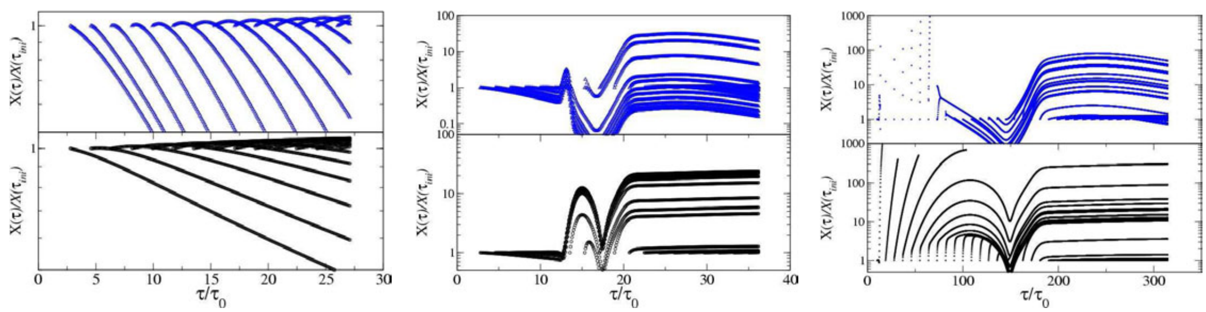
Bulk-viscosity in QCD and phenomenological implications for relativistic heavy-ion collisions

Collaborators: Giorgio Torrieri, Igor Mishustin, Boris Tomasik, Ivan Melo, Tomoi Koide, Gabriel Denicol

One of the important problems associated with heavy ion collisions is the understanding of how the dense matter created in these collisions breaks up into hadrons, a process known as hadronization. Current approaches are problematic for fundamental reasons and because they are unable to describe relevant experimental data (e.g. Particle interferometry- HBT radii) correctly.

We have proposed a scenario [1,2] which might be able to solve these problems by linking hadronization process to the behavior of bulk viscosity at the QCD phase transition. As lattice calculations show, bulk viscosity may have a sharp peak close to the phase transition temperature. This means that expanding fluid suddenly looses its liquidity and breaks into pieces like a glass. In this regime the boost-invariant Bjorken solution to hydrodynamic equations, thought to be relevant to relativistic heavy ion collisions, becomes unstable with respect to clusterization. This was explicitly shown by studying plain-wave perturbations to viscous hydrodynamics equations around a boost-invariant time-dependent background.

The explicit solutions to the equation of motion for such perturbations are shown in the Figure. As one can see from the figure, even in the case of a moderate viscosity peak (central part) the amplitude of initial perturbations may grow by about factor 10. This means that the initially almost uniform fluid will split into droplets within a short time after passing the transition point (corresponding to the deep in the curves). In ref. [3] a new method was developed which may help to find experimental signatures of this phenomenon. We are also looking for cosmological implications of this scenario, as well as similar



Behavior of the amplitude of a small instability around the Bjorken solution with time, with no peak (left), a small peak (center) and an overwhelming peak (right). Black and blue are wavenumbers of the instability in rapidity space 4 and 8 respectively

Related publications:

1) G. Torrieri, B. Tomasik and I. Mishustin, *Bulk Viscosity driven clusterization of quark-gluon plasma and early freeze-out in relativistic heavy-ion collisions,* Phys. Rev. C77, 034903 (2008)

2) G. Torrieri and I. Mishustin, *Instability of Boost-invariant hydrodynamics with a QCD inspired bulk viscosity,* Phys. Rev. C78 (2008) 021901

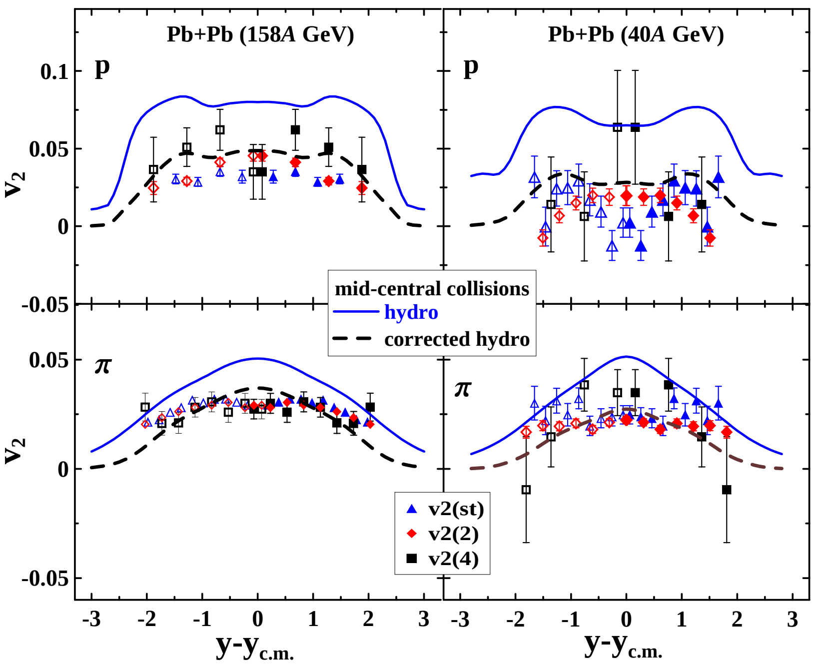
3) I. Melo, B. Tomasik, G. Torrieri, S. Vogel, M. Bleicher, S. Korony, M. Gintner, *Kolmogorov-Smirnov test and its use for the identification of fireball fragmentation*, Phys. Rev. C80 (2009) 024904

Elliptic flow and dissipation in heavy-ion collisions at AGS–SPS energies

Collaborators: I.N. Mishustin[1], L.M. Satarov[1], Yu.B. Ivanov[2], V.N. Russkikh[2]

[1]FIAS, [2]Kurchatov Institute, Moscow

Elliptic flow in heavy-ion collisions at incident energies $E_{\rm lab} \simeq (1\text{–}160)A$ GeV is analyzed within the 3-fluid dynamical model (3FD). We show that a simple correction factor, taking into account dissipative affects, allows us to adjust the 3FD results to experimental data. This single-parameter fit results in a good reproduction of the elliptic flow as a function of the incident energy, centrality of the collision and rapidity. The experimental scaling of pion eccentricity-scaled elliptic flow versus charged-hadron-multiplicity density per unit transverse area turns out to be also reasonably described. Proceeding from values of the Knudsen number, deduced from this fit, we estimate the upper limit the shear viscosity-to-entropy ratio as $\eta/s \sim 1-2$ at the SPS incident energies. These values are of the order of minimal η/s observed in water and liquid nitrogen and exceed by about of a factor ten the values extracted at RHIC energies.



Elliptic flow of protons (upper panels) and charged pions (lower panels) in mid-central Pb+Pb collisions at $E_{\rm lab} = 158A$ GeV (left panels) and 40A GeV (right panels) as a function of rapidity. The 3FD calculations are performed at $b = 5.6$ fm with the intermediate equation of state. Experimental NA49 data obtained by the standard method ($v_2(\mathrm{st})$) and by the method of n-particle correlations ($v_2(n)$) are displayed by different symbols. Full symbols correspond to measured data, while open ones are those reflected with respect to the midrapidity.

Related publications in 2009:

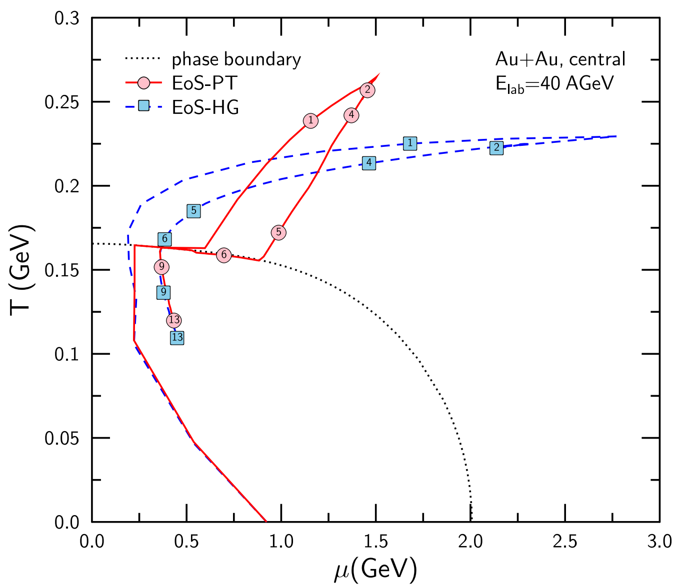
Yu.B. Ivanov, I.N. Mishustin, V.N. Russkikh, and L.M. Satarov, *Elliptic flow and dissipation at AGS-SPS energies*, Phys. Rev. C80 (2009) 064904. arXiv: 0907.4110 [nucl-th].

Hydrodynamic modeling of deconfinement phase transition in relativistic heavy-ion collisions

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

[1]FIAS, [2]Kurchatov Institute, Moscow

The equation of state (EOS) of hadron resonance gas at finite temperature and baryon density is calculated [1] taking into account finite-size effects within the excluded volume model. Calculations include contributions of all known hadrons with masses up to 2 GeV. Special attention is paid to the role of strange hadrons in the system with zero total strangeness. A density-dependent mean field is added to guarantee that the nuclear matter has a saturation point and a liquid-gas phase transition. The deconfined phase is described by the bag model with lowest order perturbative corrections. The phase transition boundaries are found by using the Gibbs conditions with the strangeness neutrality constraint. The sensitivity of the phase diagram to the hadronic excluded volume and to the parametrization of the mean-field is investigated. The possibility of strangeness-antistrangeness separation in the mixed phase is analyzed. It is demonstrated [1,2] that the peaks in the K/π and Λ/π excitation functions observed at low SPS energies can be explained by a nonmonotonous behavior of the strangeness fugacity along the chemical freeze-out line. The above EOS has been used [3] in our fluid-dynamical simulations of heavy-ion collisions at AGS, FAIR and SPS energies (see Figure).



Time evolution of strongly interacting matter created in central Au+Au collision at $E_{\rm lab} = 40$ AGeV [3]. Shown are values of temperature and baryon chemical potential (in a central box) at different time moments in c.m. frame. The solid line represents the results of fluid–dynamical calculation using the EOS with the deconfinement phase transition. The dashed line is calculated with the EOS of the ideal hadron gas.

Related publications in 2009:

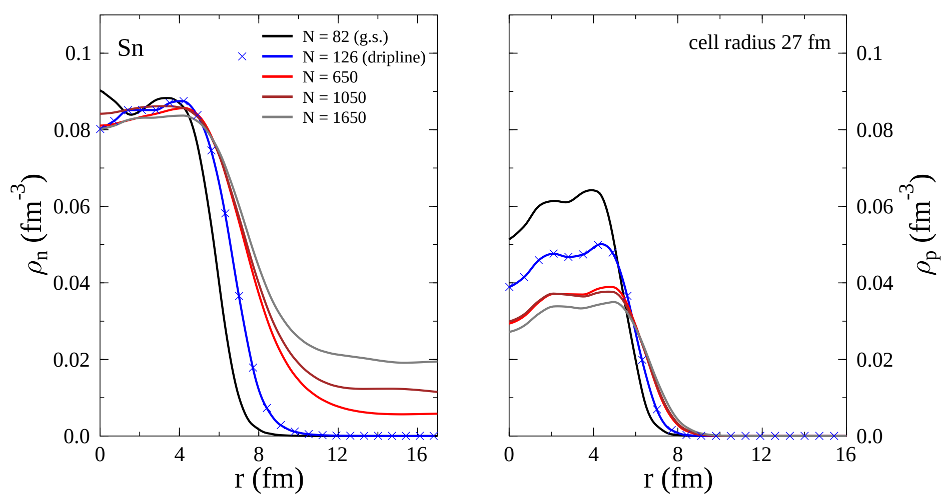
1) L.M. Satarov, M.N. Dmitriev, and I.N. Mishustin, *Equation of state of hadron resonance gas and the phase diagram of strongly interacting matter*, Yad. Fiz. 72 (2009) 1444-1469 [Phys. Atom. Nucl. 72 (2009) 1390-1415]
2) I.N. Mishustin, *Equation of state of hadron resonance gas and the "horn"*, talk at RMN meeting, GSI, 12 February 2009.
3) I.N. Mishustin, *Modeling phase transition in rapidly expanding systems*, talk at Int. Conf. CPOD-2009, 8-12 June 2009, Brookhaven. Proceedings of Science (CPOD2009), p. 12

Nuclei embedded in a neutron gas

Collaborators: Igor N. Mishustin, Thomas J. Bürvenich, and Walter Greiner

In a previous paper [1] we have studied the impact on nuclear structure of a constant electron background representing conditions in a neutron-star crust or supernova explosion. We have performed calculations within the Relativistic Mean Field (RMF) model using the Wigner-Seitz approximation. We have found that for large electron Fermi momenta, decay modes such as α decay and spontaneous fission are stabilized at high electron density. However, with growing electron density the line of β-stability moves to more neutron-rich systems, while the proton drip line moves to more proton-rich nuclei since electrons provide an attractive potential for the protons. For electron Fermi momenta of $k_F \approx 0.05$ fm^{-1}, the line of β-stability reaches the neutron drip line, hence neutron can drip out from the nuclei. In the subsequent work [2], we extend our study to include the dripping-out neutrons, i.e. the neutron in unbound states.

We still employ the Wigner-Seitz approximation by dividing the system into electrically-neutral cells, each containing a nucleus and surrounding neutron gas. The neutron and proton densities are calculated self-consistently within the RMF approach, also taking into account the screening effect of electrons. Some preliminary results are shown in the figure. Our approach can be used to quantitatively evaluate in-medium modifications of nuclear properties, such as their surface and symmetry energies. This information is needed for realistic calculations of nuclear composition and equation of state of stellar matter.



Neutron (left) and proton (right) single-particle densities for a sequence of tin isotopes in a Wigner-Seitz cell with radius $R_C = 27$ fm. The neutron drip line corresponds to N=126, and at larger N the neutrons form a rather uniform gas around the nucleus.

Related publications:

1) Thomas J. Bürvenich, Igor N. Mishustin, and Walter Greiner, *Nuclei embedded in an electron gas*, Phys. Rev. C76 (2007) 034310

2) Igor N. Mishustin, Thomas J. Bürvenich, and Walter Greiner, *Nuclei embedded in an neutron gas*, paper in preparation.

3) Igor Mishustin, *Modeling of supernova matter*, invited talk at the International Conference NUFRA2009; http://fias.uni-frankfurt.de/nufra2009/talks/mishustin.pdf

Transport calculations of $\bar{p}$-nucleus interactions

Collaborators: A.B. Larionov, I.N. Mishustin, I.A. Pshenichnov, L.M. Satarov, W. Greiner

The Giessen Boltzmann-Uehling-Uhlenbeck (GiBUU) transport model is extended and applied to the $\bar{p}$-nucleus interactions in a wide beam momentum range. The most important channels of an antinucleon-nucleon interaction, i.e. annihilation, elastic and inelastic scattering, are realistically implemented. The model includes relativistic mean fields acting on baryons and antibaryons. The comparison of the model calculations with available experimental data on $\bar{p}$-absorption at $p_{\text{lab}} = (0.1 \div 100)$ GeV/c, pion and proton production from $\bar{p}$-annihilation at $p_{\text{lab}} = 600$ MeV/c on nuclei is performed [1]. Fig. 1 shows the model results for the absorption cross section on ^{12}C for various choices of the scaling factor ξ of the antibaryon-meson coupling constants. For orientation, $\xi = 0$ and $\xi = 1$ correspond to the cases without antibaryon mean field potential and with the G-parity motivated antibaryon potential $\text{Re}(V_{\text{opt}}) \simeq -660$ MeV, respectively. Based on this comparison, we were able to put stringent constraints on the real part of an antiproton optical potential. We find that $\text{Re}(V_{\text{opt}}) = -(150 \pm 30)$ MeV is the best suited to describe the $\bar{p}$ absorption cross sections on various nuclei below 1 GeV/c, which also agrees with the values obtained from the studies of antiprotonic atoms (E. Friedman et al., 2005).

Such a deep antiproton potential is caused by a strongly attractive antinucleon-nucleon interaction. As has been shown earlier (T. Bürvenich et al., 2002, I.N. Mishustin et al., 2005), the strongly-bound $\bar{p}$-nucleus system has a high nucleon density. Currently we are studying compressional effects created in a nucleus by a moving antiproton [2,3]. Fig. 2 presents the compressional evolution of the nucleon density in the case of $\bar{p}^{16}$O system. The annihilation is switched-off in this calculation. Instead, we have traced

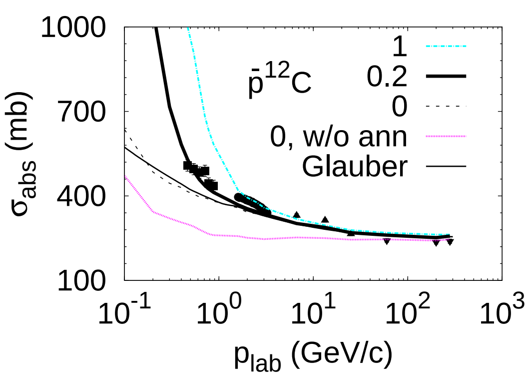


FIG. 1: $\bar{p}$ absorption cross section on ^{12}C nucleus vs the beam momentum. The lines marked with the value of a scaling factor ξ show the GiBUU results. Thin solid line represents the Glauber model calculation. A calculation with $\xi = 0$ without annihilation is additionally shown by the dotted line.

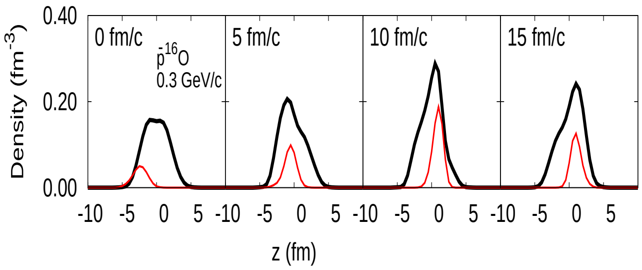


FIG. 2: Nucleon (thick solid lines) and antiproton (thin solid lines) densities along the z-axis passing through the nuclear centre for the $\bar{p}^{16}$O system at different times. The initial $\bar{p}$ momentum is directed to the nuclear centre and has a value of 0.3 GeV/c.

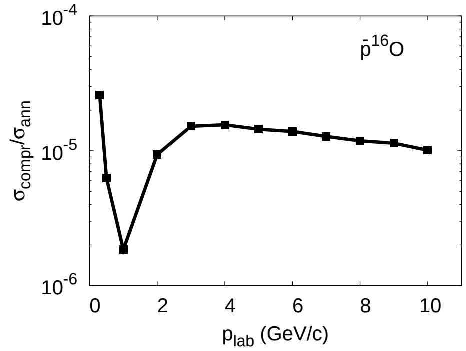


FIG. 3: The probability of antiproton annihilation at the nucleon density more than 0.3 fm^{-3} as a function of the beam momentum for $\bar{p}^{16}$O collisions.

the survival probability of the antiproton, which is $\sim 10^{-3}$ at the time of the maximal compression. In Fig. 3, we present the probability of $\bar{p}$ annihilation in a compressed zone. The rise of the ratio with the beam momentum between about 1 GeV/c and 3 GeV/c is caused by opening the pion production channels $\bar{N}N \to \bar{N}N\pi(\pi...)$, which leads to more intensive stopping of an antibaryon before annihilation, and, therefore increases the compression probability.

Publications in 2009:

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Isospin observables in multifragmentation of relativistic projectiles

FIAS group: A.S. Botvina and I.N. Mishustin
group of Selcuk University: R. Ogul and N. Buyukcizmeci
GSI group: W. Trautmann and ALADIN collaboration.

Multifragmentation is a universal phenomenon occurring when a large amount of energy is deposited in a nucleus. It was observed in high energy nuclear reactions induced by hadrons and heavy ions. It is believed to be a manifestation of nuclear liquid-gas phase transition which is also expected to occur in crusts of neutron stars and supernova explosions. This reaction gives a unique possibility to study experimentally properties of fragments imbedded in hot environment of other nuclear species. The ALADIN experiment S254, conducted in 2003 at SIS was designed to study isotopic effect in projectile fragmentation at relativistic energies. The beams of neutron-rich ^{124}Sn, and neutron-poor ^{107}Sn, and ^{124}La were used. The ALADIN set up allows for nearly complete registration of all particles with $Z \geq 2$ produced in the experiment. We have used Statistical Multifragmentation Models (SMM) for analysis of the experimental data. Previously, SMM was successfully applied for interpretation of experimental data by many groups.

By selecting a realistic ensemble of the excited residual nuclei produced after the fast dynamical stage of the reaction we have been able to describe all charge characteristics of produced fragments: fragment charge distributions, fragment multiplicity distributions, fragment-fragment correlations in events. In the following we have analysed isotope distributions of produced fragments and the corresponding observables, like isoscaling. We have found that the properties of fragments extracted from these multifragmentation reactions should be modified in comparison with cold isolated nuclei [1, 2]. In particular, the symmetry energy of fragments should be considerably decreased to fit isotope data. In Fig. 1 we show that the reduced fragment symmetry energy coefficients γ is needed to describe the data. We attribute this effect to the influence of surrounding matter and extension of hot fragments under this circumstances. It has far reaching consequences for the astrophysical processes like supernova explosions when similar temperatures and densities can be reached.

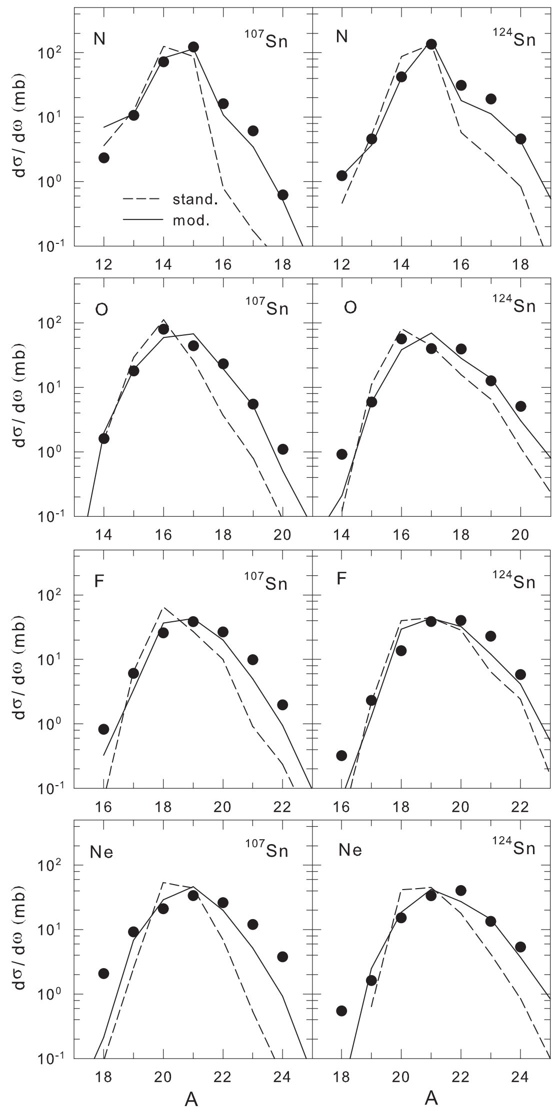

Figure 1: Comparison of experimental (circles) and calculated (lines) isotope distribution of fragments for elements with Z=7–10. Dashed lines correspond to the standard symmetry energy coefficient $\gamma = 25$ MeV, solid lines - the reduced $\gamma = 15$ MeV.

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[2] N. Buyukcizmeci et al. *Invited talk at NUFRA2009 conference*, Sep 27 - Oct 4, 2009 , Kemer, Turkey. fias.uni-frankfurt.de/nufra2009/talks/buyukcizmeci.pdf

Crossover to Cluster Plasma in the Gas of Quark-Gluon Bags

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b Bogolyubov Institute for Theoretical Physics, Kiev, Ukraine

The present and future experimental facilities such as RHIC and LHC produce strongly interacting matter in the crossover region of the QCD phase diagram. The location of the (tri)critical point that ends the line of the 1st order phase transition is unknown. It can happen that nucleus-nucleus collisions at SPS and FAIR also partially enter the crossover region.

The possibility of phase transitions in the gas of quark-gluon bags was demonstrated in 1981. Further studies allowed to obtain the 1st, 2nd, and higher order transitions. A possibility of no phase transitions was pointed out. Recently it was suggested to model also a smooth crossover transition by the gas of quark-gluon bags. Inspired by this suggestion we study in more details the high temperature behavior of the system of quark-gluon bags in case of the crossover.

The equation of state at high temperature is that of the quark-gluon plasma. However, the system consists of the bags with finite volumes which are defined by the model parameters γ and δ of the mass-volume bag spectrum. Possible structures in this *cluster* quark-gluon plasma are classified.

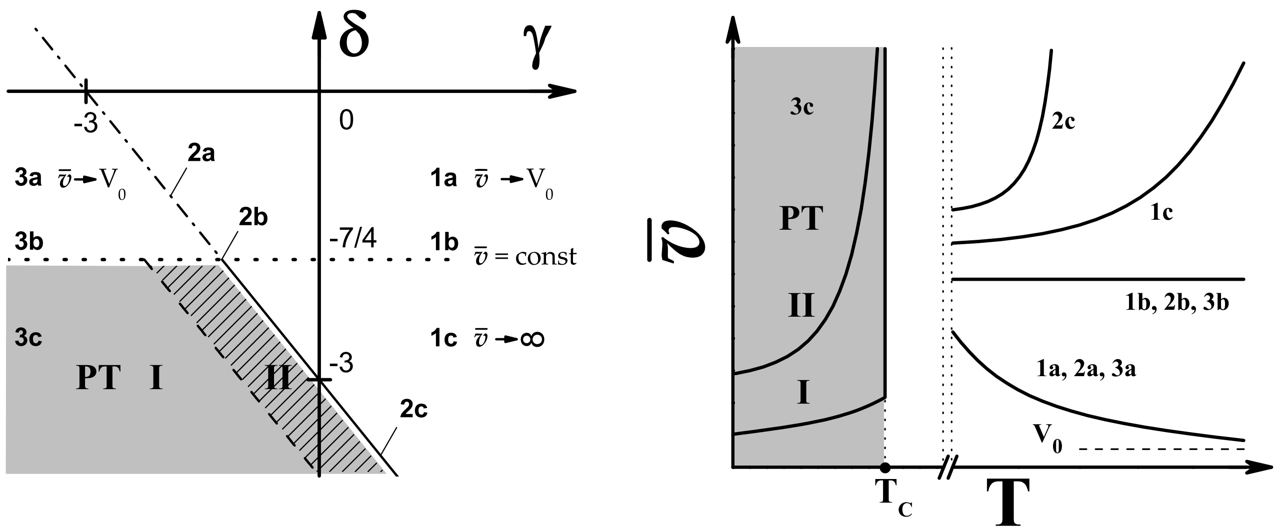

FIG. 1: *Left:* The $\gamma - \delta$ phase diagram for the gas of quark-gluon bags. *Right:* The schematic view of temperature dependence of the average volume of the bag, $\overline{v}(T)$, in different regions of $\gamma - \delta$ phase diagram.

The phase transitions in the system of quark-gluon bags take place in the only case 3c, i.e. if $\gamma + \delta < -3$ and $\delta < -7/4$. This is the lower left corner of the $\gamma - \delta$ phase diagram marked as 3c and shown by grey color in Fig. 1 *left*. The region with 1st and 2nd or higher order phase transitions are marked as I and II correspondingly. The main part of the $\gamma - \delta$ phase diagram corresponds to the case of crossover.

It was found that if the system of quark-gluon bags has no phase transition the average quark-gluon bag volume $\overline{v}(T)$ remains finite at high temperature. Such a *cluster* QGP can be rather different from the *ideal* QGP despite of the similar to that equation of state.

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Search for new reaction mechanisms leading to the formation of neutron rich heavy and superheavy nuclei

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

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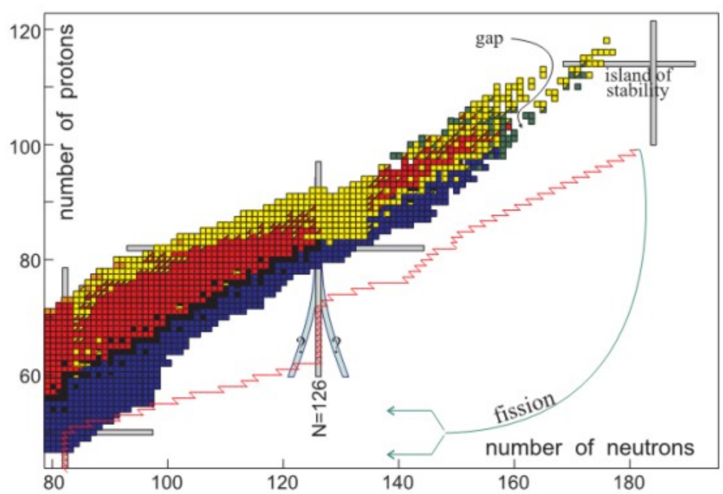
The present limits of the upper part of the nuclear map are very close to stability, while the unexplored area of heavy neutron-rich nuclides (to the east of the stability line around the neutron shell $N = 126$ and $Z \simeq 70$) is extremely important for nuclear astrophysics investigations and, in particular, for the understanding of the r-process of astrophysical nucleogenesis. This "blank spot" of the nuclear map can be reached neither in fusion-fission reactions nor in fragmentation processes widely used nowadays for production of new nuclei. A new way is found to discover and examine unknown neutron-rich heavy nuclei at the "north-east" part of the nuclear map via low-energy multi-nucleon transfer reactions. Several tens of new nuclides can be produced, for example, in near-barrier collision of ^{136}Xe with ^{208}Pb. This finding may spur new studies at heavy ion facilities and should have significant impact for future experiments. Nuclear reactions leading to formation of new superheavy (SH) elements and isotopes ("cold" and "hot" synthesis, fusion of fission fragments, transfer reactions and reactions with radioactive ion beams) are analyzed along with their abilities and limitations. We found that several isotopes of new elements with $Z = 120$ to 124 could be synthesized in fusion reactions of titanium, chromium and iron beams with actinide targets. The use of light and medium mass neutron-rich radioactive beams may help us to fill the gap between the SH nuclei produced in the "hot" fusion reactions and the mainland. In these reactions we may really approach the "island of stability". Such a possibility is also provided by the multi-nucleon transfer processes in low-energy damped collisions of heavy actinide nuclei. In many such collisions lifetime of the composite giant system consisting of two touching nuclei turns out to be rather long (more than 10^{-20} s); sufficient for observing line structure in spontaneous positron emission from super-strong electric fields, a fundamental QED process.



The top part of the nuclear map. The r-process is shown schematically.

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2) V. Zagrebaev and W. Greiner, *Production of new neutron-rich heavy nuclei*, AIP Conference Proceedings, 1098 (2009) 326.

3) A. V. Karpov, V. I. Zagrebaev, and W. Greiner, *Potential energy of heavy nuclear systems in low-energy fusion-fission processes*, submitted to Physical Review C.

Dileptons and charm as probes of the strongly interacting quark-gluon plasma (sQGP) within the parton-hadron-string dynamics (PHSD) transport

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c Institute for Theoretical Physics, University of Giessen, Germany

Our ultimate goal is understanding the dynamical properties of the partonic phase with quarks, antiquarks and gluons as dynamical degrees of freedom (sQGP) and the phase transition to an interacting hadronic system that is colorless and confined. During 2009 we focused on studying how the QGP phase transition influences the charm and dilepton production. The charm quark degrees of freedom are of particular importance since they are expected to be dominantly produced in the early, QGP state of the heavy ion collisions. The dileptons are well suited for an investigation of the violent phases of a high-energy heavy-ion collision, because they can leave the reaction volume essentially undistorted by final-state interactions. The study of dileptons produced in relativistic heavy-ion collisions allows addressing the issue of chiral symmetry restoration and in-medium effects on hadrons, too. As 'research tools' we are using effective field theory based on the high temperature QCD and the microscopic Parton-Hadron-String-Dynamics (PHSD) transport approach.

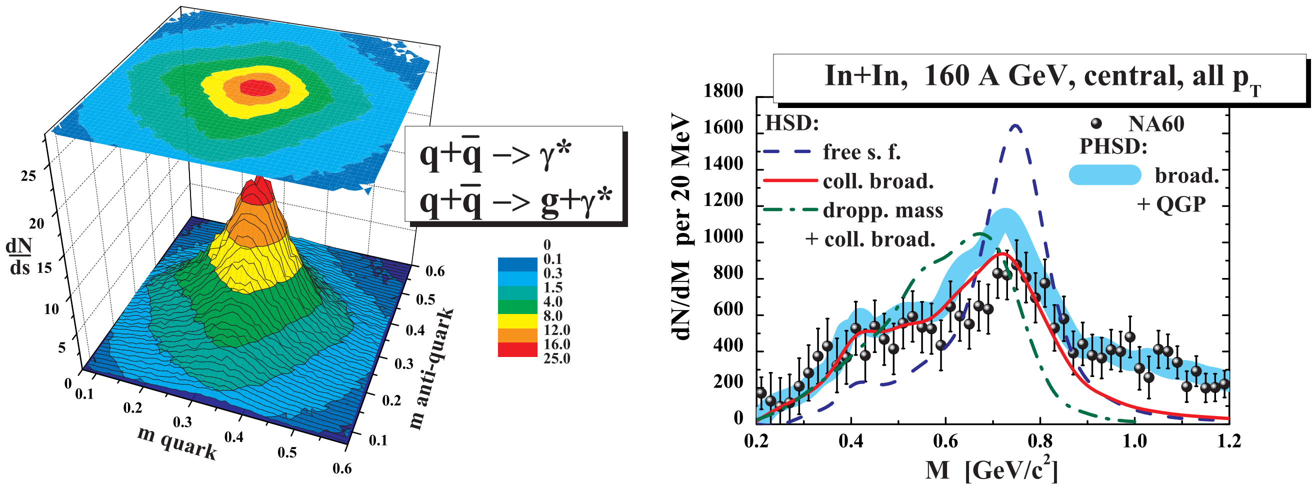

FIG. 1: Left: Quark masses in sQGP. Right: Spectra of dileptons at SPS energy.

At RHIC and LHC energies the radiation from QGP is expected to constitute a large contribution to the dilepton spectrum. On the other hand, at lower energies one probes the physics of the nuclear matter at extremely high baryonic densities as will be produced at the future experimental facility FAIR. The FAIR facility will allow the study of charm hadron production closer to the threshold for charm production in pp reactions so that in-medium effects might have a strong influence on the open and hidden charm production. The dilepton production at FAIR energies will reflect the properties of hadrons in the dense nuclear medium.

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Microscopic description of the phase transition from hadronic to partonic matter and dynamics of hadronization

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The nature of confinement and the dynamics of the phase transition from hadronic to partonic matter is an outstanding question of todays physics. The dynamics of partons, hadrons and strings in relativistic nucleus-nucleus collisions is analyzed within the novel Parton-Hadron-String Dynamics (PHSD) transport approach, which is based on a dynamical quasiparticle model for partons (DQPM) matched to reproduce recent lattice-QCD results - including the partonic equation of state - in thermodynamic equilibrium. Scalar- and vector-interaction densities are extracted from the DQPM as well as effective scalar- and vector-mean fields for the partons. The transition from partonic to hadronic degrees of freedom is described by covariant transition rates for the fusion of quark-antiquark pairs or three quarks (antiquarks), respectively, obeying flavor current-conservation, color neutrality as well as energy-momentum conservation. Since the dynamical quarks and antiquarks become very massive close to the phase transition, the formed resonant 'pre-hadronic' color-dipole states ($q\bar{q}$ or qqq) are of high invariant mass, too, and sequentially decay to the groundstate meson and baryon octets increasing the total entropy.

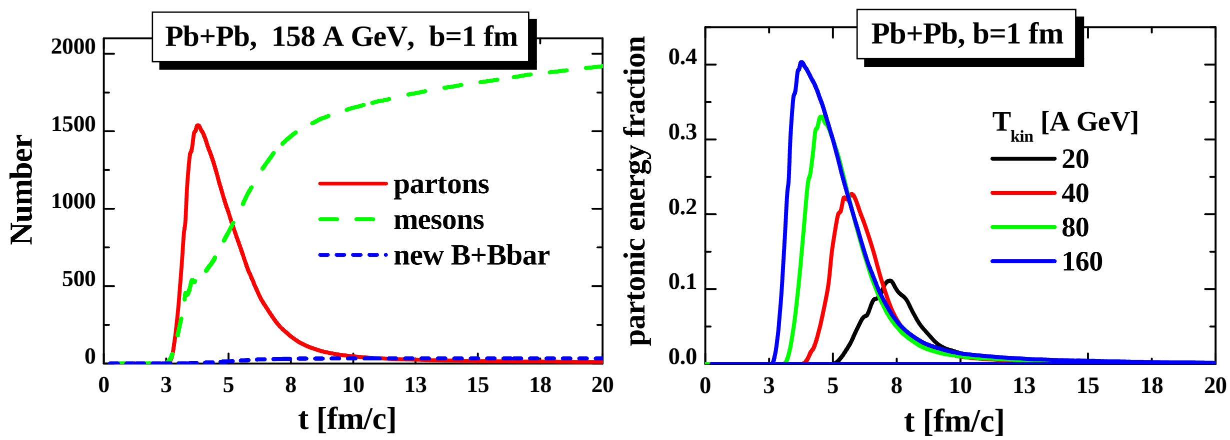

FIG. 1: L.h.s.: The number of produced partons (solid red line), mesons (long dashed green line) and newly produced baryon + antibaryons (blue dashed line) as a function of time for Pb+Pb at 158 A·GeV (for b=1fm). R.h.s.: The partonic energy fraction as a function of time for impact parameter b = 1 fm for Pb+Pb at 160, 80, 40 and 20 A·GeV.

The PHSD approach is applied to nucleus-nucleus collisions from 20 to 160 A·GeV in order to explore the space-time regions of 'partonic matter'. We find that even central collisions at the top-SPS energy of 158 A· GeV show a large fraction of non-partonic, i.e. hadronic or string-like matter, which can be viewed as a hadronic corona. Studying in detail Pb+Pb reactions from 40 to 158 A·GeV - we observe that the partonic phase has a very low impact on rapidity distributions of hadrons but a sizeable influence on the transverse mass distribution of final kaons due to the repulsive partonic mean fields. Furthermore, we find a significant effect on the production of multi-strange antibaryons due to a slightly enhanced $s\bar{s}$ pair production in the partonic phase from massive time-like gluon decay and a larger formation of antibaryons in the hadronization process.

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Fluctuations as a signature for the critical point of the parton-hadron phase transition

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b Institute for Theoretical Physics, University of Frankfurt, Germany
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The study of event-by-event fluctuations in high energy nucleus-nucleus (A+A) collisions opens new possibilities to investigate the phase transition between hadronic and partonic matter as well as the Chromodynamics (QCD) critical point. By measuring the fluctuations one might 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 and the hadron gas.

The powerful tool to study fluctuations in nucleus-nucleus collisions is a nonequilibrium microscopic transport approach HSD (Hadron-String Dynamics) which allows to completely simulate experimental collisions on an event-by-event basis including the influence of experimental acceptance as well as centrality, system size and collision energy.

The influence of participant number fluctuations on hadron multiplicity fluctuations has been emphasized and studied in detail. To make these 'trivial' fluctuations smaller, one has to consider the most central collisions. Indeed, one needs to make a very rigid selection 1% or smaller of the 'most central' collision events.

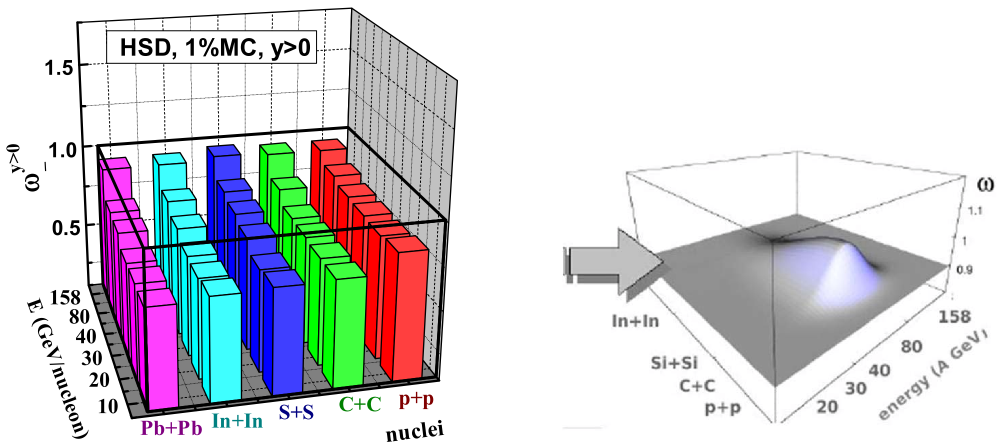

FIG. 1: HSD shows a plateau on the top of which the SHINE Collaboration expects to find increasing multiplicity fluctuations as a "signal" for the critical point

An ambitious experimental program for the search of the QCD critical point has been started by the SHINE Collaboration at the SPS, CERN (Geneva, Switzerland). High statistics multiplicity fluctuation data will be taken for p+p, C+C, S+S, In+In, and Pb+Pb collisions at bombarding energies of $E = 10$, 20, 30, 40, 80, and 158 AGeV. Our investigation is directly related to the future experimental program of the SHINE Collaboration at the SPS for a search of the critical point. The calculations were performed within the HSD microscopic transport approach.

Our findings should be helpful for the optimal choice of collision systems and collision energies for the experimental search of the QCD critical point.

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Fluctuations and Correlations in Statistical Equilibrium Ensembles

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A Monte Carlo event generator has been developed assuming thermal production of hadrons. The system under consideration is sampled grand canonically in the Boltzmann approximation. A re-weighting scheme is then introduced to account for conservation of charges (baryon number, strangeness, electric charge) and energy and momentum, effectively allowing for extrapolation of grand canonical results to the microcanonical limit. This method has two strong advantages compared to analytical approaches and standard microcanonical Monte Carlo techniques, in that it is capable of handling resonance decays as well as (very) large system sizes. In this way one can study the statistical properties of a global equilibrium system in their dependence on the size of their thermodynamic bath.

Fluctuation and correlation observables are amongst the most promising candidates suggested to be suitable for signaling the formation of new states of matter, and transitions between them. The study of event-by-event fluctuations in high energy nucleus-nucleus collisions allows to investigate the connection to quantum chromo dynamics (QCD) and its critical point.

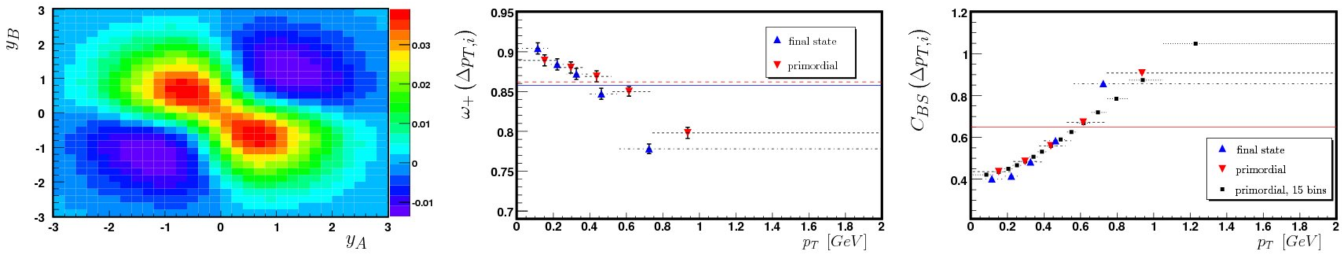

FIG. 1: The statistical hadronization model predicts a systematic behavior of fluctuation and correlation observables on acceptance cuts, conservation laws, and resonance decay. Such as long range correlations amongst particles measured in different rapidity bins (*left*), suppression of multiplicity fluctuations at high transverse momentum (*center*), or an increase of baryon number strangeness correlations also at large transverse momentum (*right*).

The statistical properties of a sample of events are, however, certainly not solely determined by critical phenomena. More broadly speaking, they depend strongly on the way events are chosen for the analysis, and on the information available about the system. We study the first and, in particular, second moments of joint distributions of extensive quantities. We concentrate mainly on particle number distributions and distributions of 'conserved' charges, and discuss the influence of acceptance cuts in momentum space, conservations laws, and resonance decay on the statistical properties of a sample of hadron resonance gas model events. This study should provide a baseline on top of which one would hope to observe new phenomena.

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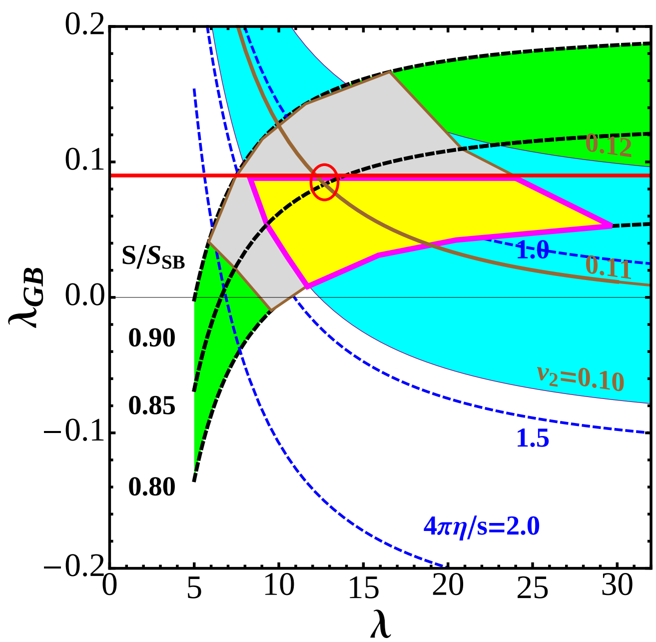
Analysis of AdS/CFT-inspired solutions

Collaborators: Giorgio Torrieri, Miklos Gyulassy, Jorge Noronha

The use of the so-called "AdS-CFT correspondence" to study the collective properties of strongly interacting systems has recently generated a lot of theoretical interest.

While CFT is different from QCD in important ways, this approach provides us with a laboratory to study the collective properties of strongly interacting systems "analytically". Recently [1] we have found ways to constrain parameters in strongly coupled theories with gravity duals using RHIC experimental data. The qualitative step in this description is that it combines data in very different regimes, including static lattice data (the equation of state), soft particle correlations (flow measurements) jet suppression and bulk measurements (multiplicity). A summary of these results is shown in the Figure.

We are also using AdS/CFT to understand to what extent strongly interacting degrees of freedom thermalize, and how they evolve after local thermalization. For instance, in [2, 3]. we examine the "exact" result of an infinitely heavy quark moving in a strongly interacting plasma. We hope to extend our analysis to other solutions in the near future in collaboration with experimental groups.



Space of possible parameters of theories with gravity duals, with experimental and lattice constraints superimposed.

[1] J. Noronha, M. Gyulassy and G. Torrieri, *Constraints on AdS/CFT Gravity Dual Models of Heavy Ion Collisions*, arXiv:0906.4099 [hep-ph].

[2] J. Noronha, G. Torrieri and M. Gyulassy, *Near Zone Navier-Stokes Analysis of Heavy Quark Jet Quenching in an $\mathcal{N}$ =4 SYM Plasma*, Phys. Rev. C78 (2008) 024903

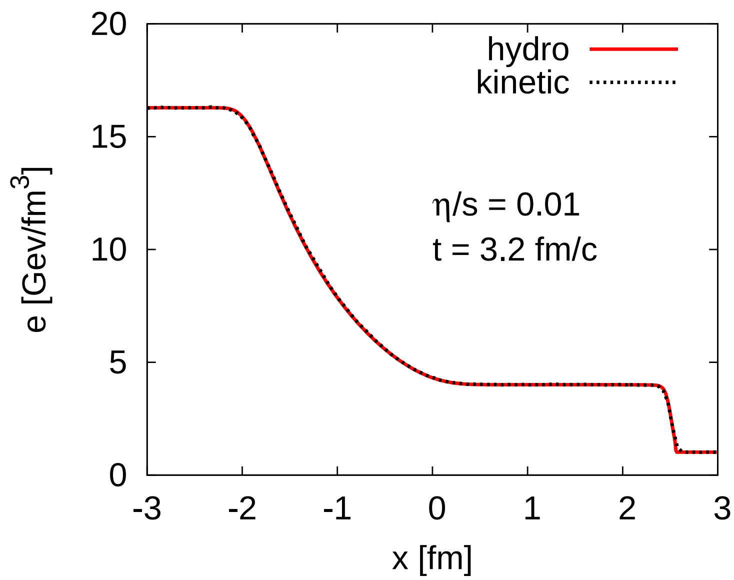
[3] J. Noronha, M. Gyulassy and G. Torrieri, *Di-Jet Conical Correlations Associated with Heavy Quark Jets in anti-de Sitter Space/Conformal Field Theory Correspondence*, Phys. Rev. Lett. 102 (2009) 10231

Applicability of the Israel-Stewart theory of relativistic dissipative hydrodynamics

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

[1] Inst. for Theor. Physics, Goethe Univ., [2] FIAS, [3] EMMI

We study the applicability of the second order Israel-Stewart theory of relativistic dissipative hydrodynamics by testing it against kinetic theory calculations. A quantity that characterizes applicability of hydrodynamical models in transport phenomena is Knudsen number, a ratio of microscopic and macroscopic length scales. We have shown that we get very good agreement between the two models when Knudsen number is small, i.e. when viscous coefficients and gradients of densities and velocity are small. We can also demonstrate that hydrodynamical approach fails when Knudsen number is large.



Energy density profile of the Riemann problem with shear viscosity to entorpy ratio $\eta/s = 0.01$. The solid curve is calculated using the Israel-Stewart theory. The dotted curve shows the result from the kinetic theory (BAMPS).

Related publications in 2009:

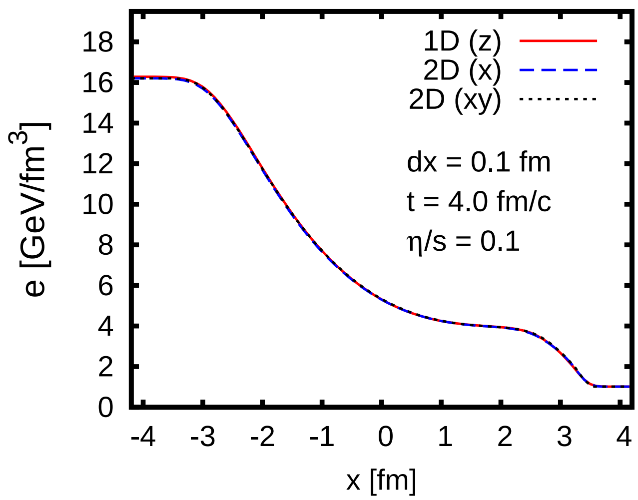
I. Bouras, E. Molnar, H. Niemi, Z. Xu, A. El, O. Fochler, C. Greiner, and D. Rischke, Phys. Rev. Lett. 103 (2009) 032301, [arXiv:0902.1927 [hep-ph]].

Numerical test of the causal relativistic dissipative hydrodynamics

Collaborators: Etele Molnar[1], Harri Niemi[1,2], Dirk H. Rischke[3,1]

[1] FIAS, [2] EMMI, [3] Inst. for Theor. Physics, Goethe Univ.

We have studied numerical algorithms suitable for solving the Israel-Stewart theory of relativistic dissipative hydrodynamics, by solving the Riemann problem in (1+1)- and (2+1)-dimensional geometries. We have shown that we can numerically reproduce the analytical solution to the (1+1)-dimensional Riemann problem in the perfect fluid limit, which shows that algoritms produce only small amount of numerical diffusion. The numerical implementation of the Israel-Stewart equations in (2+1) dimensions with non-zero shear viscosity is tested against (1+1)-dimensional implementation by solving (1+1)- and (2+1)-dimensional Riemann problems.



Energy density profile of the Riemann problem with shear viscosity to entorpy ratio $\eta/s = 0.1$. Solid curve shows result from (1+1)-dimensional implementation of the Israel-Stewart equations. Dashed and dotter curves are calculated with (2+1)-dimensional implementation with different orientations of the initial discontinuity in the xy-plane.

Related publications in 2009:

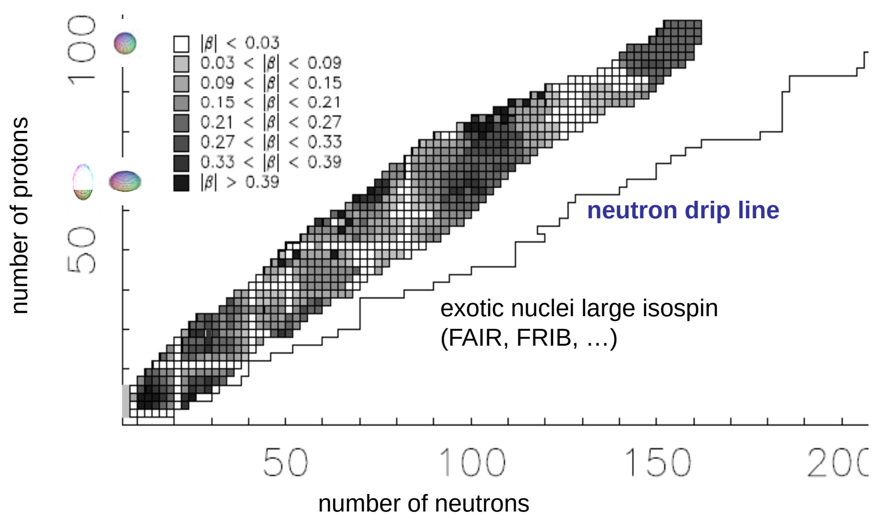
E. Molnar, H. Niemi and D. H. Rischke, arXiv:0907.2583 [nucl-th], accepted in Eur. Phys. J. C

Determination of the Neutron Drip Line

Collaborators: Stefan Schramm[1,2], Dimitry Gridnev[2], K.-N. Linn[3], L. Felipe Ruis[4], Yaser Palenzuela Martinez[4]

[1] FIAS and Center for Scientific Computing (CSC), [2] Helmholtz Postdoctoral Fellow, [3] FIGSS, now Yadanobon Univ., Burma, [4] FIGSS and HGS-HIRe

The exploration of the boundary of the realm of metastable nuclei is at the forefront of many experimental programs and is also highly relevant for nuclear astrophysics. Theoretically, this boundary, defined by the neutron drip line for neutron-rich nuclei is not very well determined. In a newly started, very computer-intensive project we investigate the isospin dependence of the neutron drip line in chiral and other relativistic models by investigating the variability of the drip line on the isospin-dependent part of the strong interactions. This will give different predictions for the existence of exotic nuclei. In the same approach the correlation of the drip line with the properties of the biggest neutron-rich "nuclei", neutron stars, can be determined.



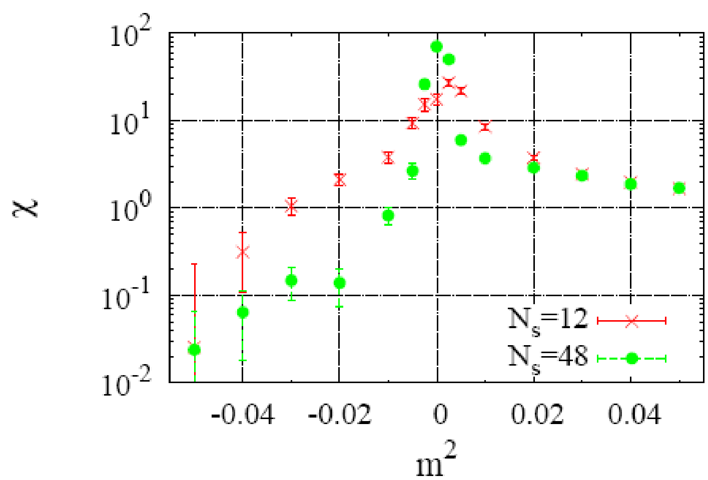
2-dimensional calculation of the deformation of all known even-even nuclei. The graph shows the neutron drip line as calculated in this model.

Lattice simulations of effective models and constrained QCD

Collaborators: Dominik Smith[1], Adrian Dumitru[2], Stefan Schramm[3],

[1] FIGSS and HGS-HIRe, [2] Brookhaven National Laboratory, [3] FIAS and Center for Scientific Computing (CSC),

Whereas QCD lattice simulations constitute in general a very useful method to tackle the problem of non-perturbative QCD, they are very computer-intensive. Therefore, effective descriptions of strongly interaction matter are still important. In a combination of both an effective Polyakov model is investigated in a simulation of the lattice. The aim of the investigation is to show that basic features of QCD can be reproduced in such a significantly simpler approach. To directly connect both methods constraints on the effective field value in a full lattice QCD calculation are introduced, which allow for eventually fixing the parameters of the effective theory via selected full QCD calculations.



Susceptibility of the Polyakov loop, signaling a second-order phase transition at coupling $m^2 = 0$.

Related publications in 2009:

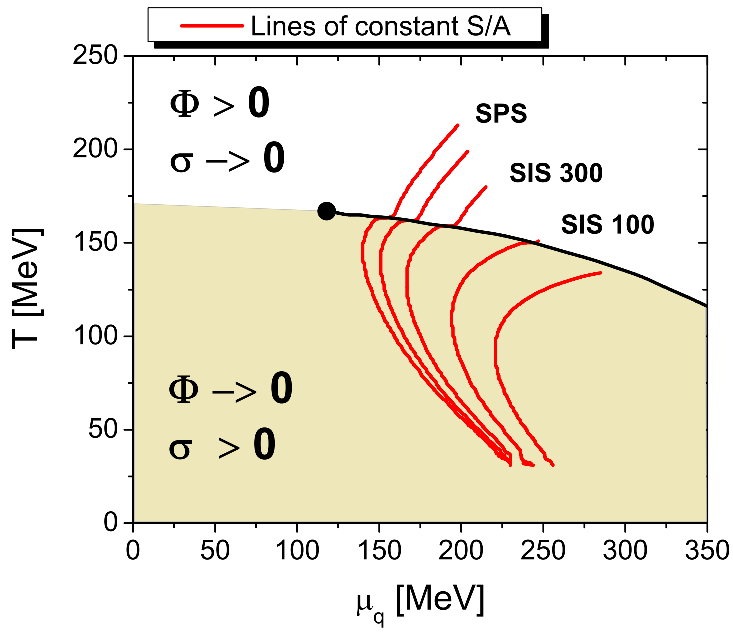
D. Smith, *Lattice simulation of a center symmetric three-dimensional effective theory for SU(2) Yang-Mills*, Nucl. Phys. A820 (2009) 227c

Implementing Quarks and Hadrons in Heavy-Ion Simulations

Collaborators: Stefan Schramm[1,2], Verônica Dexheimer[3], J. Steinheimer-Froschauer[4,5], H. Stöcker[1,4,6]

[1] FIAS, [2] Center for Scientific Computing (CSC), [3] FIGSS, now Gettysburg College, [4] Institute for Theoretical Physics, Goethe University, [5] HGS-HIRe, [6] GSI – Helmholtzzentrum für Schwerionenforschung, Darmstadt,

Most simulations of ultrarelativistic heavy-ion collisions are based on equation of states that do not reproduce the correct asymptotic properties of strongly-interacting matter, that is, quarks and gluons at high temperatures and densities and nucleons and a realistic description of nuclear matter and finite nuclei in the cold, uncompressed state. In our approach we are able to combine both regions in a single coherent model. We employ this framework for the study of the phase structure of strongly interaction matter at high temperatures and densities as well as a source for the equation of state that we use in hydrodynamical simulations.



Isentropes of heavy-ion collisions at different beam energies. A possible critical endpoint in the phase diagram is indicated.

Related publications in 2009:

J. Steinheimer, V. Dexheimer, H. Petersen, M. Bleicher, S. Schramm, H. Stöcker, *Hydrodynamics with a chiral hadronic equation of state including quark degrees of freedom*, submitted to Phys. Rev. C, arXiv:0905.3099 [hep-ph]

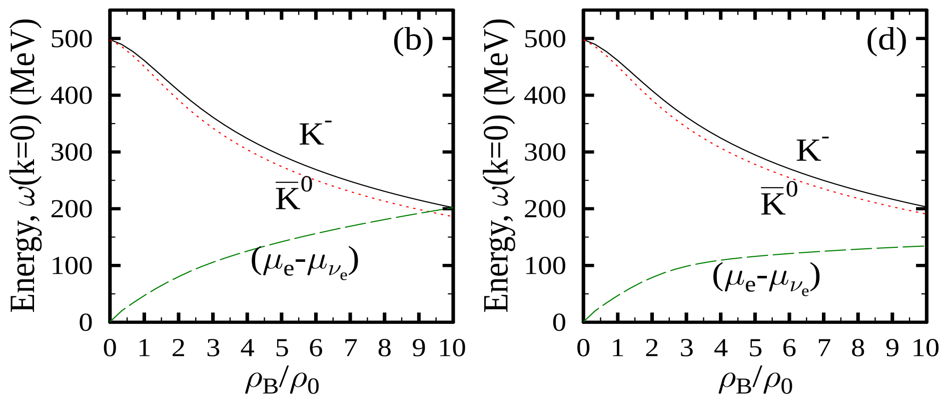
J. Steinheimer, S. Schramm, H. Stöcker, *An effective chiral Hadron-Quark Equation of State Part I: Zero baryochemical potential*, submitted to Phys. Rev. C, arXiv:0909.4421 [hep-ph]

The properties of kaons and possible kaon condensates in dense and hot matter

Collaborators: Stefan Schramm[1], Verônica Dexheimer[2], Amruta Mishra[3]

[1] FIAS and Center for Scientific Computing (CSC), [2] FIGSS, now Gettysburg College, [3] IIT New Delhi, Alexander von Humboldt Visiting Fellow

Understanding the properties of kaons in hadronic matter is essential in understanding heavy-ion collisions as well as the general problem of strangeness in matter. There is a long-standing speculation about the possibility of bose condensates of kaons in extremely dense matter. This effect might have drastic consequences for the stability and cooling behavior of neutron stars, effectively prohibiting large-mass stars, which would be in contradiction to observation. In the project we study the kaon properties under various conditions of density and temperature and determine the onset of the kaon condensate. The stability of the star with respect to condensation in its evolution after the supernova explosion is investigated.



Kaon energies in the hot proto-neutron stars. The critical density for kaon condensation shifts to values beyond ten times nuclear matter groundstate density. This prevents a massive neutron star from collapsing into a black hole during its cooling phase.

Related publications in 2009:

A. Mishra, A. Kumar, S. Sanyal, V. Dexheimer, S. Schramm, *Kaon properties in (proto) neutron stars*, submitted to Phys. Rev. C., arXiv 0905.3518 [nucl-th].

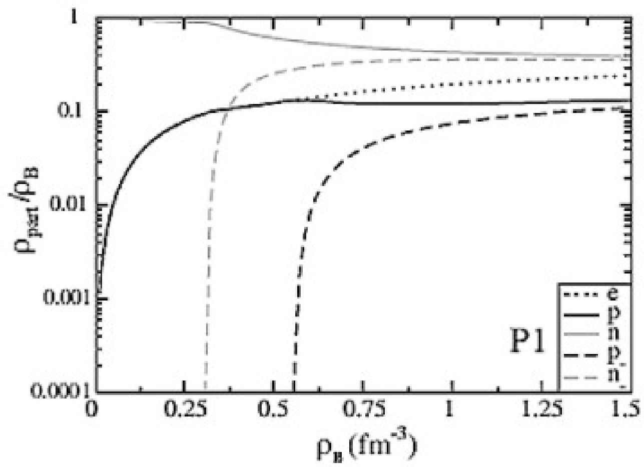
A. Mishra, A. Kumar, S. Sanyal, S. Schramm, *Kaon and antikaon optical potentials in isospin-asymmetric hyperonic matter*, Eur. Phys. J. A41 (2009)205

Hadronic Matter in a SU(3) Parity Model

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

[1] FIAS and Center for Scientific Computing (CSC), [2] Institute for Theoretical Physics, Goethe University, [3] FIGSS, now Gettysburg College

At high densities and temperatures chiral models are in general used to describe the transition to the chirally restored phase with degenerate parity partners like the σ and π meson. In standard approaches this does not hold for the nucleons which become massless but do not have parity partners. In the parity model the nucleonic state with opposite parity is taken into account, which becomes degenerate with the nucleon in the chirally restored phase (see the figure). Thus, new particle species appear under these extreme conditions as produced in heavy-ion collisions and found in neutron stars. After successfully studying this effect in the flavor-$SU(2)$ case we extend the description to include the hyperons, which has not been done before. This is a very new project in development, but the basic theoretical framework has been formulated and first calculations have been performed.



Population of particle species as function of nuclear density. The chiral partners appear at about twice the saturation density of nuclear matter.

Related publications in 2009:

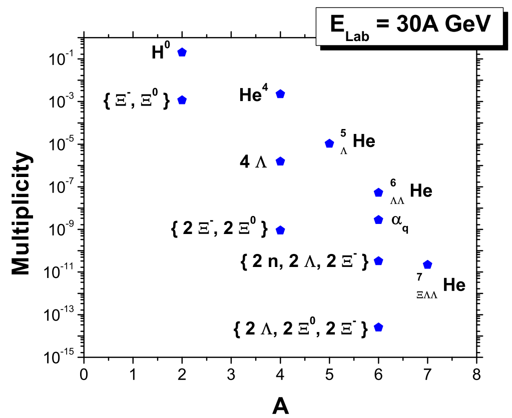
S. Schramm and V. Dexheimer, *Phase structure in hadron-quark models and its implementation in heavy-ion simulations*, Proceedings PANIC 2008, p. 546.

Strangeness fluctuations and the productions of multistrange baryonic objects

Collaborators: M. Mitrovski, H. Petersen, T. Schuster, J. Steinheimer, M. Bleicher

[1] FIAS and Institute for Theoretical Physics, Frankfurt

A coupled transport-hydrodynamics model is used to describe the production of multi-strange meta-stable objects in Pb+Pb reactions at the FAIR facility. Beside the prediction for the yields, also rapidity and transverse momentum distributions were calculated. Our calculations showed that the FAIR energy regime is the optimal place to search for multi-strange baryonic objects, due to the high baryon density, favoring a distillation of strangeness. Using the UrQMD model we calculate the strangeness separation in phase space which might lead to an enhanced production of MEMOs compared to models that assume global thermalization.



Multiplicities of various types of MEMOs and strangelets in central Pb+Pb reactions at $E_{\mathrm{lab}} = 30A$ *GeV.*

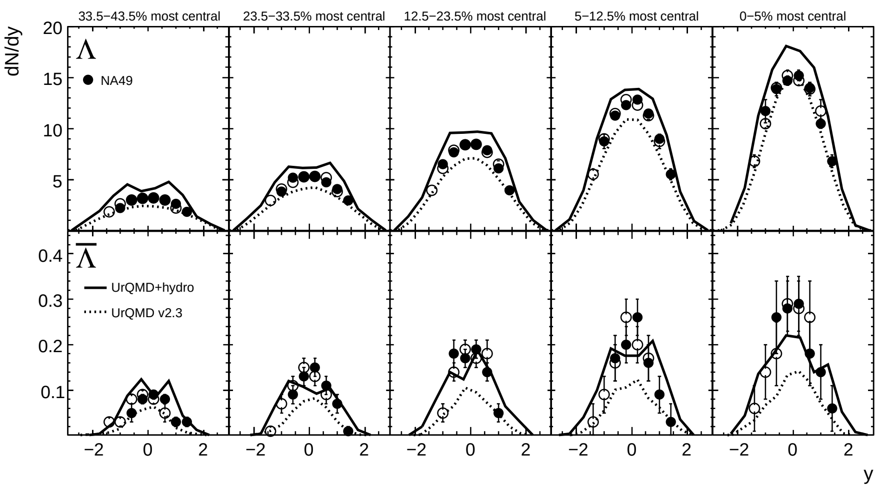
Related publications in 2009:

1) T. Anticic et al. [NA49 Collaboration], *System-size dependence of Lambda and Xi production in nucleus-nucleus collisions at 40A and 158A GeV measured at the CERN Super Proton Synchrotron*, Phys. Rev. C 80 (2009) 034906
2) T. Anticic et al. [NA49 Collaboration], *Inclusive production of protons, anti-protons and neutrons in p+p collisions at 158 GeV/c beam momentum*, arXiv:0904.2708 [hep-ex]
3) A. Adare et al. [PHENIX Collaboration], *Measurement of Bottom versus Charm as a Function of Transverse Momentum with Electron-Hadron Correlations in p+p Collisions at* $\sqrt{(s)} = 200$ *GeV*, Phys. Rev. Lett. 103 (2009) 082002
4) A. Adare et al. [PHENIX Collaboration], *Photon-Hadron Jet Correlations in p+p and Au+Au Collisions at* $\sqrt{s_{NN}} = 200$ *GeV*, Phys. Rev. C 80 (2009) 024908
5) T. Schuster, M. Nahrgang, M. Mitrovski, R. Stock and M. Bleicher, *Analysis of the baryon-, proton-, and charged particle kurtosis in heavy ion collisions within a relativistic transport approach*, arXiv:0903.2911 [hep-ph]
6) H. Petersen, M. Mitrovski, T. Schuster and M. Bleicher, *Centrality and system size dependence of (multi-strange) hyperons at 40A and 158A GeV*, Phys. Rev. C80 (2009) 054910
7) M. Mitrovski, T. Schuster, G. Graf, H. Petersen and M. Bleicher, *Charged particle (pseudo-) rapidity distributions in* $p^+\bar{p}$ */* p^+p *and Pb+Pb/Au+Au collisions from SPS to LHC energies from UrQMD*, Phys. Rev. C 79 (2009) 044901
8) T. Anticic et al. [NA49 Collaboration], *Energy dependence of transverse momentum fluctuations in Pb+Pb collisions at the CERN Super Proton Synchrotron (SPS) at 20A to 158A GeV*, Phys. Rev. C 79 (2009) 044904
9) J. Steinheimer, M. Mitrovski, T. Schuster, H. Petersen, M. Bleicher and H. Stöcker, *Strangeness fluctuations and MEMO production at FAIR*, Physics Letters B 676 (2009) 126
10) C. Alt et al. [NA49 Collaboration], *Energy dependence of particle ratio fluctuations in central Pb+Pb collisions from* $\sqrt{s_{NN}} = 6.3$ *to 17.3 GeV*, Phys. Rev. C 79 (2009) 044910
11) B. I. Abelev et al. [STAR Collaboration], *Longitudinal Spin Transfer to* Λ *and* $\bar{\Lambda}$ *Hyperons in Polarized Proton-Proton Collisions at* $\sqrt{s} = 200$ *GeV*, arXiv:0910.1428 [hep-ex]
12) B. I. Abelev et al. [STAR Collaboration], *Identified particle production, azimuthal anisotropy, and interferometry measurements in Au+Au collisions at* $\sqrt{s_{NN}} = 9.2$ *GeV*, arXiv:0909.4131 [nucl-ex]

An Integrated Boltzmann+Hydrodynamics Approach to Heavy Ion Collisions

Collaborators: Hannah Petersen, M. Mitrovski, T. Schuster, J. Steinheimer, M. Bleicher, H. Stöcker

The integrated approach allows for a systematic investigation of expansion dynamics of the fireball created in heavy ion collisions in the energy regime of CERN-SPS and the future FAIR facility. The newly developed hybrid approach is based on the Ultra-relativistic Quantum Molecular Dynamics (UrQMD) model including an ideal hydrodynamic evolution for the hot and dense stage. This combined microscopic and macroscopic approach aims at the exploration of observables sensitive to the quark gluon plasma phase transition. Furthermore, the differences in the expansion dynamics of a hadronic transport vs. ideal fluid dynamics, with an hadronic equation of state, are investigated.



Rapidity distribution of Λ (top) and $\overline{\Lambda}$ (bottom) from NA49 measured for different centralities in Pb + Pb collisions at 158A GeV. Solid (dashed) lines: UrQMD + hydro (UrQMD only) calculations.

Related publications in 2009:

1) H. Petersen, M. Mitrovski, T. Schuster and M. Bleicher, *Centrality and system size dependence of (multi-strange) hyperons at 40A and 158A GeV: A comparison between a binary collision and a Boltzmann+hydrodynamic hybrid model*; Phys. Rev. C 80 (2009) 054910

2) H. Petersen, J. Steinheimer, G. Burau and M. Bleicher, *A transport calculation with an embedded (3+1)d hydrodynamic evolution: Elliptic flow as a function of transverse momentum at SPS energies*; Nucl. Phys. A830 (2009) 283c

3) J. Steinheimer, M. Mitrovski, T. Schuster, H. Petersen, M. Bleicher and H. Stöcker, *Strangeness fluctuations and MEMO production at FAIR*; Phys. Lett. B 676 (2009) 126-131

4) H. Petersen and M. Bleicher, *Ideal hydrodynamics and elliptic flow at SPS energies: Importance of the initial conditions*; Phys. Rev. C 79 (2009) 054904

5) M. Mitrovski, T. Schuster, G. Graef, H. Petersen and M. Bleicher, *Charged particle (pseudo-)rapidity distributions in proton+anti-proton/proton+proton and Pb+Pb/Au+Au collisions from SPS to LHC energies from UrQMD*; Phys. Rev. C79 (2009) 044901

5) H. Petersen, J. Steinheimer, M. Bleicher and H. Stöcker, $\langle m_T \rangle$ *excitation function: Freeze-out and equation of state dependence*; J. Phys. G: Nucl. Part. Phys. 36 (2009) 055104

6) Q. Li, J. Steinheimer, H. Petersen, M. Bleicher, H. Stöcker, *Effects of a phase transition on HBT correlations in an integrated Boltzmann+Hydrodynamics approach*; Phys. Lett. B674 (2009) 111-116

7) J. Steinheimer, H. Petersen, G. Burau, M. Bleicher and H. Stöcker, *Strangeness production and local thermalization in an integrated Boltzmann+Hydrodynamics approach*; Acta Phys. Polon. B40 (2009) 999

8) H. Petersen, J. Steinheimer, G. Burau, M. Bleicher, *Elliptic flow in an integrated (3+1)d microscopic+macroscopic approach with fluctuating initial conditions*; Eur. Phys. J. C62 (2009, 31-36

Dissipative hydrodynamics and stochastic dynamics

Collaborators: T. Koide, X. Huang, T. Kodama, E. Nakano, S. Pu, D. Rischke, M. Mine, M. Okumura, Y. Yamanaka

Project 1: Microscopic formula for transport coefficients in Causal Dissipative Hydrodynamics

The most important result is the derivation of the transport coefficients. Since the relativistic fluid becomes a non-Newtonian fluid because of causality and stability, we cannot use the traditional Green-Kubo-Nakano (GKN) formula to calculate the coefficients. We proposed a new microscopic formulae to calculate the shear viscosity η and the corresponding relaxation time τ_π, and show that, in the leading order approximation, there are simple relationships,

$$\eta = \eta_{GKN}, \quad \tau_\pi = \eta_{GKN}/P,$$

where P is the pressure and η_{GKN} is the GKN formula for the shear viscosity of relativistic Navier-Stokes theory.

Project 2: Stability and causality in Causal Dissipative Hydrodynamics

The naive relativistic extension of Navier-Stokes theory suffers from the problem of relativistic acausality. However, it is sometimes claimed that the violation of causality is not pragmatically important and we can still use the relativistic Navier-Stokes theory to discuss the collective behaviors of relativistic heavy-ion collisions.
In this project, we showed that the problem of acausality and instability are related, that is, if the theory violates causality it leads to the instability of the theory. This indicates that causality is a pragmatic problem and we should not use the relativistic Navier-Stokes theory.

[Project 3: Fluctuation theorem and Stochastic Dynamics

The fluctuation theorem is derived from the different behavior of the time-forward and -backward processes. In the deterministic dynamics such as the Liouville equation, the evolution of the time reversed process is trivially obtained by changing the sign of time. On the other hand, the reverced process is not obtained by this simple manipulation.
We proposed a new model for non-equilibrium stochastic model including the time reversed evolution explicitly and showed that several different fluctuation theorems are unified by extending the concept of thermodynamic relation.

Related publications in 2009:

1) T. Koide, E. Nakano and T. Kodama, *Shear viscosity coefficient and relaxation time of causal dissipative hydrodynamics in QCD*, Phys. Rev. Lett. 103 (2009) 052301
2) S. Pu, T. Koide and D. H. Rischke, *Does stability of relativistic dissipative fluid dynamics imply causality?*, arXiv:0907.3906
3) T. Koide, M. Mine, M. Okumura and Y. Yamanaka, *Extended Thermodynamic Relation and Fluctuation Theorem in Stochastic Dynamics with Time Reversed Process*, arXiv:0907.3383

The horn, the hadron mass spectrum and the QCD phase diagram

A. Andronic[1], P. Braun-Munzinger[1,2,3,4], and J. Stachel[5]

[1]GSI Darmstadt, Germany; [2]ExtreMe Matter Institute, GSI Darmstadt, Germany; [3]Technical University Darmstadt, Germany; [4]FIAS, J.W Goethe University, Frankfurt, Germany; [5]University of Heidelberg, Germany

The analysis of hadron yields measured in central heavy ion collisions from AGS up to RHIC energies has shown [2] that hadron multiplicities can be described very well with a hadro-chemical equilibrium approach which is governed by the chemical freeze-out temperature T, baryochemical potential μ_b, and the fireball volume V. The main result of these investigations was that the extracted temperature values rise rather sharply from low energies on towards $\sqrt{s_{NN}}$ $\simeq$10 GeV and reach afterwards constant values near T=160 MeV, while the baryochemical potential decreases smoothly as a function of energy. While in general all hadron yields are described rather quantitatively [2], a notable exception was up-to-now the energy dependence of the K^+/π^+ ratio which exhibits a rather marked maximum, "the horn" [3], near $\sqrt{s_{NN}} \simeq$ 10 GeV [4].

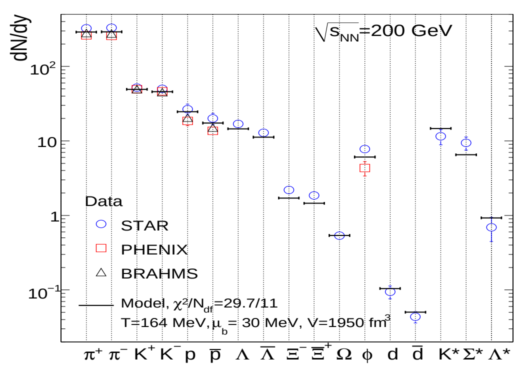


Figure 1: Experimental hadron yields and model fit at 200 GeV.

We have performed recently [1] a new analysis of hadron production in central nucleus-nucleus collisions, with the aim to explore the consequences of an improved hadronic mass spectrum in which the σ meson and many higher-lying resonances are included. An example of a fit to the data is shown in Fig. 1 for the energy of 200 GeV. The model is successful in reproducing the measurements and this applies to all energies, from 2 AGeV beam energy (fixed target) up to the top RHIC energy of $\sqrt{s_{NN}}$=200 GeV. The reduced χ^2 values are reasonable. In most cases the fit quality is improved compared to our earlier analysis [2], even though the experimental errors are now smaller. An important result of our analysis is that the resulting thermal parameters are close to those obtained earlier [2].

We employ parametrizations of T and μ_b to investigate the energy dependence of the relative production yields K^+/π^+ and Λ/π^-, shown in Fig. 2. The K^+/π^+ ratio shows a rather pronounced maximum at a beam energy

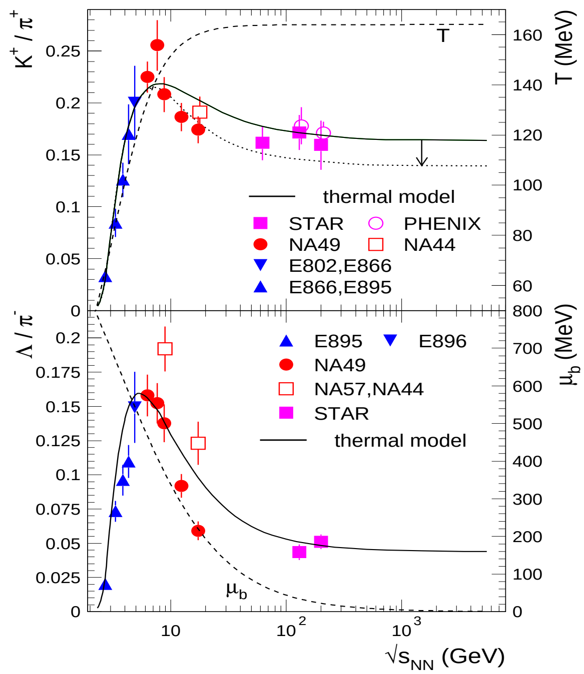


Figure 2: Energy dependence of the relative production ratios K^+/π^+ and Λ/π^-. The dashed lines show the energy dependence of T (upper panel) and μ_b (lower panel).

of 30 AGeV [4], and the data are well reproduced by the model calculations. In the thermal model this maximum occurs naturally at $\sqrt{s_{NN}}$ $\simeq$8 GeV [5]. It is due to the counteracting effects of the steep rise and saturation of T and the strong monotonous decrease in μ_b. The competing effects are most prominently reflected in the energy dependence of the Λ hyperon to pion ratio (lower panel of Fig. 2), which shows a pronounced maximum at $\sqrt{s_{NN}}$ $\simeq$5 GeV. This is reflected in the K^+/π^+ ratio somewhat less directly; it appears mainly as a consequence of strangeness neutrality, assumed in our calculations.

References

[1] A. Andronic, P. Braun-Munzinger, J. Stachel, Phys. Lett. B **673** (2009) 142 [arXiv:0812.1186], Erratum: ibid. B **678** (2009) 516; Acta Phys. Pol. **40** (2009) 1005 [arXiv:0901.2909].

[2] A. Andronic, P. Braun-Munzinger, J. Stachel, Nucl. Phys. A **772** (2006) 167.

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[5] P. Braun-Munzinger, J. Cleymans, H. Oeschler, K. Redlich, Nucl. Phys. A **697** (2002) 902.

Statistical hadronization of heavy flavor quarks in elementary collisions: successes and failures

A. Andronic[1], F. Beutler[6], P. Braun-Munzinger[1,2,3,4], K. Redlich[5,2], and J. Stachel[6]

[1]GSI Darmstadt, Germany; [2]ExtreMe Matter Institute, GSI Darmstadt, Germany; [3]Technical University Darmstadt, Germany; [4]FIAS, J.W Goethe University, Frankfurt, Germany; [5]University of Wrocław, Poland; [6]University of Heidelberg, Germany

We analyze recently compiled data on the production of open heavy flavor hadrons and quarkonia in e^+e^- as well as pp and p-nucleus collisions in terms of the statistical hadronization model [1].

In Fig. 1 we show a comparison of data and model prediction. for charmed and bottom hadron yields in e^+e^- annihilations at $\sqrt{s}$=91 GeV. For the model we have used the parameter set: T=170 MeV, V=16 fm^3 and γ_s=0.66, which represents the best fit of multiplicities of hadrons with lighter quarks [1].

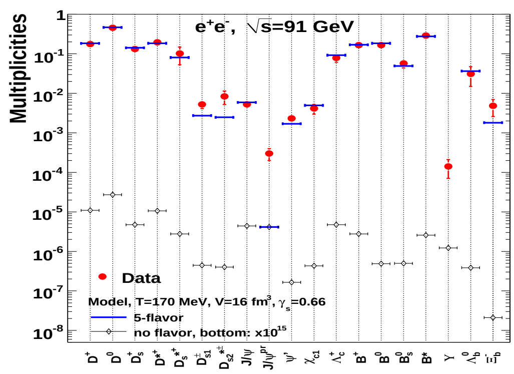

Figure 1: Multiplicities of hadrons with charm and bottom quarks in e^+e^- collisions compared to the thermal model calculations for two cases: i) the 5-flavor jet scheme (thick lines) and ii) no (net) flavor jet scheme (thin lines with diamonds). Note, for case ii) the factor 10^{15} used to scale the model calculations for bottom hadrons to fit in the plotting range.

The calculation employing the 5-flavor scheme is in very good agreement with the data. Despite this overall agreement, the exceptions are significant: the Υ meson yield is underpredicted by the model by 17 orders of magnitude, while the prompt J/ψ yield is underpredicted by almost 2 orders of magnitude. Obviously, the production of quarkonia is expected to be strongly suppressed in the statistical model. The disagreement is a consequence of the separate hadronization of the c and $\bar{c}$ quarks. The measured prompt J/ψ production in Z^0 decays (into hadrons) is about 3×10^{-4}. The thermal model predicts a prompt yield for J/ψ of 4.1×10^{-6} (1.6×10^{-7} for ψ' and 4.3×10^{-7} for χ_{c1}), identically for the two calculation schemes. Whenever the model seems to describe the yields of charmonia the measured yields are dominated by the feed down from bottom hadrons and the agreement only reflects the agreement seen for the open bottom hadrons and their branching ratios to charmonia, properly considered in the model.

The calculation employing a purely thermal ansatz underpredicts all the measurements by many oders of magnitude, while for the light quark sector the differences between calculations with a pure thermal model and with the 5-flavor quark-antiquark scheme were found to be small [1]. This reflects the fact that a negligible number of c and b quarks are formed in the fragmentation process.

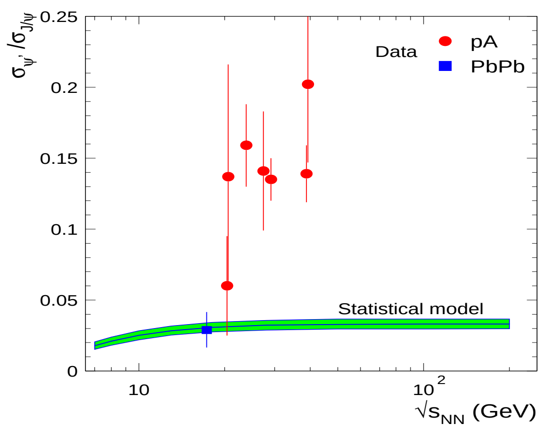

Figure 2: Production cross section of ψ' relative to J/ψ.

In Fig. 2 we show the model comparison to data for the relative production cross section of J/ψ and ψ' charmonia. The measurements in pA collisions are about a factor 4 above the model values. The relative production cross sections of charmonium states cannot be described in the thermal approach. This is in sharp contrast to the (only currently existing) measurement in central nucleus-nucleus collisions, performed at the SPS by the NA50 experiment, which is well described. We recall that it was in part the observation of this measurement that brought forward the idea of statistical production of charmed hadrons in nucleus-nucleus collisions [2]. We note that the pA data exhibit a constant $\psi'/J/\psi$ production ratio as a function of energy. In the model, the value is determined only by the temperature and this is reflected in the slight decrease of the ratio towards low energies. A constant value, also up to the LHC energies, is predicted beyond $\sqrt{s_{NN}}$ $\simeq$20 GeV.

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Nuclear composition in supernova explosions and multifragmentation reactions

A.S. Botvina and I.N. Mishustin, FIAS

During the collapse of massive stars, and the supernova type-II explosions, stellar matter reaches baryon densities $\rho \approx (10^{-5} \div 2)\rho_0$ ($\rho_0 \approx 0.15$ fm^{-3} is the normal nuclear density), and temperatures $T \approx (0.5\div 10)$ MeV. These conditions are similar to those which are reached in nuclear multifragmentation reactions. Multifragmentation, i.e., a break-up of nuclei into many small fragments, has been observed and investigated in nearly all types of reactions when a large amount of energy is deposited in nuclei. It is believed that this process is a manifestation of a liquid-gas phase transition in nuclear matter. As demonstrated by many calculations this type of reactions can be very successfully described by the Statistical Multifragmentation Models (SMM). Analyses of experimental data show that the properties of fragments imbedded in hot environment are modified in comparison with cold isolated nuclei. In particular, their symmetry energy is decreased. It has important consequences for astrophysical processes proceeding through similar conditions of matter. For example, a nearly adiabatic collapse of the massive stars with typical entropies of 1-2 per baryon passes exactly through the liquid-gas coexistence region in the nuclear phase diagram.

The SMM was generalized for supernova conditions by including electron, neutrino, and photon interactions in stellar matter. In Fig. 1 we present the results of SMM calculations [1, 2] of fragment yields for two situations: 1) multifragmentation of *Au* sources at different excitation energies (3, 5, 8 MeV per nucleon), and 2) clusterization of stellar matter with density ρ, electron fraction Y_e, and temperatures T expected during the collapse of massive stars and supernova explosions. One can see that the evolution of mass distributions with increasing excitation energy is qualitatively the same for the both considered systems. However, in the supernova environments much heavier and neutron-rich nuclei can be formed, because of the screening effect of surrounding electrons. Moreover, the nuclei become very large when the fragment symmetry energy coefficients γ is reduced from 25 to 15 MeV, as obtained in multifragmentation reactions. This provides a new mechanism for producing heavy and superheavy nuclei in supernova environments. Rates of weak reactions (e.g., electron capture, neutrino scattering) also depend crucially on the nuclear composition and fragment symmetry energy. As was discussed in [2, 3, 4] these effects are important in constructing a realistic EOS of stellar matter for numerical simulations of supernova explosions.

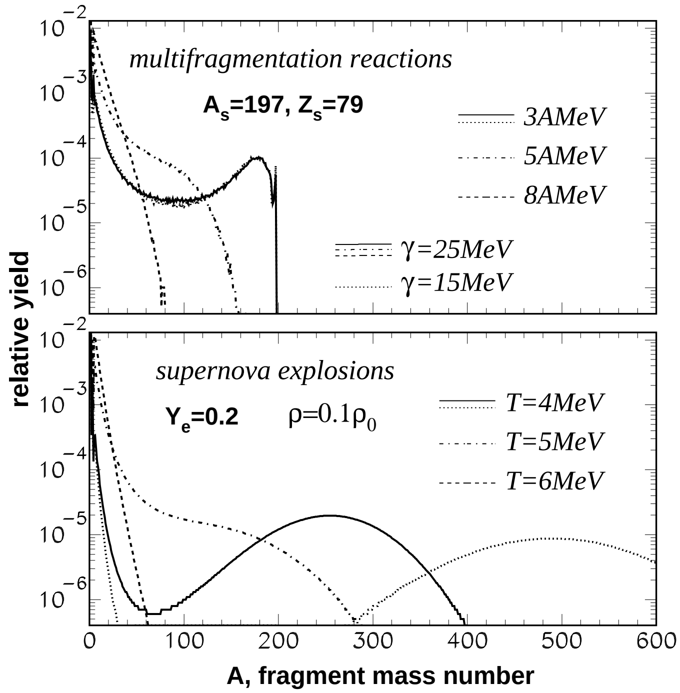

Figure 1: Composition of nuclear fragments produced in multifragmentation and in supernova environment.

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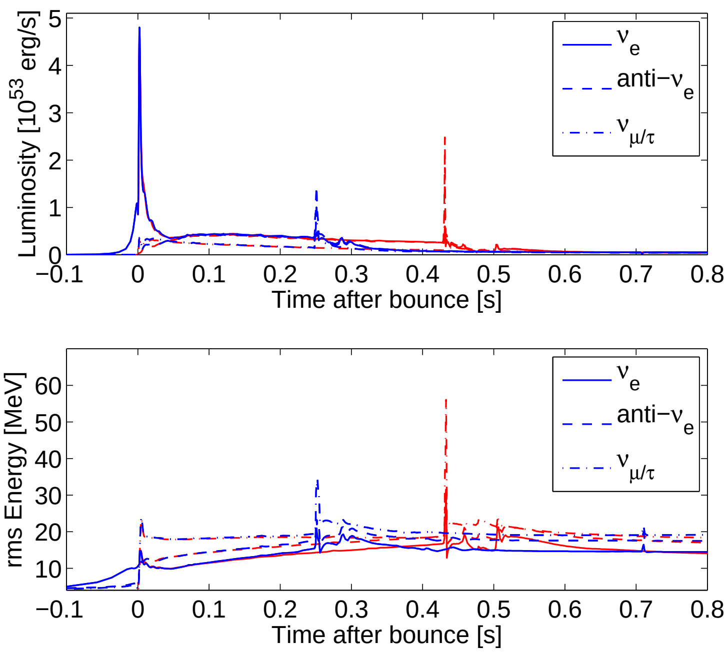
Strange Quark Matter in Explosive Astrophysical Systems

Collaborators: Matthias Hempel[1,2,3], Giuseppe Pagliara[4], Irina Sagert[3], Jürgen Schaffner-Bielich[4]

[1] FIAS, [2] GP-HIR, [3] H-QM, [4] EMMI

We work on a strange quark matter equation of state constructed as an input for modeling explosive astrophysical systems. The hadronic part is taken from an existing equation of state for astrophysical simulations, while for the quark equation of state we chose the MIT Bag Model. We explore the implications of the QCD phase transition during the early postbounce evolution of core-collapse supernovae, where the phase transition produces a second shock wave that triggers a delayed supernova explosion, accompanied by a burst of neutrinos, which will be observable by today's and future neutrino detectors. Furthermore simulations of strange star mergers were performed, combined with estimates of stellar binary populations. We found that the flux disappears for high values of the bag constant leading to the possibility that strange stars could coexist with ordinary neutron stars as the latter are not converted by the capture of cosmic ray strangelets.



Neutrino signal for different bag constants for the supernova explosion of a 10 $M_\odot$ progenitor. The second anti-neutrino burst is caused by the appearance of quark matter.

Related publications in 2009:

1) I. Sagert, M. Hempel, G. Pagliara, J. Schaffner-Bielich, T. Fischer, A. Mezzacappa, F.-K. Thielemann, M. Liebendörfer, Phys. Rev. Lett. 102 (2009) 081101
2) A. Bauswein, H.-T. Janka, R. Oechslin, G. Pagliara, I. Sagert, J. Schaffner-Bielich, M.M. Hohle, and R. Neuhäuser, Phys. Rev. Lett 103 (2009) 011101
3) I. Sagert, M. Hempel, D. Pagliara, J. Schaffner-Bielich, T. Fischer, A. Mezzacappa, F.-K. Thielemann, and M. Liebendörfer, J. Phys. G Nucl. Phys. 36 (2009) 064009
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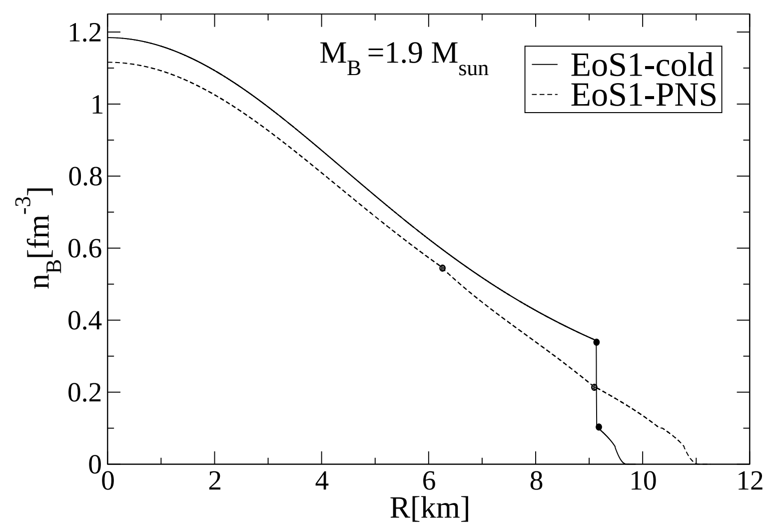
Phase Transitions in Supernovae, Proto-Neutron and Neutron Stars

Collaborators: Matthias Hempel[1,2,3], Giuseppe Pagliara[4], Jürgen Schaffner-Bielich[4], [1] FIAS, [2] GP-HIR, [3] H-QM, [4] EMMI

In astrophysical systems plenty of first order phase transitions can occur, as e.g. the liquid-gas phase transition of nuclear matter or the hadron-quark phase transition. Such phase transitions can have significant consequences on the stars evolution and its stability. E.g. the phase transition to quark matter may trigger the collapse to a black hole. In this research project we study the general properties of phase transitions but also investigate the details and peculiarities of selected systems. The aim is to find imprints of phase transitions on astrophysical scenarios which then can be confronted with astronomical observations.



Density profiles for a neutron star with a baryon mass of $1.9M_\odot$ for the proto-neutron star stage and the cold configuration. The dots mark the onset and the end of the phase transition for a mixed phase with locally charge neutral phases. It can be seen that the mixed phase disappears during the cooling which may lead to the collapse to a black hole.

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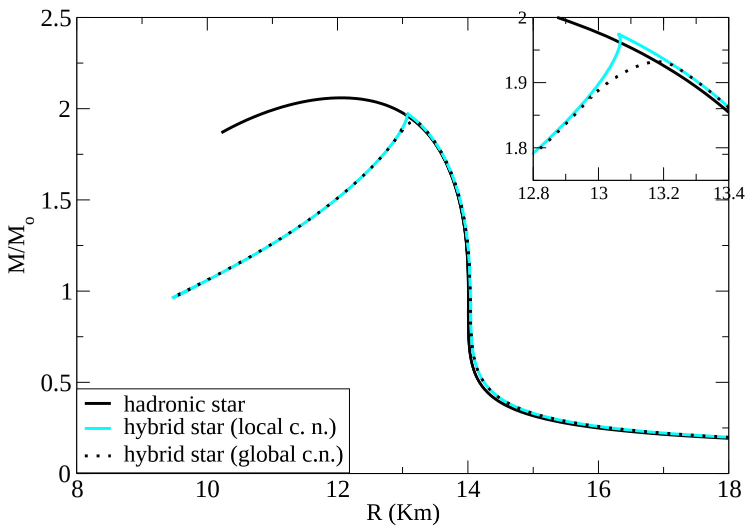
1) B.W. Mintz, E. Fraga, G. Pagliara, and J. Schaffner-Bielich, arXiv:0910.3927
2) G. Pagliara, M. Hempel, and J. Schaffner-Bielich, Phys. Rev. Lett. 103 (2009) 171102
3) M. Hempel, G. Pagliara, and J. Schaffner-Bielich, Phys. Rev. D80 (2009)125014

Description of neutrons stars and hybrid quark-hyper stars

Collaborators: Stefan Schramm[1], Verônica Dexheimer[2]

[1] FIAS and Center for Scientific Computing (CSC), [2] FIGSS, now Gettysburg College,

We study the evolution of neutron stars in a three-flavor chiral effective model. In this approach also finite nuclei can be calculated which allows for the direct comparison of the effect of isospin-dependent interactions on the properties of stars as well as nuclei, connecting both fields of research. A new approach of including quark and gluon degrees of freedom has been introduced. On this basis the study of compact stars is possible that consist of nucleons, hyperons, as well as quarks in the core of the star at zero and finite temperature. Results show that the quarks inside of the star generate a softening of the equation of state, limiting the maximum star mass that is attainable.



The figure shows hybrid star masses and radii. The relatively sharp structure at about 1.95 solar masses is generated by the influence of quarks inside of the star.

Related publications in 2009:

V. Dexheimer and S. Schramm, *A Novel Approach to Model Hybrid Stars*, submitted to Phys. Rev. C; arXiv:0901.1748 [astrop-ph].

V. Dexheimer and S. Schramm, *Neutron Stars as a Probe for Dense Matter*, Nucl. Phys. A827 (2009) 579c.

V. Dexheimer and S. Schramm, *Chiral Symmetry Restoration and Deconfinement to Quark Matter in Neutron Stars*, preprint arXiv:0910.1312 [astro-ph].

Stellar electron capture rates

A.A. Dzhioev[3], A.I. Vdovin[3], V.Yu. Ponomarev[4], J. Wambach[2,4], K. Langanke[1,2,4], G. Martínez-Pinedo[2], A. Juodagalvis[5], R.W. Hix[6], and J.A. Sampaio[7]

[1]Frankfurt Institute of Advanced Studies, Frankfurt, Germany; [2]GSI Helmholtzzentrum für Schwerionenforschung, Germany; [3]Bogoliubov Laboratory, Dubna, Russia; [4]Technische Univeristät Darmstadt, Institut für Kernphysik, Germany; [5]VU ITPA, Vilnius, Lithuania; [6]Oak Ridge National Laboratory, USA; [7]CFNUL, Lisboa, Portugal

Electron captures on nuclei play an important role for the dynamics of the collapsing core in the supernova explosion of a massive star [1]. We have proposed a new method to calculate stellar weak-interaction rates [2]. It is based on the thermo-field-dynamics formalism and allows the calculation of the Gamow-Teller and forbidden strength distributions in nuclei at finite temperatures. The thermal evolution of the GT_+ distributions has been studied in details for the sample nuclei ^{54,56}Fe and ^{76,78,80}Ge. We show that in our model thermal effects shift the GT_+ centroid to lower excitation energies and make possible negative- and low-energy transitions (Fig. 1). Using ^{78}Ge as an example, we demonstrate that the unblocking effect for GT_+ transitions in neutron-rich nuclei is sensitive to increasing temperature. The obtained GT_+ distributions are used to calculate electron capture rates and are compared to those obtained from shell model calculations.

Recent tabulations of stellar electron capture rates were based on microscopic models which account for relevant degrees of freedom [3, 4]. Due to computational limitations such calculations were restricted to a modest number of nuclei, mainly in the mass range $A = 45 - 110$. Recent supernova simulations show that this pool of nuclei, however, omits the very neutron-rich and heavy nuclei which dominate the nuclear composition during the last phase of the collapse before neutrino trapping. Assuming that the composition is given by Nuclear Statistical Equilibrium we have presented electron capture rates for collapse conditions derived from individual rates for around 2700 nuclei [5]. For those nuclei which dominate the early stage of the collapse the individual rates are derived within the framework of microscopic models, while for the nuclei which dominate at high densities we have derived the rates based on the Random Phase Approximation with a global parametrization of the single particle occupation numbers. Finally we have improved previous rate evaluations by properly taking screening corections into account.

This work is supported by the HIC for FAIR and EMMI Programs.

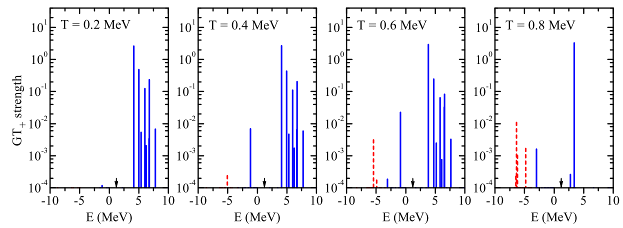


Figure 1: Temperature evolution of GT_+ strength distribution, calculated in the TQRPA model for ^{54}Fe.

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The νp-process in gamma-ray burst accretion disks

L.T. Kizivat[2,3], K. Langanke[1,2,3], G. Martínez-Pinedo[2], R. Surman[4], and G.C. McLaughlin[5]

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The νp-process has recently been associated to proton-rich supernova ejecta, where the absorption of antineutrinos on free protons produce neutrons which later, via (n,p) reactions, help to overcome waiting point nuclei with long beta-decay half lives. In this way light-p nuclei and in particular ^{92,94}Mo and ^{96,98}Ru can be synthesized, which had been an outstanding problem in the understanding of the origin of the elements in the Universe [1].

Similar conditions as in supernova ejecta are also found in proton-rich outflows from gamma-ray bursts accretion disks (Fig. 1). In our work we have explored the possibility that such outflows are a site of the νp-process. The efficancy of the νp-process depends on thermodynamic and hydrodynamic factors like entropy of the material, the outflow rate, the initial ejection point and accretion rate of the disk. We have performed detailed nucleosynthesis simulation to check whether gamma-ray burst accretion disks are indeed another site for the νp process and to identify the sensitivity of the νp-process abundances from those quantities which determine the outflows. We find that in some cases the νp-process pushes the nucleosynthesis out to $A \sim 100$ and produces light p-nuclei. An example is shown in Fig. 2. However, even when these nuclei are not produced, neutrino induced interactions can significantly alter the abundance pattern and cannot be neglected.

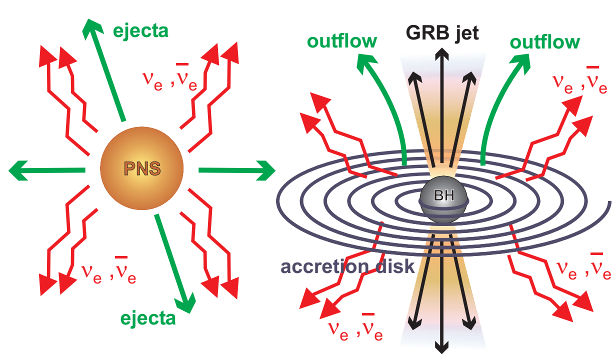

Figure 1: Scheme of the geometry in core collapse supernovae and gamma-ray burst accretion disks. 'PNS' is the nascent remnant, the proto-neutron star. Neutrinos and matter in the early ejecta are emitted radially. 'BH' denotes the Black Hole, the central engine in a gamma-ray burst accretion disk. The outflows leave the disk vertically.

This work is supported by the HIC for FAIR and EMMI Programs.

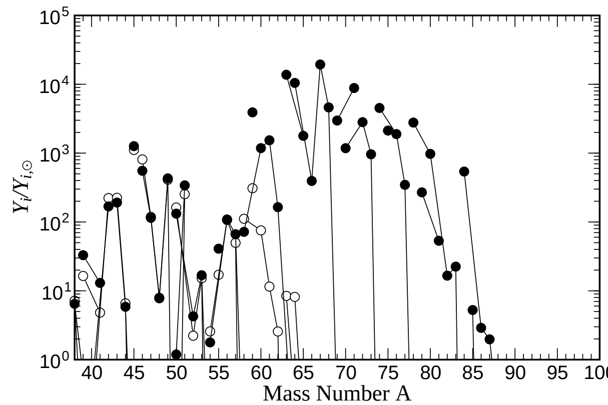

Figure 2: Final isotopic abundances for the nucleosynthesis in a specific disk model. The dotted line shows the abundances obtained with the same nucleosynthesis network, however, switching off neutrino and anti-neutrino capture reactions once the freeze-out value for the electron-to-nucleon value is reached.

Publications

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[2] L.-T. Kizivat, G. Martinez-Pinedo, K. Langanke, R. Surman and G.C. McLaughlin, submitted to Phys. Rev. C; arXiv:1001.3009

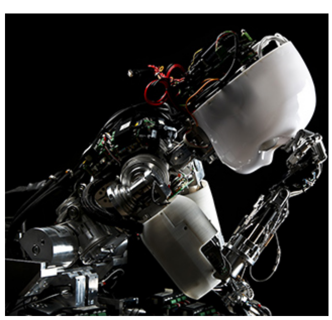
4.2 Neuroscience

IM-CLeVeR: Intrisically Motivated Cumulative Learning Versatile Robots

Project leader at FIAS: Jochen Triesch

Collaboration partners
CNR-ISTC: Consiglio Nazionale delle Richerche, Istituto di Scienze e Tecnologie della Cognizione and LOCEN: Laboratory of Computational Embodied Neuroscience (Team Leader: Gianluca Baldassarre)
CNR-ISTC / UCP: Unit of Cognitive Primatology (Team Leader: Elisabettta Visalberghi)
UMASS: University of Massachusetts Amhers and ALL: Autonomous Learning Laboratory (Team Leader: Andrew Barto)
UCBM: Universitàă Campus Biomedico and BRBL: Biomedical Robotics and Biomicrosystems Laboratory (Team Leader: Eugenio Guglielmelli)
USDF: University of Sheffield and ABRG: Adaptive Behaviour Research Group (Team Leader: Peter Redgrave)
UU: University of Ulster, Cognitive Robotics (Team Leader: Ulrich Nehmzow)
AU: Aberystwyth University, Intelligent Robotics (Team Leader: Mark Lee)
IDSIA-SUPSI: Scuola Universitaria Professionale della Svizzera Italiana, Istituto Dalle Molle sull'Intelligenza Artificiale, Reinforcement Learning Research Group (Team Leader: Jürgen Schmidhuber)

The IM-CLeVeR project (funded by the EU) aims at developing a new methodology for designing robot controllers that can: (a) cumulatively learn new skills through autonomous development based on intrinsic motivations, and (b) reuse such skills for accomplishing multiple, complex, and externally-assigned tasks. This goal will be pursued by investigating three fundamental issues:
- The mechanisms of abstraction of sensorimotor information;
- The mechanisms underlying intrinsic motivations;
- Hierarchical architectures that permit cumulative learning.
The study of these issues will be conducted on the basis of empirical experiments run with monkeys, children, and human adults, with bio-mimetic models aimed at reproducing and interpreting the results of such experiments, and through the design of innovative machine learning systems. The models, architectures, and algorithms so developed will be validated with experiments and demonstrators run with the simulated and real iCub humanoid robot. Within this project, our group is concerned with the development of hierarchial control architectures capable of cumulative learning and quantitative models of physiological and behavioral data produce by other project partners.



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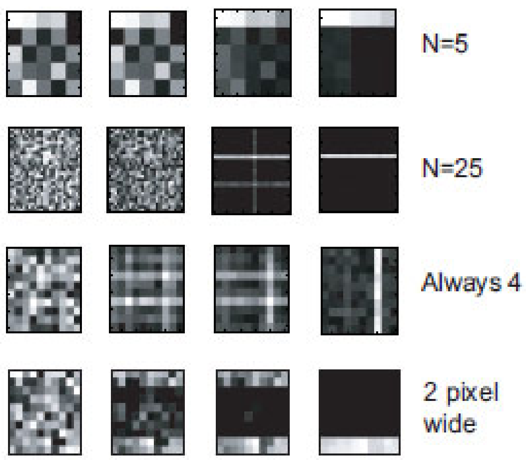
S. Saeb, C. Weber and J. Triesch, *Goal-Directed Learning of Features and Forward Models*, Neural Networks, 22(5-6), pp. 586–92, 2009.
C. Weber and J. Triesch, *Goal-Directed Feature Learning*, in Proceedings of the International Joint Conference on Neural Network (IJCNN), Atlanta, 14-19 June 2009, pp. 3319–3326. 2009.

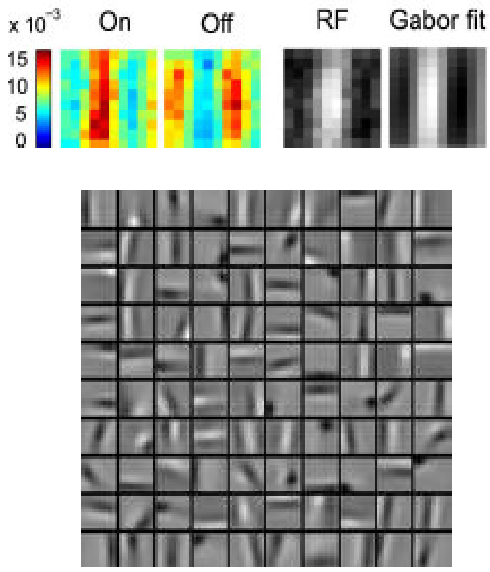
Independent component analysis in spiking neurons

Collaborators: Cristina Savin, Prashant Joshi and Jochen Triesch

How the brain learns to encode and represent sensory information is a core question for neuroscience. Computational theories predict that sensory neurons should reduce redundancies between their responses to a given stimulus set in order to maximize the amount of information they can encode. Specifically, ICA and related models, e.g. sparse coding, have emerged as a standard for learning efficient codes for sensory information, as they have been able to explain several aspects of sensory representations in the brain, such as the shape of receptive fields of neurons in primary visual cortex. It remains unclear how networks of spiking neurons using realistic plasticity rules can realize such computation.

RF development for Foldiak's bars (one IC) and natural scenes (one IC and full basis)





Here, we propose a biologically plausible mechanism for ICA-like learning with spiking neurons. Similar to our previous work, the model combines spike-timing dependent plasticity and synaptic scaling with an intrinsic plasticity rule that regulates neuronal excitability to maximize information transmission. We show that a stochastically spiking neuron learns one independent component for inputs. Interestingly, this is true regardless whether inputs are encoded as rates or using spike-spike correlations, unlike other attempts in this direction. Furthermore, different independent components can be recovered, when the activity of different neurons is decorrelated by adaptive lateral inhibition.

Related publications in 2009

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

P. Joshi, and J. Triesch, Rules for information-maximization in spiking neurons using intrinsic plasticity, Proc. IJCNN, pages 1456–1461, 2009

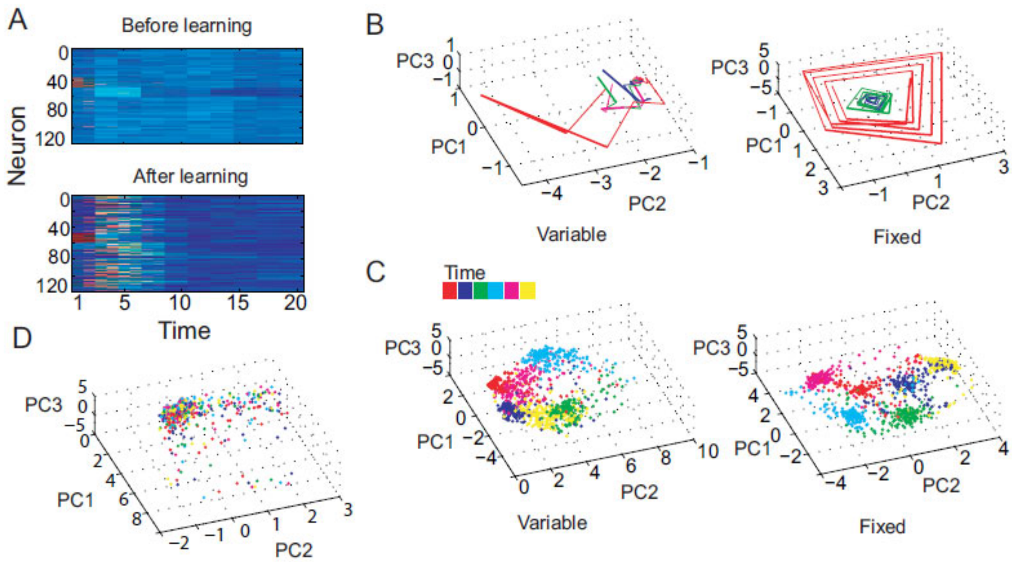
Gerhard, F., Savin, C., Triesch, J. A robust biologically plausible implementation of ICA-like learning ESANN 2009

Working memory development by reward-dependent STDP

Collaborators: Cristina Savin and Jochen Triesch

Working memory (WM) is critical for various cognitive processes. This temporary storage of stimulus-specific information is thought to have as neural correlate the selective persistent neuronal activity during delay period. Additionally, recent experimental evidence suggests that additional information is encoded in time-varying neural response which can convey as much information about the initial stimulus as persistent firing. Importantly, these neuronal responses can be significantly shaped by experience. The mechanisms by which this type of adaptation could occur have received little attention in computational modeling, however .

Emergent stimulus specific and time-dependent representations



Here, we ask if an initially unstructured neural network can acquire WM properties as it learns to perform a delayed response task. Although we make no a priori assumptions on stimulus encoding, reward-dependent learning leads to representations similar to those observed in various WM experiments. Our model demonstrates that WM dynamics may emerge naturally in a recurrent network with reward-modulated STDP, suggesting that reward-dependent learning may be a central driving force for the development of WM.

Related publications in 2009

Savin, C. and Triesch, J. A recurrent network acquires working memory properties by reward-dependent STDP, in Proc MSRL, June 2009

Savin, C., Triesch, J. Developing a working memory with reward-modulated STDP Frontiers in Computational Neuroscience. Conference Abstract: Computational and systems neuroscience. doi: 10.3389/conf.neuro.10.2009.03.276

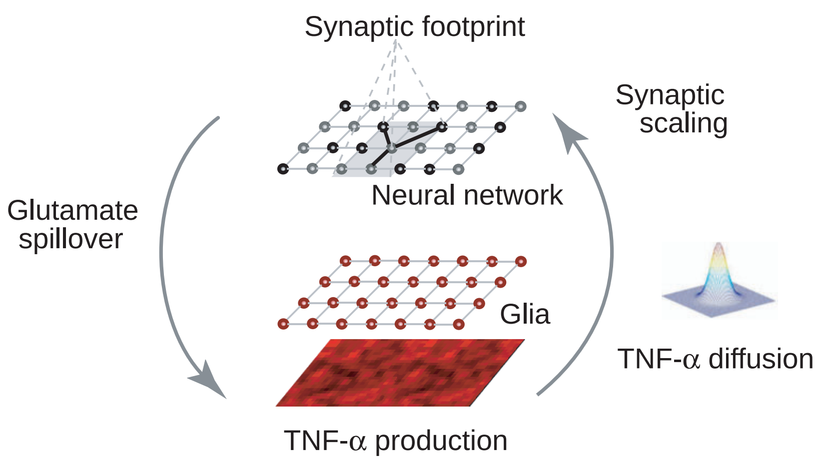
Seizure induction by glia-mediated synaptic scaling

Collaborators: Cristina Savin, Jochen Triesch, Michael Meyer-Hermann

Homeostatic mechanisms are required for maintaining the activity of cortical networks in some desired dynamic regime that allows for efficient information processing. A powerful mechanism for regulating overall network activity is synaptic scaling, which scales all excitatory synapses of a neuron to compensate for changes in synaptic drive.It has recently been demonstrated that a specific form of homeostatic synaptic scaling is mediated by glia cells that interact with neurons through the diffusible messenger TNF-α .

Interestingly, TNF-α is also used by the immune system as a pro-inflammatory messenger, suggesting potential interactions between immune system signalling and the homeostatic regulation of neuronal activity. Specifically, we hypothesize that the interference between different signaling pathways could explain some of the recent evidence suggesting an immune system influence in seizure initiation in certain pathological conditions.

To investigate this hypothesis, we have developed a computational model of TNF-α -mediated synaptic scaling. Our model shows that an overall increase in TNF-α levels following chronic inflammation or TNF-α overexpression by glia can push the network activity into a paroxysmal regime. In addition, it shows that neuronal hyperexcitability also arises after localized disruptions in network structure, resulting from simulated local lesions. In particular, following partial deafferentation, TNF-α produced by glial cells within the lesion area diffuses to the neighboring tissue and triggers network bursts.



Related publications in 2009:

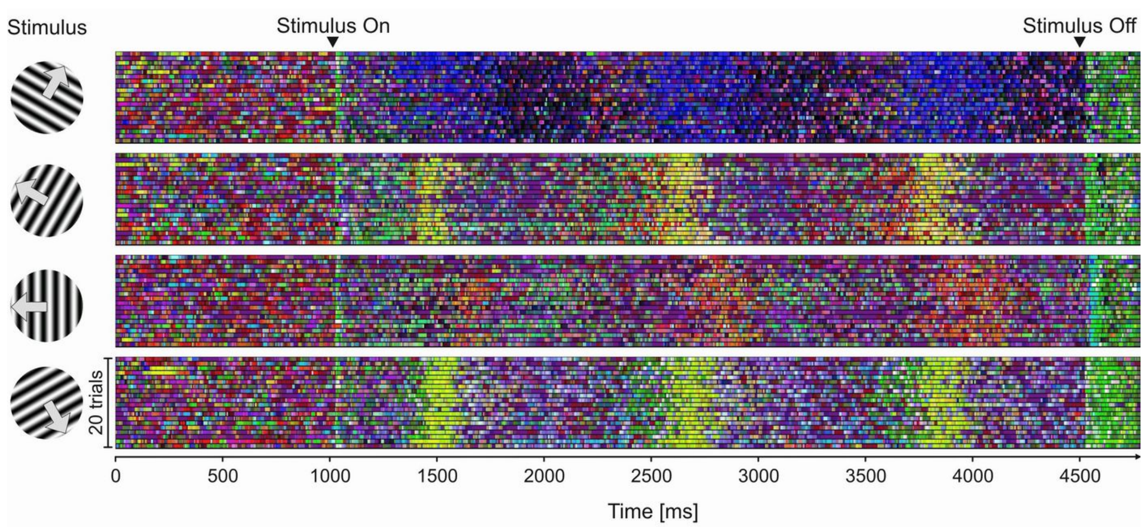
C. Savin, J. Triesch and M. Meyer-Hermann, *Epileptogenesis due to glia-mediated synaptic scaling*, J. Roy. Soc. Interface 6 (2009) 655

Processing information in the visual cortex by means of multineuronal spike patterns

Collaborators: Ovidiu Jurjuţ, 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 aims to find out how populations of neurons in the primary visual cortex process information about visual scenes. More precisely, we are interested in finding out what properties of multineuronal activity are correlated with features of visual stimuli and what are the temporal scales on which these correlations evolve. The data used to address these issues consist of simultaneous recordings of multiple neurons from the primary visual cortex of anesthetized cats while the animals were presented visual stimuli of various temporal dynamics. To handle such data, which are complex and often difficult to investigate, we developed a framework that enables the analysis and visualization of multineuronal datasets. Using Kohonen maps and classification, we provide on one hand intuitive means of visualizing large multineuronal datasets with the help of colors, and on the other hand, means of identifying multineuronal spiking patterns and their expression motifs with respect to stimulus features. This way, properties of the neuronal activity (time scale, stimulus specificity, stimulus time-locking, etc) can be efficiently investigated and conclusions about the mechanisms of information coding in the visual cortex can be drawn.



Activity of 26 neurons from cat visual cortex stimulated with drifting sinusoidal gratings. Colors represent the identity of multineuronal activation patterns. Horizontal color-lines correspond to trials that are grouped by stimulus (20 trials per stimulus).

Related publications in 2009:

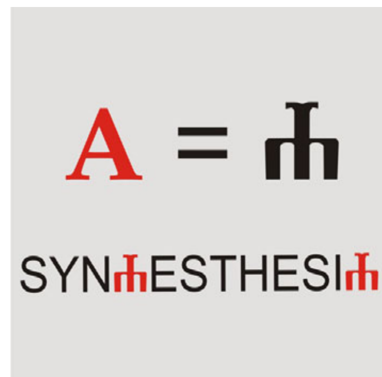
O.F. Jurjuţ, D. Nikolić, G. Pipa, W. Singer, D. Metzler, R.C. Mureşan, *A Color-Based Visualization Technique for Multi-electrode Spike Trains*. Journal of Neurophysiology 102 (2009) 3766

The nature of synaesthesia

Collaborators: D. Nikolić, A. Mroczko, T. Metzinger, W. Singer

Synaesthesia is a rare phenomenon in which real sensory experiences in one modality evoke sensory experiences in another modality. For example, when a synaesthete hears a name, it can experience certain taste that is unique for this particular name. Thus, for a synaesthete person, 'John' could always taste as chocolate. We investigate another, more common, form of synaesthesia in which letters and digits are associated with perception of color. This phenomenon is known as grapheme-color synaesthesia. The illustration shows grapheme-color associations for one synaesthete who volunteered as a participant in our study.

Importantly, the associations in grapheme-color synaesthesia are acquired in early childhood and remain robust throughout the lifetime. Synesthetic associations can transfer to novel inducers in adulthood as one learns a second language that uses another writing system. However, it was not known how long this transfer takes. We found that grapheme-color associations can transfer to novel graphemes after only a 10-minute writing exercise (see the illustration). Most subjects experienced synesthetic associations immediately after learning a new Glagolitic grapheme. Using a Stroop task, we provide objective evidence for the creation of novel associations between the newly learned graphemes and synesthetic colors (Mroczko et al., 2009). Also, these associations generalized to graphemes handwritten by another person. The fast learning process and the generalization suggest that synesthesia begins at the semantic level of representation with the activation of a certain concept (the inducer), which then, uniquely for the synesthetes, activates representations at the perceptual level (the concurrent).



The results imply that synesthesia is not a sensory-sensory phenomeon, as it has been largely held. Instead, this is a semantic-sensory phenomenon and a more accurate name is then ideaesthesia (Nikolić, 2009).

Related publications in 2009:

1) A. Mroczko, T. Metzinger, W. Singer, D. Nikolić, *Immediate transfer of synesthesia to a novel inducer*, Journal of Vision 9:25 (2009) 1

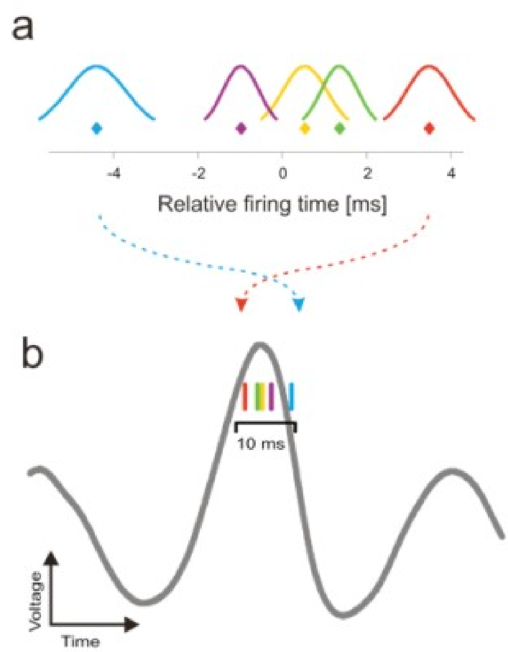
2) D. Nikolić, *Is synaesthesia actually ideaestesia? An inquiry into the nature of the phenomenon*, Proceedings of the Third International Congress on Synaesthesia, Science & Art, Granada, Spain, April 26-29, 2009

Temporal coding by relative spiking delays in the visual cortex

Collaborators: D. Nicolić, M. N. Havenith, G. Hahn, T. Petermann, S. Yu, W. Singer, D. Plenz, A. Zemmar, S.M. Baudrexel, J. Biederlack, N-H. Chen, P. Uhlhaas, G. Pipa, B. Lima, L. Melloni, S. Neuenschwander

For long time, the wisdom was that neuronal synchrony occurs with zero-delay precision. However, now we know that this is not true. Precise neuronal synchrony occurs most commonly with small (< 15 ms) but precise and reliable time delays detectable already from cross-correlation (Havenith et al, 2009). More accurately, one neuron tends to fire action potentials earlier than the other one (reviewed in e.g., Uhlhaas et al. 2009). For a given stimulus, each neuron has its own firing time relative to other neurons (Fig. 1a) and to the ongoing gamma oscillations in e.g., LFP (Fig. 1b).

A number of computational functions could be achieved if i) these small time delays contain stimulus-related information and ii) this information can be decoded by cortical neurons at later stages of processing. We discovered that, in cat visual cortex, these delays are stimulus dependent and can carry about as much information about stimuli as firing rates (Havenith et al., submitted). In other words, a novel brain code has been discovered.



In addition, we found a tight relationship between the presence of narrow synchronization peaks in cross-correlograms of spontaneous activity on one side and the existence of neuronal avalanches on another side (Hahn et al., submitted).

These discoveries have important implications for advancing the theory of cortical oscillatory dynamics (Nikolić, 2009).

Related publications in 2009:

1) G. Hahn, T. Petermann, M. N. Havenith, S. Yu, W. Singer, D. Plenz, and D. Nikolić, *Neuronal avalanches in spontaneous activity in vivo* (submitted)
2) M.N. Havenith, A. Zemmar, S. Yu, S.M. Baudrexel, W. Singer and D. Nikolić, *Measuring sub-millisecond delays in spiking activity with millisecond time-bins*, Neuroscience Letters 450 (2009) 296-300.
3) M. N. Havenith, S. Yu, J. Biederlack, N-H. Chen, W. Singer, and D. Nikolić, *Synchrony makes neurons fire in sequences – and stimulus properties determine who is ahead* (submitted)
4) D. Nikolić, *Model this! Seven empirical phenomena missing in the models of cortical oscillatory dynamics*, in Proceedings of the International Joint Conference on Neural Networks (IJCNN), Atlanta, 14-19 June 2009, p. 2272.
5) P. Uhlhaas, G. Pipa, B. Lima, L. Melloni, S. Neuenschwander, D. Nikolić, and W. Singer, *Neural synchrony in cortical networks: history, concept and current status*, Frontiers in Integrative Neuroscience 3 (2009) 17.

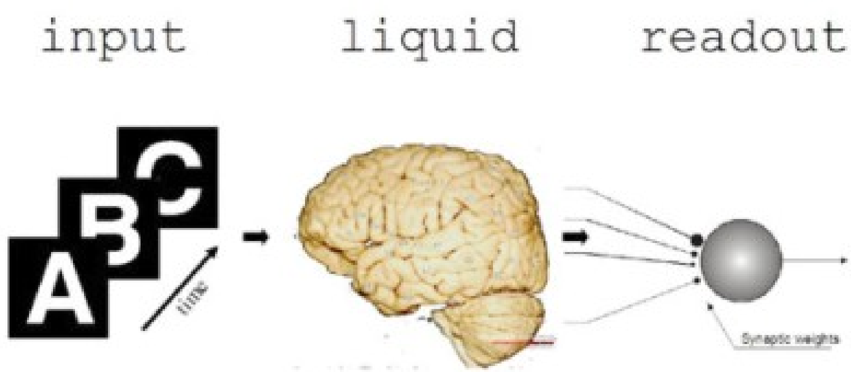
Liquid computing in the wet brain and spatio-temporal patterns

Collaborators: D. Nikolić, W. Maass, S. Häusler, O.F. Jurjuţ, G. Pipa, D. Metzler, R.C. Mureşan, W. Singer

In this project we investigate how an artificial neuron (simulated on a computer) can extract information from the activity recorded from a number of real neurons simultaneously. As shown in the figure, the attached readout neuron uses a computer-implemented algorithm to learn the weights of connections (strengths of 'synapses') to the real neurons. These connections need to be optimized for detection of a certain visual stimulus.

These experiments have several goals. For one, we learn about the mechanisms by which information is represented in distributed neuronal activity. We can investigate the conditions under which the information is available in neuronal activity and the time course of the available information. By doing so, we can investigate the current theories about cortical information processing (e.g., liquid state machine).

Also, important insights have been obtained about the nature of iconic memory. We discovered that the brain has a one-back memory for visual stimuli. Neural responses to an image contain as much information about that image as about another image presented immediately before (Nikolić et al., 2009).



These experiments have also important practical implications for advancement of neuroprostetic technologies. To connect electronic or robotic devices to the brains of impaired human patients, it is necessary to understand the principles of information coding, the types of information detectable from neuronal activity, the pitfalls and the limitations of such technologies. Our experiments investigate these questions by extracting stimulus-related information from the primary visual cortex.

Precise spike timing produces spatio-temporal patterns. A new method has been developed for their detection and analysis (Jurjuţ et al., 2009). press).

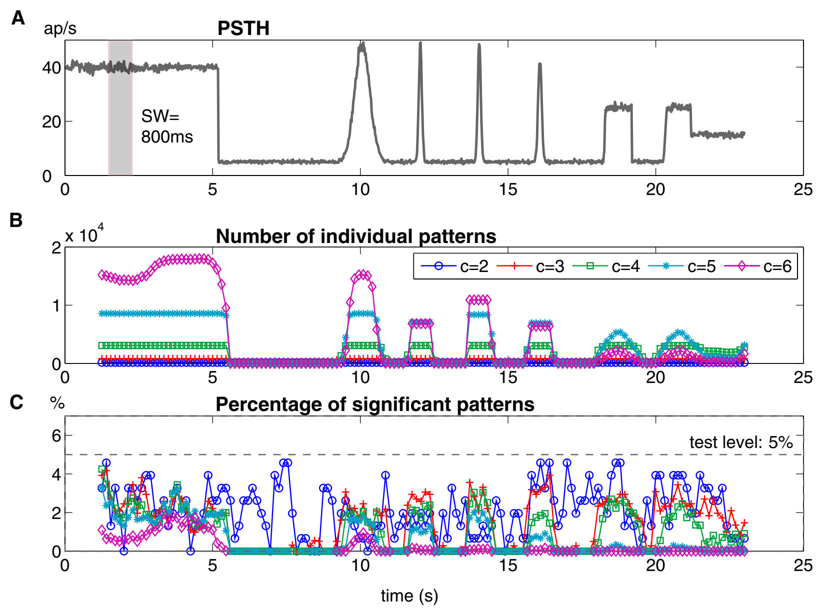
Related publications in 2009:

1) D. Nikolić, S. Häusler, W. Singer and W. Maass, *Distributed fading memory for stimulus properties in the primary visual cortex*, PLoS Biology 7 (2009) e1000260
2) O.F. Jurjuţ, D. Nikolić, G. Pipa, W. Singer, D. Metzler, R.C. Mureşan, *A Color-Based Visualization Technique for Multielectrode Spike Trains*. Journal of Neurophysiology 102 (2009) 3766

Detection of changes in neuronal coupling

Collaborators: Wei Wu, Diek W. Wheeler, Ovidiu Juruţ, Danko Nikolić, Raul C. Mureşan, Wolf Singer, Gordon Pipa

Synchronous neuronal firing has been proposed as a potential neuronal code. To determine whether synchronous firing is really involved in different forms of information processing, one needs to directly compare the amount of synchronous firing due to various factors, such as experimental or behavioral conditions. In order to address this issue, we developed two new methods. The first is a extended version of the previously published method, NeuroXidence. The improved method incorporates bi- and multivariate testing to determine whether different factors result in synchronous firing occurring above the chance level. We demonstrate through the use of simulated data sets that bi- and multivariate NeuroXidence reliably and robustly detects joint-spike-events across different factors. The second method is used to visualize high large numbers of simultaneously recorded spike trains, and to map the high dimensional data an a low embedding dimension.



False-positives for two non-stationary processes evaluated by bivariate NeuroXidence. Feature a (period 11) describes the changing rates across trials and neurons, such that neurons $1-9$ *were modeled by a homogenous Poisson process with a background rate of* 15 *spikes/sec, while the rates of neurons* $10-18$ *changed from trial to trial from* 15 *to* 30 *spikes/sec. (b) The peristimulus time histogram (PSTH) displays the rate profile of the non-stationary processes. (c) The number of individual spike-patterns of complexities* $2-6$ *that were detected in each sliding window. (d) The percentage of JS-patterns that are significant.*

Related publications in 2009:

1) P. Ulhaas, G.Pipa, B. Lima, L. Melloni, S. Neuenschwander, and W. Singer, *Neural synchrony in cortical networks: History, concept and current status*, Review. Front. Integr. Neurosci. 3:17. (2009), doi:10.3389/neuro.07.017.2009

2) G. Pipa, E.S. Städtler, E.F. Rodriguez, J.A. Waltz, L.F. Muckli,W. Singer, Rainer Goebel, and M. H. J. Munk, *Performance-and coding-dependent oscillations in monkey prefrontal cortex during short-term memory*, Frontiers in Neuroscience-Integrative Neuroscience 3:25 (2009) 1

3) W. Wu, D. Wheller, G. Pipa, *Multivariate analysis of spike train coupling*, in preparation

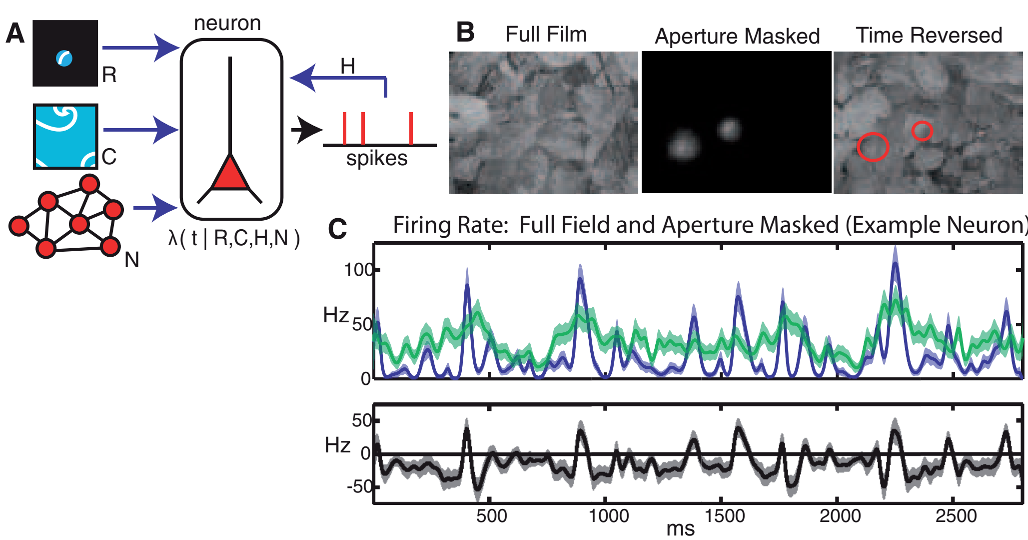
4) O.F. Jurjuţ, D. Nikolić, G. Pipa, W. Singer, D. Metzler, R.C. Mureşan, *A Color-Based Visualization Technique for Multielectrode Spike Trains*. Journal of Neurophysiology 102 (2009) 3766

Modeling surround effect in the monkey visual cortex

Collaborators: Rob Haslinger[1], Gordon Pipa[2,3], Sergio Neuenschwander[3], Emery Brown[1]

[1]MIT, [2]FIAS, [3]Max Planck Institut für Hirnforschung

Even in V1, where neurons have well characterized receptive fields, it has been difficult to deduce which features of complex natural scene stimuli neurons respond to. This may be partly due to network activity, either ongoing or dictated by the stimulus in the entire visual field, not only that in the classical receptive field (CRF). Here we quantify the extent to which V1 neuronal activity in the behaving macaque monkey is modulated by stimuli outside the classical receptive field, by the neuron's previous spiking activity and by ongoing network activity as reflected local field potentials (LFPs. We simultaneously recorded spikes and LFPs in V1 during stimulation by various natural scenes movies for which the portion of the movie within the CRF remained the same but for which the surround was variable. To quantify changes the spiking response to the different movies we fit Generalized Linear Models (GLMs) of the spike probability to the data. The GLM included a spline based PSTH-like terms accounting for the stimulus an auto-regressive-type term accounting for the neuron's previous spiking history and a term dependent upon the power and phase of different LFP frequency bands decomposed using a Daubechies stationary multiresolution analysis (sMRA).



A) A V1 neuron's spiking is influenced not only by its classical receptive field (CRF) but also the surround context of the stimulus, the neuron's previous spiking history and the embedding network. B) Frames from Full Film (FF), Aperture Masked (AM) and Time Reversed (TR) movies (see text) used to probe the influence of the stimulus surround. Movie within the CRF (red circles) remains unchanged across conditions. C) Top panel: GLM fitted PSTH of a representative neuron during FF (blue) and AM (green) movies. Shaded bands are 95% confidence regions on the fits. Bottom panel: Difference between the FF and AM movies.

Related publications in 2009:

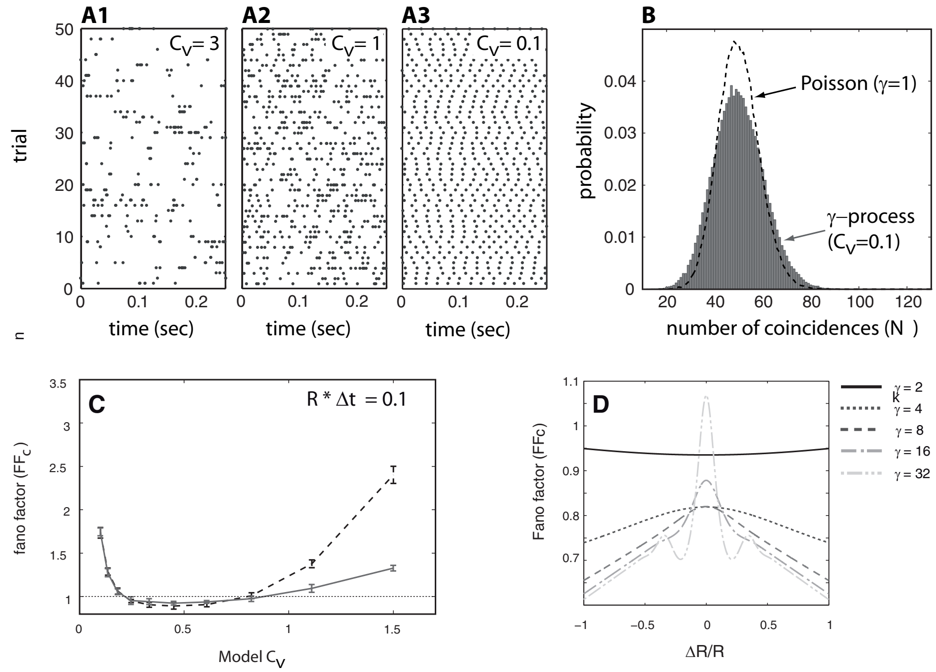
1) R. Haslinger, E.N. Brown, and G. Pipa, *Discrete Time Rescaling Theorem: Determining Goodness of Fit for Discrete Time Statistical Models of Neural Spiking*, Journal of Neural Computation, submitted

2) R. Haslinger, G. Pipa, E.N. Brown, and Sergio Neuenschwander, *Surround effects in V1*, Science, in preparation.

Impact of Non Poissonian Point processes on Structure Formation in neuronal networks

Collaborators: M. Castellano, B. Scheller, R. Vicente, C. van Vreeswijk, G. Pipa

In this project we study the impact of presynaptic activity that is deviating from Poissonian firing onto the postsynaptic firing of a conductance based integrate and fire neurons. We first show that the compound activity of a large group of neurons, e.g. presynaptic cells, cannot be described by a Poisson process in general. Then we demonstrate that the auto-structure of the presynaptic drive has strong impact onto the auto-structure of the postsynaptic spike-train. And finally, we discuss the potential impact of non-Poissonian presynaptic activity on the structure formation in recurrent networks based on Spike Timing Dependent Plasticity.



Raster plot for 50 trials of Gamma-processes with 3 different coefficient of variations of the inter-spike interval distribution (A1: C_V=0.1; A2: C_V=1, A3: C_V=3). (***B****) Distribution of coincidence counts shared by pairs of mutually independent Gamma-processes of the same kind as shown in A. Dashed curves in (****B****) shows the coincidence count distribution for the cases of Poisson processes ($\gamma = 1$) and a Gamma-process with C_V=0.1. (****C****) Fano factor of the coincidence count distribution as a function of the model C_V (****D****) Analytically determined Fano Factor FF_C of the coincidence count distribution for two neurons with different rate $R_1 = R + \Delta R$ and $R_2 = R - \Delta R$ as function of $\Delta R/R$.*

Related publications in 2009:

1) G. Pipa, S. Grün, C. van Vreeswijk, *Impact of spike-train auto-structure on probability distribution of joint-spike event*, Joural of Neural Computation, under revision
2) G. Pipa, C. van Vreeswijk, S. Grün, *Impact of spike-train auto-structure on significance estimation of joint-spike event by the unitary event method*, Joural of Neural Computation, under revision
3) M. Castellano, B. Scheller, R. Vicente, G. Pipa, *Impact of Non Poissonian Point processes on Structure Formation in neuronal networks*, in preparation

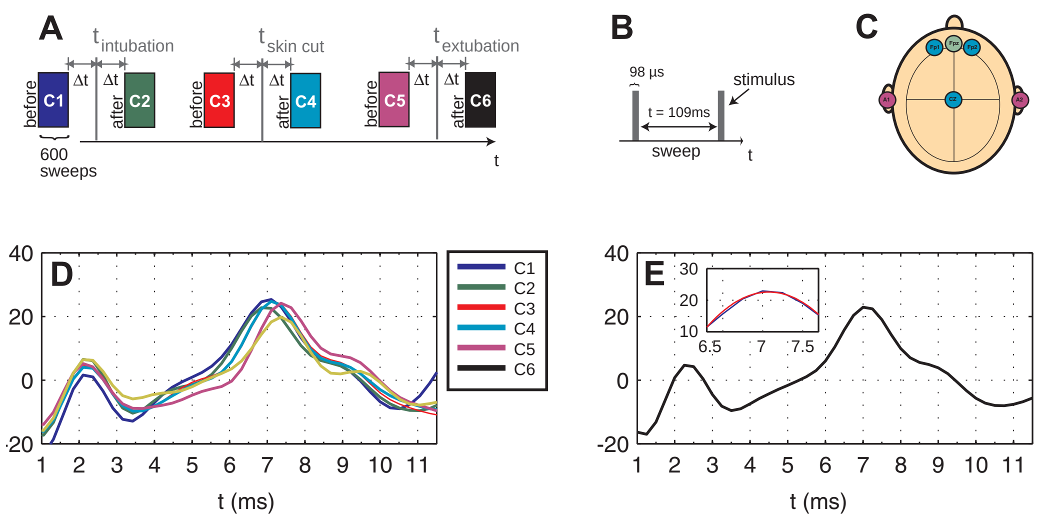
General Anesthesia Affects Temporal Precision and Power of the Brainstem Auditory Evoked Response

Collaborators: Gordon Pipa, Bertram Scheller

We investigated the brainstem auditory evoked responses, in particular wave V, under the influence of general anaesthesia for. Clinically, brainstem auditory evoked responses have attracted a great deal of attention and serve i.e. as diagnostic tool in neurosurgical procedures as well as in the testing of hearing ability in the newborn.

We recorded auditory evoked potentials in 427 patients with comparable distributions of age and body mass index, scheduled for elective surgery under general anaesthesia. Anaesthetic regimen was randomized as a combination of one of 4 hypnotic drugs supplemented by one of 4 opioids, as such resulting in a balanced anaesthesia, widely in clinical use. Neuroelectric signals were recorded from prior induction of general anaesthesia to post general anaesthesia. Broadband wavelet-filtered signals were evaluated on the base of the stimulus associated EEG-segments used for averaging the evoked potential. Multi scale analysis reveals a highly significant reduction in power, accompanied by a highly significant rise in the locking of the neuroelectric signals to the stimulus.

We demonstrated that General anaesthesia affects the brainstem auditory evoked potential wave V. Thus the role of the brainstem in processing and/or conducting sensory information and it's role in conditions of general anaesthesia have been underestimated.



Stimuli consisted of brief binaural clicks at 80 dB, sweeps were defined as following EEG-segments with a length of 111 ms (1B), collected as a differential signal at A1/Fp1, A2/Fp2, A1/Cz, A2/Cz with Fpz as common ground according to the 10/20-system (1C). Normalized grand means for the brainstem auditory evoked potential. (1D) fit of a polynom 2nd order for the great grand mean (1E). Latency and Amplitude of the peak of BAEP wave V.

Related publications in 2009:

G.B.C.A. Scheller, M. Daunderer, and G. Pipa, *General anesthesia increases temporal precision and decreases power of the brainstem auditory evoked response*, Journal of Anesthesiology, accepted

V. V. Moca, B. Scheller, R. C. Muresan, M. Daunderer, and G. Pipa, *EEG under anesthesia Ű Feature extraction with TESPAR,* Comput. Meth. Programs Biomed. 95 (2009) 191

Using transfer entropy to unveil effective connectivity in neuronal datasets

Collaborators: Raul Vicente[1,2], Michael Wibral[3], Gordon Pipa[1,2], Wei Wu[1,2], Jochen Triesch[2], German Gomez-Herrero[4]

[1]Max Planck Institut für Hirnforschung, [2] FIAS, [3]Brain Imaging Center Frankfurt, MEG unit, [4]Tampere University

The functional connectivity of the brain describes the network of statistically correlated activities of different brain areas. However, as it is well known correlation does not imply causality and most of synchronization measures are not able to distinguish context-dependent causal interactions (who drives whom?) among remote neural populations. There exists a great interest in the detection of this type of effective or causal networks since they can help in unveiling the neural circuitry of brain areas and its directed interactions involved in the processing of information.

In this project we use an information theoretic functional (transfer entropy) as a tool to discover patterns of causal relationships within the context of neurophysiological datasets. Transfer entropy can be understood as a direct implementation of the original concept of Wiener causality into an information theoretic framework and, thus naturally generalizing the limited linear regression modeling assumed in Granger causality. In particular, we have studied the robustness of transfer entropy to estimate causality against two common problems in neurophysiological recordings, namely, volume conduction and noise contamination. To go beyond the original pair-wise formulation of the transfer entropy, we have also extended its definition and numerical estimator to the multivariate case which allows the distinction of direct from indirect causal interactions. We have also make use of the typical multi-trial structure of a data set to propose a time resolved definition of transfer entropy able to capture causal relations between certain types of non-stationary time series. Current work is focused on the application of this causality approach to MEG datasets recorded during the performance of different paradigms, such for example a Simon task.

Related publications in 2009:

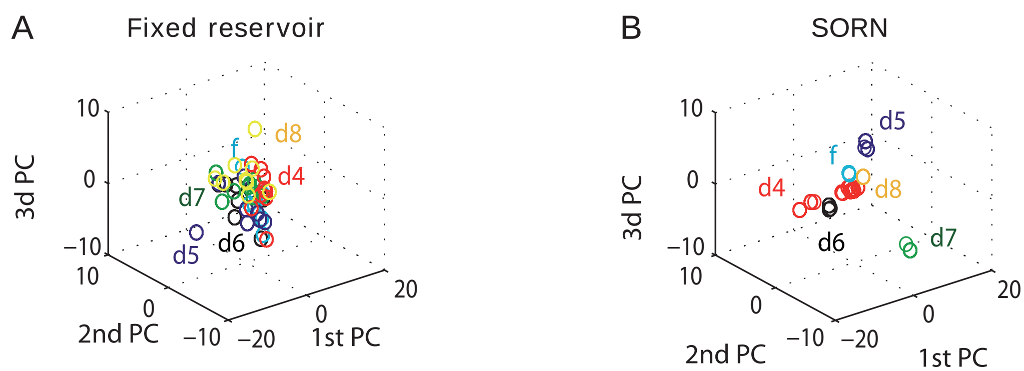
1) German Gomez-Herrero, Raul Vicente, Wei Wu, Gordon Pipa, and Karen Egiazarian, *Assessing coupling dynamics from an ensemble of multivariate time series*, in preparation.

2) Raul Vicente, Gordon Pipa, Michael Lindner, and Michael Wibral, *Using transfer entropy to unveil effective connectivity in neuronal datasets*, in preparation.

Self-organization in Recurrent Neural Networks

Collaborators: Andreea Lazar, Gordon Pipa and Jochen Triesch

Understanding the dynamics of recurrent neural networks is crucial for explaining how the brain processes information. In the neocortex, a range of different plasticity mechanisms are shaping recurrent networks into effective information processing circuits that learn appropriate representations for time-varying sensory stimuli. However, it has been difficult to mimic these abilities in artificial neural network models. In this collaboration we study self-organization phenomena in recurrent neural networks that combine different forms of learning and plasticity rules. In particular, we have proposed a new type of neural network that combines three forms of plasticity. While anaylzing these networks, we have discovered that only the combination of all three plasticity mechansisms manages to keep the networks' dynamics in a healthy regime suitable for learning. Furhermore, these networks learn to encode information in the form of trajectories through their high-dimensional state space, which is reminiscent of recent biological findings on cortical coding. We managed to show that only the combination of all three types of plasticity allows the network to (a) maintain a dynamical regime suitable for computation that makes efficient use of all the network's resources; (b) learn to effectively represent the spatio-temporal structure of its inputs, and (c) perform much better on prediction tasks compared to a comparable reservoir computing approach, which is considered the current state-of-the-art in the field.



Result of PCA on the network's internal representations corresponding to the last 6 letters of the input sequence 'edddddddddf' which we refer to as 'd4', 'd5', 'd6', 'd7','d8' and 'f'. A: For the fixed reservoir, identical input conditions are spread far apart and strongly overlap with other input conditions. B: For the SORN, the different input conditions form compact clusters that are well separated for different input conditions, suggesting a more orderly dynamics in the SORNs.

Related publications in 2009:

A. Lazar, G. Pipa, and J. Triesch, *SORN: a Self-organizing Recurrent Neural Network*, Front. Comput. Neurosci. 3:23 (2009)

Interactions between global and local functional network structures in visual cortex

Collaborators: Katharina Schmitz, Ralf Galuske, Gordon Pipa

This project combines theoretical work with electrophysiological data analysis: First, graph theoretical methods for the analysis of neuronal network dynamics are to be developed. Second, they will be applied to electrophysiological data recorded in the primary visual cortex of anaesthetized cats while a part of their brain, namely area pMS, is reversibly deactivated by cooling. The effect of this deactivation on the network dynamics in primary visual cortex is to be examined.

Graphs are obtained detecting synchronous events in the multi-unit signals of each two of 16 electrodes in a 4x4 grid, which are interpreted as nodes of the graph. Whenever the number of synchronous events is significantly high, an edge is inserted between the respective nodes.

We compared the distribution of edges and the degree in the observed graphs to those of Erd"os-Rényi graphs. We also checked the edge probabilities for homogeneity. Furthermore, we compared entire networks to each other using the Hamming distance $d_h(X,Y) := \sum_i |X_i - Y_i|$, $i = 1, ..., N$, as a measure of (dis-)similarity.

We found that the observed networks did not match the features of Erd"os-Rényi graphs. A comparison of 'short' and 'long' connections showed a stronger representation of short links. For graphs obtained under the same experimental conditions, the Hamming distance was significantly small, indicating that there are stable configurations of edges.

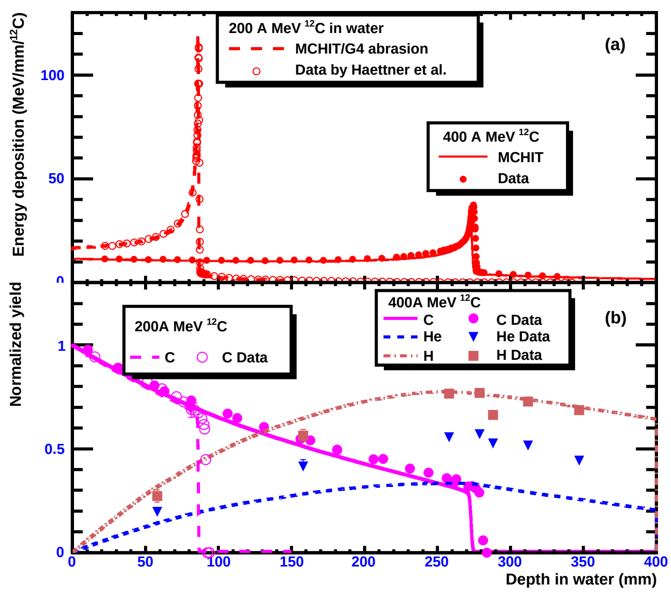
In the next step the focus will be on comparing graphs from different experimental conditions, i.e. with and without deactivation of pMS cortex, to quantify the effect of the deactivation and the resulting loss of feedback information.

4.3 Biology, Immunology, Medicine

Modeling heavy-ion transport in extended media for cancer therapy applications

Collaborators: I.A. Pshenichnov, A.S. Botvina, I.N. Mishustin, W. Greiner, A. Solov'yov, E. Surdutovich, E. Scifoni

We use the Monte Carlo model for Heavy Ion Therapy (MCHIT) based on Geant4 toolkit to study the energy deposition and fragmentation reactions occurring when various nuclei propagate through tissue-like media (see details in ref. [1]). The MCHIT model has been developed in FIAS and it is currently based on the Geant4 toolkit of version 9.3. Depth-dose distributions and yields of secondary fragments produced by ion beams were calculated and compared with experimental data, see the figure. The calculations were performed with various de-excitation models for light and medium-size nuclei formed in nuclear reactions. Besides the traditional evaporation models they include the Fermi break-up model and the Statistical Multifragmentation model. This allowed us to estimate the role of multifragment decays on the depth-dose, depth-yield and charge distributions of secondary fragments produced in tissue-like media. While the energy deposition is not very sensitive to decay mechanisms of excited nuclei, the fragment yields can not be properly described without accounting for multifragment decays. The validity of the Statistical Multifragmentation model of Geant4 has been confirmed in a set of stand-alone tests, following several updates and fixes introduced to this component of the toolkit. Now the MCHIT model can be used for reliable calculations of 3D dose distributions for ion-beam cancer therapy. These results will be used also for modeling radiation effects on nano-scales within the multi-scale approach proposed in ref. [2] (see report of the Meso-Bio-Nano Group).



Calculated depth-dose distributions and normalized yields of secondary hydrogen and helium fragments for 200 and 400 A MeV ^{12}C ions in water. Experimental data by E. Haettner et al., 2006, are shown by points.

Related publications in 2009:

1) I. Pshenichnov, A. Botvina, I. Mishistin, W. Greiner, *Nuclear fragmentation in extended media studied with Geant4 toolkit,* to be submitted to NIM B.

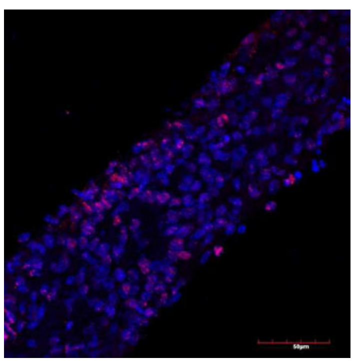
2) Andrey V. Solov'yov, Eugene Surdutovich, Emanuele Scifoni, Igor Mishustin, Walter Grainer, *Physics of ion beam cancer therapy: a multi-scale approach*, Phys. Rev. E 79 (2009) 011909

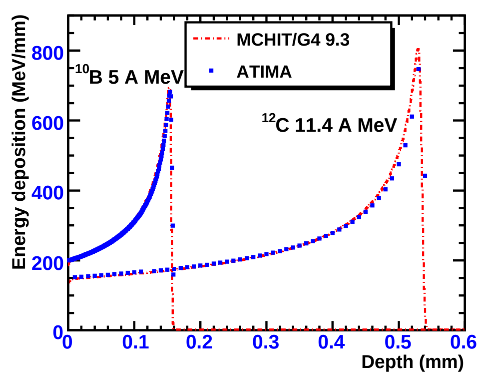
Effects of X-rays and heavy ions on cell death, proliferation, and DNA damage in hippocampal tissue slice cultures

Collaborators: Mareike Müller[1,3,4,⋆], Felicitas Merz[2], Horst Stöcker[3,4], Marco Durante[4], Gisela Taucher-Scholz[4], Franz Rödel[5], Horst-Werner Korf[1], Igor Mishustin[3], Igor Pshenichnov[3], Ingo Bechmann[2]

[1]Dr. Senckenbergische Anatomie, Institut für Experimentelle Neurobiologie, Goethe Universität Frankfurt, [2]Institut für Anatomie, Universität Leipzig, [3]Frankfurt Institute for Advanced Studies, [4]Gesellschaft für Schwerionenforschung, Darmstadt, [5]Klinik für Strahlentherapie und Onkologie, Universitätsklinikum Frankfurt
⋆M. Müller is a PhD student of the HGS-HIRe, funded by a Puschmann-scholarship

Heavy ions offer an advantageous depth-dose-profile in comparison to conventional radiotherapy using X-rays, due to the fact that they have an enhanced energy deposition (dose) close to the end of their range . This and an increased relative biological effectiveness of heavy ions such as ^{12}C offers the possibility to deliver the prescribed dose to the tumor while healthy surrounding tissue is preserved. Although heavy ions are already being used to treat patients, most of the biological research was done using cell lines. Thus, only little is known about the effects of radiation on tissue. In this project, rat brains are used to prepare organotypic hippocampal slice cultures. These tissue slices have the advantage over cell cultures and cell lines that they preserve the 3D-environment of the native, genetically non-modified cells. This leads to the assumption that the tissue slice cultures will be a more accurate model in the analysis of reactions to irradiation such as DNA damage, cell death (necrosis and apoptosis), and proliferation in comparison to in vivo models than cell lines. So far, the tissue slices cultures were irradiated with X-rays at the radiation facility of the university hospital in Frankfurt/Main at doses of up to 40 Gy. Heavy ion irradiations were performed at the UNILAC and SIS at GSI with different ions. First results show that the antibody stainings for necrosis, apoptosis, proliferation, and DNA damage bind specifically. Further analysis for statistical purposes will follow.





Left: *a 40× magnification of a slice irradiated with* 8×10^6 *p/cm*^{2} ^{12}*C at an initial energy of 11.4 MeV/u. Hoechst-staining (blue) visualizes the cell nuclei, gamma-H2Ax-staining (red) visualizes DNA damage. The gamma-H2Ax-staining nicely shows ion tracks in the tissue - the ions entered the tissue from the top left corner.* Right: *Comparison of MCHIT and ATIMA results for* ^{10}*B at an energy of 5 MeV/u and* ^{12}*C at 11.4 MeV/u in water. For light ions at low energies, the results show a very good agreement for the two codes.*

Planning of the heavy ion irradiation experiments is done using simulation programs developed at GSI (ATIMA) and FIAS (MCHIT). In the scope of these plannings, the results of these two codes (ATIMA being a deterministic code and MCHIT a Monte Carlo code) were compared to each other and differences analysed according to the physical models used in each code.

Related publications in 2009:

1) F. Merz, M. Müller, F. Rödel, H. Stöcker, K. Schopow, G.Taucher-Scholz, F. Dehghani, M.Durante, I. Bechmann, *Tissue slice cultures from humans or rodents: a new tool to measure biological effects of heavy ions,* to be submitted

2) M. Müller, M. Durante, H. Stöcker, I. Bechmann, *Modeling radiation effects at the tissue level,* to be submitted

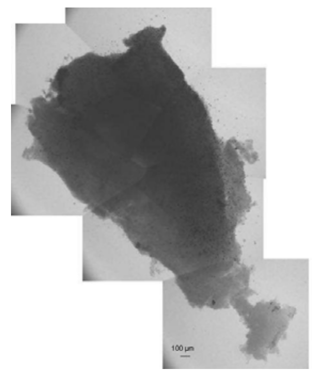
Human tissue slice cultures: a new tool in medical research to avoid complications from species-differences

Collaborators: Mareike Müller[1,3,4], Felicitas Merz[2], Horst Stöcker[3,4], Marco Durante[4], Gisela Taucher-Scholz[4], Franz Rödel[5], Horst-Werner Korf[1], Volker Seifert[5], Johannes Rieger[7], Michel Mittelbronn[7], Patrick Harter[7], Ingo Bechmann[2]

[1]Dr. Senckenbergische Anatomie, Institut für Experimentelle Neurobiologie, Goethe Universität, [2]Institut für Anatomie, Universität Leipzig, [3]Frankfurt Institute for Advanced Studies, [4]Gesellschaft für Schwerionenforschung, Darmstadt, [5]Klinik für Strahlentherapie und Onkologie, Universitätsklinikum Frankfurt, [6]Klinik und Poliklinik für Neurochirurgie, Universitätsklinikum Frankfurt, [7]Dr. Senckenbergisches Institut für Neuroonkologie, Universitätsklinikum Frankfurt
M. Müller is a PhD student of the HGS-HIRe, funded by a Puschmann-scholarship.

A new drug or therapy is always tested first in cell culture experiments, then in animals (usually mice or monkeys), and only if these experiments do not show serious implications, further testing is done on human volunteers. The catastrophic results this procedure may have became clear in what is known as the "London tragedy": an in-human trial in which six volunteers showed severe side-effects up to organ failure after they had been applied the drug TGN1412. In all previous trials, this drug showed no significant side-effects and had been approved in Germany and England.

One possibility to avoid species-differences is the use of human tissue slice cultures. They are advantageous to murine tissue slice or cell cultures because they pose as a workaround concerning these problems of species-differences while conserving the native, 3D-organotypic environment of the cells. We established human brain slice cultures in order to analyse and compare the biological effects of heavy ions and X-rays such as cell death (necrosis and apoptosis), proliferation, and DNA damage. This is done in light of the fact that heavy ions have a so-called inverted doseprofile, and thus may be more suited to treat deep-seated tumors than X-rays.



10× magnified, merged image of a viable glioblastoma tissue slice which has been kept in culture for 15 days.

For the lack of effective treatment, we focused on the glioblastoma, the most aggressive brain tumor. Within ethical restrictions, glioblastoma tissue slice cultures were prepared from tissue taken from glioblastoma surgery patients. These slice cultures were then irradiated with X-rays of doses up to 40Gy at the radiation facility of the university hospital in Frankfurt/Main. One experiment using ^{12}C was done at the SIS at GSI.

First results show that glioblastoma tissue can successfully be kept in culture for at least 21 days. Antibody staining for biological endpoints such as programmed cell death, proliferation, and DNA damage was successful and will be analyzed further for statistical purposes.

Related publications in 2009:

F. Merz, M. Müller, F. Rödel, H. Stöcker, K. Schopow, G.Taucher-Scholz, F. Dehghani, M. Durante, I. Bechmann, *Tissue slice cultures from humans or rodents: a new tool to measure biological effects of heavy ions*, to be submitted

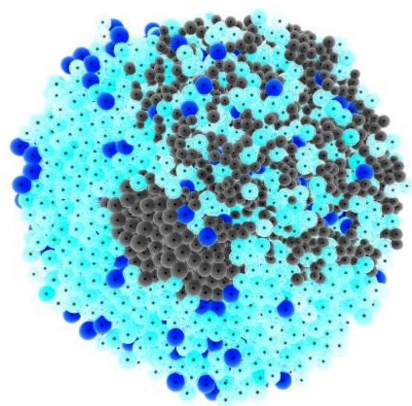
M. Müller, M. Durante, H. Stöcker, I. Bechmann, *Modeling radiation effects at the tissue level*, to be submitted

Tumour growth dynamics during irradiation treatment

Collaborators: Harald Kempf[1], Michael Meyer-Hermann[1]

[1] FIAS

The irradiation of cancer with heavy-ions has proven to be a most efficient and successful treatment strategy for specific types of cancers. In view of the precision of irradiation, this treatment can also be applied in cases that are not accessible to surgery, like in the vicinity of the optical nerve. The treatment protocols have been optimised based on a mathematical extrapolation of photon treatment to the case of heavy-ion. We aim to understand the changes and the development of irradiated tumours during and between treatment sessions. This is done by agent-based simulations of tumour growth under realistic conditions. In 2009 we have established the framework of the model based on the method of Delaunay-Object-Dynamics which was developed in house before and allows for an efficient and fast localisation of interaction partners in biological cellular systems. This model has the potential to include soluble factors as well as mechanical interactions between cells on a quantitative level. In addition, it can distinguish cells in different phases of the cell cycle which are known to change the efficiency of radiation. This simulation tool is currently being adapted to real experimental and clinical set-ups and is expected to become very helpful for the planning of cancer treatments. Harald Kempf finished his diploma thesis on this project and now got a PhD project "Heavy-Ion Irradiation of Cancer" funded for three years by the Polytechnische Gesellschaft.



Snap shot of a growing three-dimensional tumour spheroid. Light blue cells are actively proliferating, blue cells are quiescent, and grey cells are dying in response to heavy-ion irradiation. It is visible that upon irradiation a large part of the tumour cells restarts to proliferate while most of these cells were quiescient before irradiation.

Related publications in 2009:

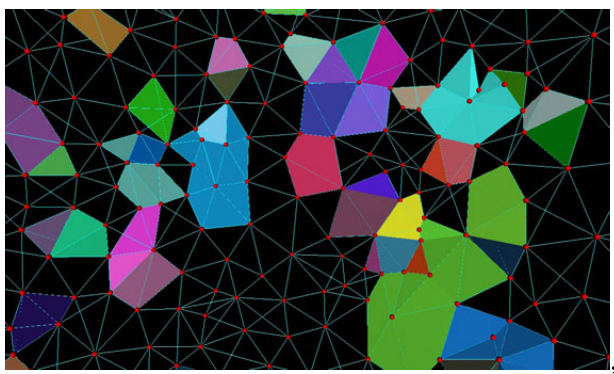
Harald Kempf, Diploma thesis, *Agent-based modelling of tumour spheroid growth and treatment.* Frankfurt am Main (2009)

Cell migration and shape on the subcellular level

Collaborators: Graziela Grise[1], Michael Meyer-Hermann[1]

[1] FIAS

Mathematical modelling of biological cells encounters the necessity of an extension of currently available methods. Up to now cells were modelled as single units (in the best case including biomechanical and chemical properties). Only a few models exist (Potts model, hyphasma, the subelement method) that start to shed light on the internal structure of the cell at an agent-based level. If one is interested in the intracellular content of the investigated cells, this is mostly done on a space-averaged level. However, there are a number of examples showing that the space-distribution (or: spatial distribution) of molecules in the cell are essential for their functionality. Novel methods allowing for the measurement of intracellular molecular distributions call for corresponding methods that, on one the hand, respect the individuality of the cells and on the other hand correctly describe diffusion and transport processes of molecules inside the cell. Based on the method of Delaunay-Object-Dynamics the Delaunay-derived neighbourhood relations are extended to the subcellular level. This induces a number of technical problems related to surface reconstruction problems which, in parts, have been solved in the framework of a PhD thesis in 2009. Possible applications of this agent-based subcellular model ranges from electrophysiology of cells to intracellular signalling and signalling in response to interactions between cells.

,

Delaunay-triangulation of a simulated cell built by membrane and internal particles. The coloured regimes are three-dimensional structures in the cell membrane that need tobe reduced to a realistic description of the two-dimensional cell surface.

Related publications in 2009:

Grise, G., Meyer-Hermann, M.; *Cell shape and migration in subcellular modeling.* Submitted 2009.

Optimising antibodies in germinal centres

Collaborators: Michael Meyer-Hermann[1], Marc Thilo Figge[1], Marie Kosco-Vilbois[2], Kai-Michael Toellner[3], Anja Hauser[4], Matthias Gunzer[5]

[1] FIAS, [2] NovImmune, Geneva, CH, [3] Birmingham University, UK, [4] Deutsches Rheuma-Forschungszentrum (DRFZ), Berlin, [5] Magdeburg University

The germinal centre reactions is the physiological site in which new types of antibodies are generated. Resulting from germinal centre reactions, high affinity antibodies are generated by plasma cells and memory cells and are made to allow for a fast and optimised response to subsequently encountered pathogenic substances. This process is at the basis of vaccination and is of great importance to public health. However, there is still an ongoing debate about the selection mechanisms that drive this in-body evolutionary process, during which lymphocytes are diversified and then selected for high-affinity of the encoded antibodies. In 2009 we have interpreted intravital two-photon imaging data of cells in germinal centres and derived a new model for cell migration and selection. We expect that this knowledge will help to better control related autoimmune diseases and to optimise vaccination protocols. These issues have been discussed in the 16th Germinal Centre Conference which was hosted and organised by Michael Meyer-Hermann in Frankfurt am Main, July 5th-9th. The running EU project MAMOCELL was successfully extended to 2010.

Cover of Trends in Immunology 30 in 2009 showing B cells on a cat walk that are enlighted by mathematical spots.

Related publications in 2009:

1) M. Meyer-Hermann, M.T. Figge, and K.M. Toellner, *Germinal centres seen through the mathematical eye: B cell models on the catwalk.* Trends Immunol. 30 (2009) 157-164.

2) M. Kosco-Vilbois, M. Meyer-Hermann, *The 16th international conference on lymphatic tissues and germinal centres in immune responses.* Eur. J. Immunol. 39 (2009) 2311-2312.

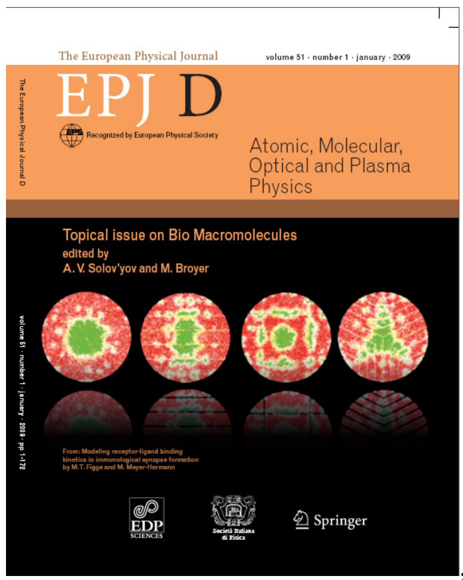
3) A. Garin, M. Meyer-Hermann, M. Contie, M.T. Figge, V. Buatois,M. Gunzer, K.-M. Toellner, G. Elson, and M.H. Kosco-Vilbois, *TLR4 signaling by follicular dendritic cells impacts germinal center reactions and the subsequent humoral response.* Submitted 2009.

The immunological synapse

Collaborators: Marc Thilo Figge[1], Michael Meyer-Hermann[1], Matthias Gunzer[2]

[1] FIAS, [2] Magdeburg University

The immunological synapse is the analogon of the synapses between neurons in the nervous system. Immune cells that get into contact to antigen-presenting cells and form in a dynamic process molecular complexes between their receptors and ligands that result into peculiar molecular patterns at the contact area. This, in particular, allows the exchange of toxic substances without harming other surrounding cells. The toxic substances can induce programmed cell death in the target cell, which is referred to as the kiss-of-death. In an agent-based mathematical model we have analysed the intracellular processes responsible for the dynamic molecular patterns at the synapse and have previously found that intermolecular adhesion, long-range attraction mediated by the cell cytoskeleton, and short-range repulsion between molecular sub-types are necessary to understand the genesis of these patterns. The results have been extended to realistic receptor-ligand binding kinetics and it was found that the resulting pattern depends on the affinity of the respective receptor-ligand pairs. This explains the diversity of the synapse patterns found in nature.



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Cover of European Physics Journal D 51 in 2009 showing simulations of immunological synapses resulting from barrier manipulation of the motility of molecules in the cellular plasma membrane. Adhesion molecule complexes are shown in red and complexes forming between the T-cell-receptor and peptid-major-histocompatibility-complexes are shown in green.

Related publications in 2009:

M.T. Figge and M. Meyer-Hermann, *Modeling receptor-ligand binding kinetics in immunological synapse formation.* Eur. Phys. J. D 51 (2009) 153-160.

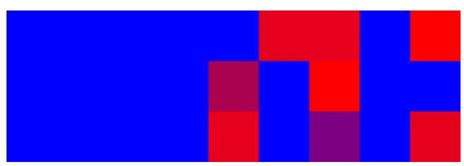
Electrophysiology and granule dynamics in diabetes

Collaborators: Jaaber Dehghani[1], Michael Meyer-Hermann[1], Michele Solimena[2], Eugenio Fava[3], Richard Benninger[4]

[1] FIAS, [2] Technische Universität Dresden, [2] Deutsches Zentrum für Neurodegenerative Erkrankungen (DZNE), Bonn, [4] Vanderbilt University, Nashville, TN

In type-II diabetes, insulin secretion by pancreatic betacells is impaired. The reason for disregulation of exocytosis of insulin carrying granules in the cells is not understood. In response to elevated glucose levels and after intracellular metabolism, the ATP/ADP-ratio in the cell is increased and induces so-called burst events in the membrane potential. These control the calcium level in the cell. It is known that the release of insulin carrying granules at the plasma membrane involves several calcium-dependent processes. In addition to this coupling of glucose to insulin release, the betacell has to synthesise insulin and to pack it in granules. This process is regulated by a number of factors including feedback mechanisms from exocytosis to the nucleus.

We plan to understand the processes leading to granule exocytosis and homeostasis in a comprehensive model covering betacell electrophysiology, granule dynamics, granule motility and exocytosis. The predictive power of the modelling approach is optimised by using an approach that is based on a single transmembrane protein and is fully derived from experimental data. In 2009 we have achieved a surprising result, in a combination of experiment, image analysis and mathematical modelling, setting in question the generally assumed homeostatic number of granules per betacell. We have also extended the earlier model of the betacell electrophysiology to a realistic islet of many betacells that are connected by gap-junctions and show an interesting pattern of betacell activity in the islet.



A snap-shot of the activity of betacells coupled by gap-junctions in a pancreatic islet is shown (blue and red correspond to low and high activity, respectively). These inhomogenous activity patterns and dynamics exhibit the characteristics of chaotic systems.

Related publications in 2009:
2 publications in preparation.

The interaction of subsystems: Nervous and immune system

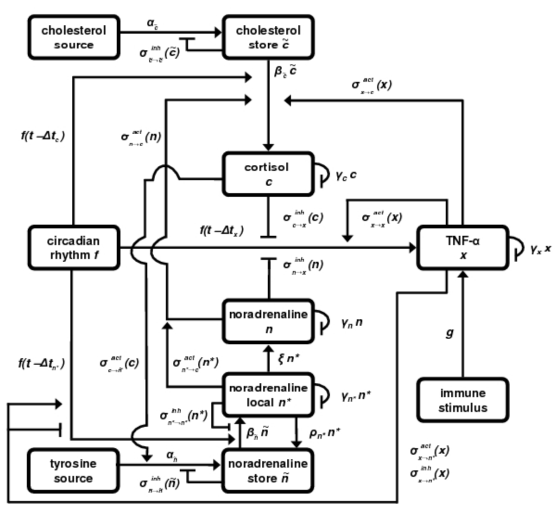
Collaborators: Michael Meyer-Hermann[1], Jochen Triesch[1], Marc Thilo Figge[1], Cristina Savin[1], Rainer Straub[2]

[1] FIAS, [2] Regensburg University

In recent years there is increasing evidence that the well studied nervous and immune systems are not isolated subsystems, despite the blood-brain-barrier suggesting this, but that their interaction is most important for the control of the organism as a whole. In two subprojects we have enlighted this complex relationship between the two systems:

A) Rheumatoid arthritis refers to the inflammatory degeneration of joints that is of tremendous relevance to public health. Disease progression is associated with the generation of new antibodies in tertiary lymphoid tissue newly generated in the joints on the one hand, and with the reduction of anti-inflammatory nerve endings in these joints on the other hand. In a mathematical model, we have analysed the circadian rhythm of endocrine and immune factors and their interaction and found that the effect of anti-inflammatory drugs strongly depends on the in-day time the drug is given. This result has strong impact on the pharmaceutical industry.

B) The relation of seizures with inflammatory molecules is not intuitive. However, it was recently found that pleiotopic moleculs like TNF-alpha are pro-inflammatory molecules in the periphery and, at the same time, induce synaptic scaling in the nervous system. We have shown that a neuronal network becomes more prone to seizures under inflammatory stimuli in the brain. Indeed, it is observed in clinics that patients with brain injury have a higher probability of developing seizures.



Interaction network of serum tumor-necrosis-factor-alpha, cortisol, and noradrenaline in response to a circadian pace maker signal.

Related publications in 2009:

1) M. Meyer-Hermann, M.T. Figge, and R. Straub, Mathematical modeling of the circadian rhythm of key neuroendocrine immune players in rheumatoid arthritis: A systems biology approach. Arthritis & Rheumatism 60 (2009) 2585-2594.

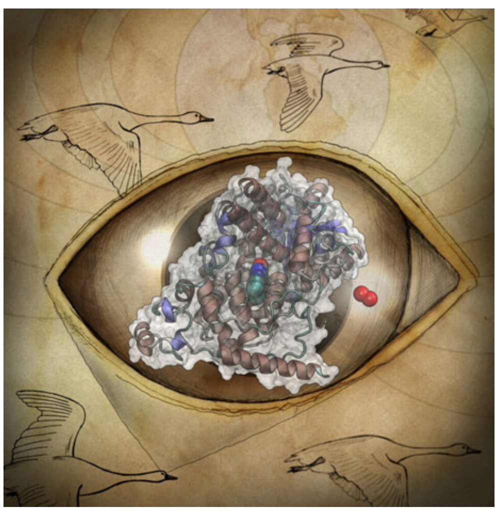
2) C. Savin, J. Triesch, and M. Meyer-Hermann, *Seizure induction by glia-mediated synaptic scaling.* J. Roy. Soc. Interface 6 (2009) 655-668.

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

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

[1]Frankfurt Instiute for Advanced Studies, [2]Department of Physics, University of Illinois at Urbana-Champaign, and Beckman Institute for Advanced Science and Technology, 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. In sensing the earth's magnetic field, cryptochrome relies on redox reactions, which exchange electrons between molecules. Such reactions are crucial for life, but can also be damaging. Antioxidants to keep them in check are produced and used naturally in the body and marketed commercially in pharmacology and as dietary supplements. For magnetoreception, cryptochrome requires small quantities of negatively charged molecular oxygen, superoxide (O_2^-). It is fortunate that only low doses are needed, because superoxide is toxic, despite being used elsewhere in the body for signaling.



Structure of cryptochrome, likely involved in avian magnetoreception. The protein internally binds the FADH (the semireduced form of flavin adenine dinucleotide) cofactor, which governs its functioning capabilities. Signaling is terminated by the superoxide radical O_2^-. The figure has been adapted from the cover image of the Biophysical Journal, volume 96, number 12 (2009).

Related publications in 2009:

1. I. A. Solov'yov and K. Schulten, *Understanding how birds navigate*, SPIE Newsroom, DOI: 10.1117/2.1200909.1804 (2009)
2. I. A. Solov'yov and W. Greiner, *Micromagnetic insight into a magnetoreceptor in birds: existence of magnetic field amplifiers in the beak*, Physical Review E80 (2009) 041919
3. I. A. Solov'yov and K. Schulten, *Magnetoreception through Cryptochrome May Involve Superoxide*, Biophysical Journal 96 (2009) 4804-4813
4. I. A. Solov'yov and W. Greiner, *Iron-mineral-based magnetoreceptor in birds: polarity or inclination compass?*, European Physical Journal D51 (2009) 161-172

Report by Prof. Peter Güntert

NMR-based Computational Structural Biology

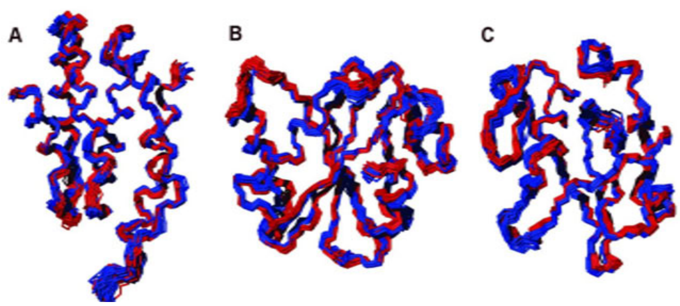
Computation methods to study biomolecular systems, in particular by nuclear magnetic resonance (NMR), are the focus of our research. The relationship between structure, dynamics and function of biological macromolecules is of fundamental importance for understanding life at a molecular level, and a key element of rational drug design. The three-dimensional structure has a pivotal role, since its knowledge is essential to understand the physical, chemical, and biological properties of a protein. Until recently NMR protein structure determination was a laborious undertaking that occupied a trained spectroscopist for months or years for each new protein structure. This situation has changed by the introduction of automated, computational systems. We are extending NMR protein structure analysis to hitherto inaccessible systems, including proteins larger than 40 kDa, membrane proteins, and proteins studied directly inside living cells.

Prof. Dr. Peter Güntert
Institut für biophysikalische Chemie
and
Frankfurt Institute for Advanced Studies
http://www.bpc.uni-frankfurt.de/guentert/

Protein structure analysis

Collaborators: T. Ikeya, R. Schmucki, D. Gottstein, F. Hefke, E. Schmidt, D. Kirchner, L. Buchner, P. Güntert

Three-dimensional (3D) structures of proteins in solution can be calculated on the basis of conformational restraints derived from NMR measurements. Our CYANA program package, based on simulated annealing by molecular dynamics simulation in torsion angle space and the automated assignment of NOE distance restraints, is one of the most widely used algorithms for this purpose. Automated methods for protein structure determination by NMR have increasingly gained acceptance and are now widely used for the automated assignment of distance restraints and the calculation of 3D structures. Our FLYA algorithm for the fully automated NMR structure determination of proteins yields, without human intervention, 3D protein structures starting from a set of multidimensional NMR spectra. As in the classical manual approach, structures are determined by a set of experimental NOE distance restraints without reference to already existing structures or empirical molecular modeling information. In addition to the 3D structure of the protein, FLYA yields backbone and side-chain chemical shift assignments, and cross peak assignments for all spectra.



Fully automated NMR structure determination: *Three protein structures obtained by fully automated structure determination with the FLYA algorithm (blue) are virtually identical to the corresponding NMR structures determined by conventional methods (red).*

Related publications in 2009:

1) Hamada, T., Matsunaga, S., Iwamoto, M., Shimizu, H., Fujiwara, M., Fujita, K., Muramatsu, I., Hirota, H., Schmucki, R., Güntert, P., Fusetani, N., Oiki, S., *Channel-forming non-ribosomal peptide from marine sponge.* Nature Chemistry.

2) Coutandin, D., Löhr, F., Niesen, F. H., Ikeya, T., Weber, T. A., Schäfer, B., Bullock, A. N., Yang, A., Güntert, P. , Knapp, S., McKeon, F., Der Ou, H. & Dötsch, V., *Conformational stability and activity of p73 require a second helix in the tetramerization domain.* Cell Death Diff. 16(2009) 1582.

3) Khayrutdinov, B. I., Bae, W. J., Yun, Y. M., Lee, J. H., Tsuyama, T., Kim, J. J., Hwang, E., Ryu, K. S., Cheong, H. K., Cheong, C., Ko, J. S., Enomoto, T., Karplus, P. A., Güntert, P., Tada, S., Jeon, Y. H., Cho, Y., *Structure of the Cdt1 C-terminal domain: Conservation of the winged helix fold in replication licensing factors.* Prot. Sci. 18, 2252-2264.

4) He, F., Saito, K., Kobayashi, N., Harada, T., Watanabe, S., Kigawa, T, Güntert, P., Unzai, S., Muto, Y. & Yokoyama, S., *Structural and functional characterization of the NHR1 domain of the Drosophila Neuralized E3 ligase in the Notch signaling pathway.* J. Mol. Biol. 393 (2009) 478-495.

5) Tsuda, K., Kuwasako, K., Takahashi, M., Someya, T., Inoue, M., Terada, T., Kobayashi, N., Shirouzu, M., Kigawa, T., Tanaka, A., Sugano, S., Güntert, P., Muto, Y. & Yokoyama, S., *Structural basis for the sequence specific RNA-recognition mechanism of human CUG-BP1 RRM3.* Nucl. Acids Res. 37 (2009) 5151-5166.

6) He, F., Dang, W., Saito, K., Watanabe, S., Kobayashi, N., Güntert, P., Kigawa, T, Tanaka, A., Muto, Y. & Yokoyama, S. *Solution structure of the cysteine-rich domain in Fn14, a member of the tumor necrosis factor receptor superfamily.*, Protein Sci. 18 (2009) 650-656.

7) Peroza, E. A., Schmucki, R., Güntert, P., Freisinger, E. & Zerbe O. *The E-domain of Ec-1 metallothionein: A metal-binding domain with a distinctive structure.*, J. Mol. Biol. 387 (2009) 207-218.

8) He, F., Dang, W., Abe, C., Tsuda, K., Inoue, M., Watanabe, S., Kobayashi, N., Kigawa, T, Matsuda, T., Yabuki, T., Aoki, M., Seki, E., Harada, T., Tomabechi, Y., Terada, T., Shirouzu, M., Tanaka, A., Güntert, P., Muto, Y. & Yokoyama, S., *Solution structure of the RNA binding domain in the human muscleblind-like protein 2.* Protein Sci. 18 (2009) 80-91.

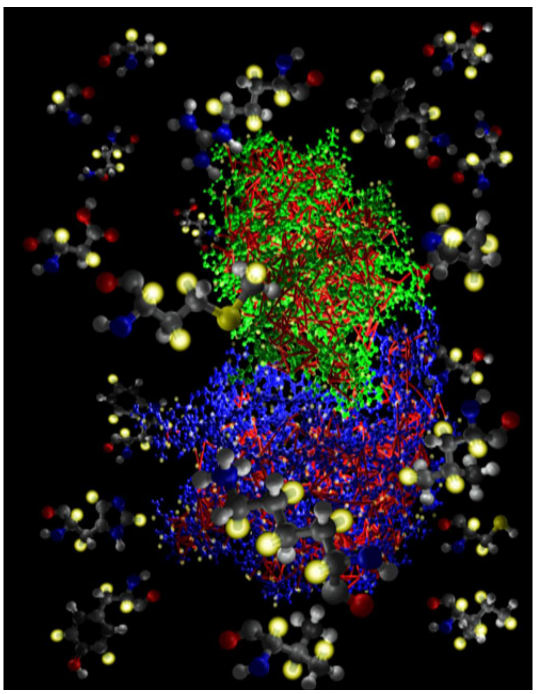
9) Güntert, P., *Automated structure determination from NMR Spectra.*, Eur. Biophys. J. 38 (2009) 129-143.

10) Ohnishi, S. Pääkkönen, K., Koshiba, S., Tochio, N., Sato, M., Kobayashi, N., Harada, T., Watanabe, S., Muto, Y., Güntert, P., Tanaka, A., Kigawa, T. & Yokoyama, S., *Solution structure of the GUCT domain from human RNA helicase II/Guβ reveals the RRM fold, but implausible RNA interactions.* Proteins 74 (2009) 133-144.

Stereo-array isotope labeling

Collaborators: T. Ikeya, E. Schmidt, P. Güntert

NMR spectroscopy can determine the three-dimensional structure of proteins in solution. Nevertheless, its potential has been limited by the difficulty of interpreting NMR spectra in the presence of broadened and overlapped resonance lines and low signal-to-noise ratios. Stereo-array isotope labelling (SAIL) can overcome many of these problems by applying a complete stereo- and regiospecific pattern of stable isotopes, which is optimal with regard to the quality and information content of the resulting NMR spectra. SAIL utilizes exclusively chemically and enzymatically synthesized amino acids for cell-free protein expression such that in all methylene groups, one ^{1}H is stereo-selectively replaced by ^{2}H, in all single methyl groups, two ^{1}H are replaced by ^{2}H, and in the prochiral methyl groups of Leu and Val, one methyl is stereo-selectively -$^{12}C(^2H)_3$ and the other is -$^{13}C^1H(^2H)_2$. In six-membered aromatic rings, the 12C-2H and 13C-1H moieties alternate with each other. SAIL achieves a 4-7-fold increase in signal-to-noise, sharper resonance lines, and a 40-60% reduction in the number of signals without sacrificing essential information about the backbones and the side chains of all amino acid residue types. The resulting reduction of spectral overlap, the higher accuracy of the frequency determination, the complete stereospecific assignment, and the measurement of longer ^{1}H–^{1}H distances makes it possible to determine high-quality solution structures of proteins larger than 30 kDa.



Stereo-array isotope labeling (SAIL): *The 20 standard amino acids are labeled such that each CHn group carries at most a single NMR-visible ^{1}H nucleus, the others being replaced by NMR-invisible ^{2}H. The remaining ^{1}H nuclei, shown as lights in the Figure, provide data that allows the NMR structure determination of proteins about twice as large as by conventional NMR approaches. The structure of the 42 kDa maltodextrin-binding protein MBP that is shown in the center of the Figure was solved in collaboration with the laboratory of Prof. Masatsune Kainosho at Tokyo Metropolitan University, Japan, using SAIL in conjunction with the structure calculation program CYANA.*

Related publications in 2009:

1) Kainosho, M. & Güntert, P., *SAIL - Stereo-array isotope labeling.* Q. Rev. Biophys. In press.

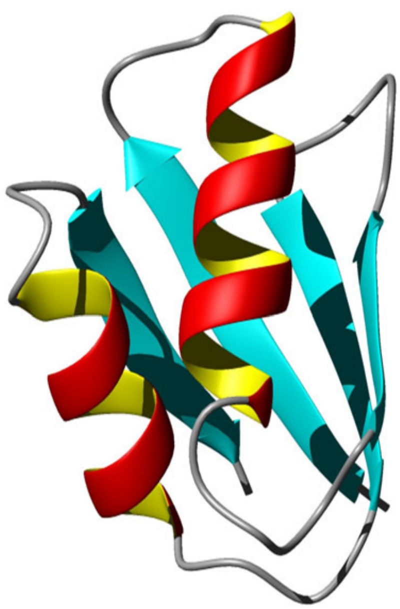
2) Ikeya, T., Jee. J. G., Kainosho, M. & Güntert, P., *NMR protein structure determination using exclusively NOESY spectra.* J. Am. Chem. Soc. Submitted.

3) Ikeya, T., Takeda, M., Yoshida, H., Terauchi, T., Jee, J., Kainosho, M. & Güntert, P., *Automated NMR structure determination of stereo-array isotope labeled ubiquitin from minimal sets of spectra using the SAIL-FLYA system.* J. Biomol. NMR. 44 (2009) 261-272.

Protein structure determination in living cells by in-cell NMR spectroscopy

Collaborators: T. Ikeya, P. Güntert

Proteins in living cells work in an extremely crowded environment where they interact specifically with other proteins, nucleic acids, co-factors and ligands. Methods for the three-dimensional structure determination of purified proteins in single crystals or in solution are widely used and have made very valuable contributions to understanding many biological processes. However, replicating the cellular environment *in vitro* is difficult. *In vivo* observations of three-dimensional structures, dynamics and interactions of proteins are required for fully understanding the structural basis of their functions inside cells. Investigating proteins "at work" in a living environment at atomic resolution is thus a major goal of molecular biology. Recent developments in NMR hardware and methodology have enabled the measurement of high-resolution heteronuclear multi-dimensional NMR spectra of macromolecules in living cells (in-cell NMR). Various intracellular events such as conformational changes, dynamics and binding events have been investigated by this method. However, the low sensitivity and short life time of the samples have so far prevented the acquisition of sufficient structural information to determine protein structures by in-cell NMR. Recently we presented the first three-dimensional protein structure calculated exclusively on the basis of information obtained in living cells. The in-cell NMR approach can thus provide accurate high-resolution structures of proteins in living environments.



Protein structure determined in living cells: *The first three-dimensional protein structure calculated exclusively on the basis of information obtained in living cells was solved by in-cell NMR for the putative heavy metal-binding protein TTHA1718 from* Thermus thermophilus *HB8 overexpressed in* E. coli *cells. A major hurdle for determining in-cell NMR structures is the limited lifetime of the cells inside the NMR sample tube. Standard NMR experiments usually require 1-2 days of data collection, which is an unacceptably long time for live cells. This time could be shortened to 2-3 hours by preparing a fresh sample for each experiment and by applying a nonlinear sampling scheme in combination with maximum entropy processing for the indirectly acquired dimensions.*

Related publications in 2009:

1) Sakakibara, D., Sasaki, A., Ikeya, T., Hamatsu, J., Hanashima, T., Mishima, M., Yoshimasu, M., Hayashi, N., Mikawa, T., Wälchli, M., Smith, B. O., Shirakawa, M., Güntert, P. & Ito, Y., *Protein structure determination in living cells by in-cell NMR spectroscopy.* Nature 458 (2009) 102-105.

2) Ikeya, T., Sasaki, A., Sakakibara, D., Shigemitsu, Y., Hamatsu, J., Hanashima, T., Mishima, M., Yoshimasu, M., Hayashi, N., Mikawa, T., Nietlisbach, D., Wälchli, M., Smith, B. O., Shirakawa, M., Güntert, P. & Ito, *Y. Protein structure determination in living E. coli cells by in-cell NMR spectroscopy.* Nature Protocols. Submitted.

3) Ito, Y. & Güntert, P. *Seeing proteins in living cells.* BIOforum Europe 13 (2009) 25-27.

4.4 Atoms, Molecules, Nanosystems

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

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.

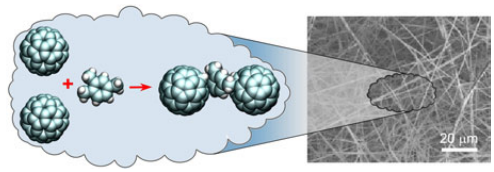
Research directions and sub-directions (the year 2009) include:

1. Structure, structure formation and dynamics of MBN systems:
   - Structure and dynamics of nanosystems.
   - Photo processes in nanostructures.
   - Phase transformations at 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.
   - Multiscale approach to ion beam cancer therapy.
3. Software development.

1. Research direction: 'Structure and dynamics of nanosystems'

Collaborators: C. Bréchignac (CNRS, France), B. Johnson (Cambridge, UK), W. Greiner (FIAS), D. Poenaru (Nat. Inst. Phys., Romania), V. Ivanov (St. Petersburg State Polytech. Univ., Russia), E.A. Vinogradov (Inst. Spectrosc., Troitsk, Russia).

Short description: a systematic 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 surfaces'

Main results: Theoretical study of the process of fractal growth on a surface by means of the deposition, diffusion, and aggregation method is performed. The analysis of the deposition process of nanoparticles on various substrates at different temperatures and of their dynamics on the surface is carried out. It is demonstrated that the pattern formation depends crucially on the ratio of the flux of nanoparticles to their mobility on the surface.

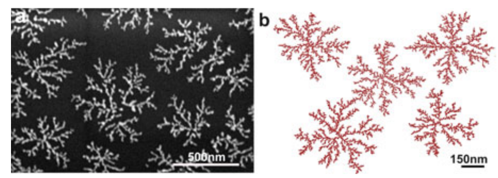


Fig.1. (a) Structures of silver cluster fractals grown by clusters deposition technique on the graphite surface [C. Bréchignac and et al., PRL 97 (2006) 133402]; (b) Fractal structures grown by the DDA method.

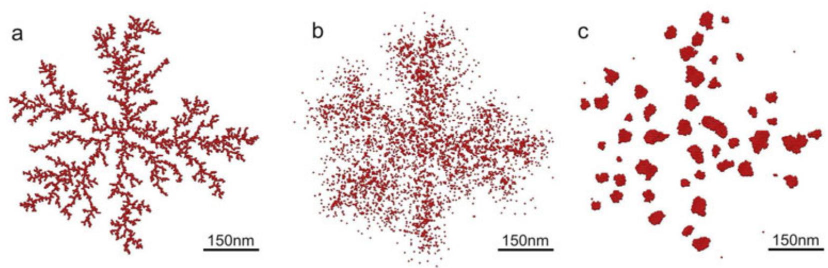


Fig.2. Evolution of the fractal structure: (a) initial structure of the fractal; (b) rapid fragmentation of the fractal (c) fragmentation of the fractal due to the diffusion of the particles along the branches.

The dependence of fractal pattern stability and the paths of fragmentation on the concentration of impurities and temperature were investigated by means of the developed method which accounts for the internal dynamics of fractal particles. We demonstrated that particle diffusion and detachment controls the shape of the emerging stable islands on surface. We considered different scenarios of fractal post-growth relaxation and analyzed the time evolution of the island's morphology. The results of our calculations were compared with available experimental observations, and experiments in which the post-growth relaxation of deposited nanostructures can be probed were suggested.

Related publication in 2009:

1) V. Dick, I.A. Solov'yov, A.V. Solov'yov, *Theoretical study of fractal growth and stability on surface*, AIP Conf. Proc. 1197 (2009) 76-88.

1.2. Research project: 'Structure and dynamics of fullerene-based nanotubes'

Main results: We have performed a thorough theoretical analysis, aiming at gaining an in-depth understanding of the exceptionally large aspect ratio of C_{60}-based nanowires exceeding 3000. By accounting for different interactions in the system we have calculated the structures of the unit cell and determined the role of the fullerene and of the solvent molecules in the crystallization process of the nanowires [1]. We have calculated the adhesion energy of C_{60} molecules to the nanowire surface, and on the basis of this explained the growth anisotropy of the crystal.

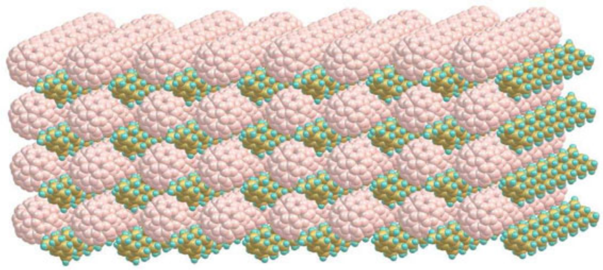


Fig. 1. Solvent-controlled growth of a C_{60}-based nanowire. The growth of nanowires is strongly solvent-dependent: in abundance they grow from the 1,2,4-trimethylbenzene solution of C_{60}, while only flake-like small particles nucleate, e.g., in toluene.

We demonstrated theoretically that at room temperature the effect of electron polarization is negligibly small and, therefore, cannot become the driving force for nanowire growth along one preferential direction [2]. Experimental measurements are in agreement with the theoretical analysis [2,3]: the nanowires have been observed to emerge from the polar 1,2,4-trimethylbenzene and non-polar 1,3,5-trimethylbenzene solution of C_{60}, while no nanowires from polar toluene, 1,2,3-trimethylbenzene and non-polar benzene solutions could be recorded (see Fig. 2).

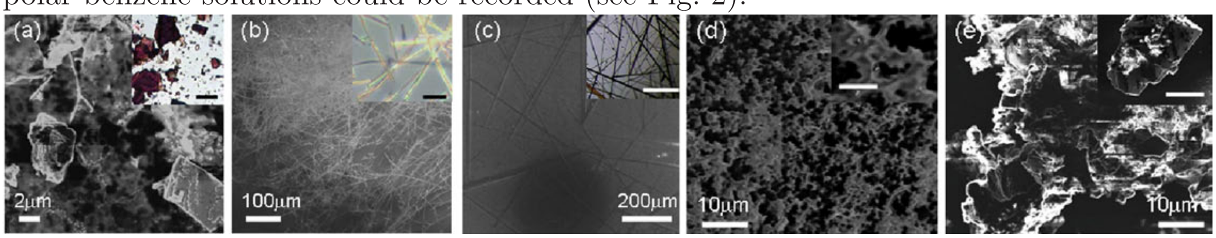


Fig. 2. Scanning electron microscopic images of C_{60} crystals (either in the form of wires or particles) grown by using the solvents of 1,2,3-trimethylbenzene (a), 1,2,4-trimethylbenzene (b), 1,3,5-trimethylbenzene (c), benzene (d), and toluene (e).

Related publications in 2009:

1) J. Geng, I.A. Solov'yov, W. Zhou, A.V. Solov'yov, B.F.G. Johnson, *Uncovering a solvent-controlled preferential growth of buckminsterfullerene C_{60} nanowires,* J. Phys. Chem. C113 (2009) 6390.

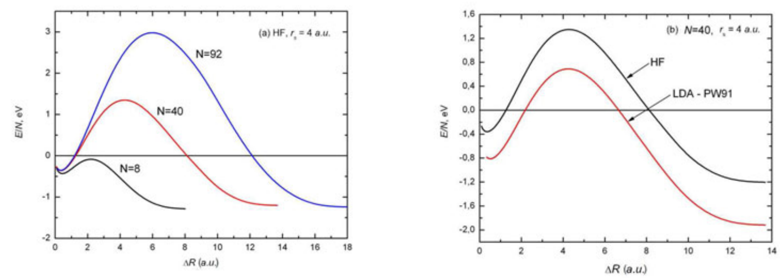
2) I.A. Solov'yov, J. Geng, A.V. Solov'yov, B.F.G. Johnson, *On the possibility of the electron polarization to be the driving force for the C60-TMB nanowire growth,* Chem. Phys. Lett. 472 (2009) 166.

3) I.A. Solov'yov, J. Geng, A.V. Solov'yov, B.F.G. Johnson, *Understanding the formation process of exceptionally long fullerene-based nanowires,* AIP Conf. Proc. 1197 (2009) 89-102.

1.3. **Research project: 'Structure and dynamics of clusters'**

Main results:

• The stability of the volume and the hollow metallic cluster systems within the spherical jellium model approach based on the Hartree-Fock approximation and the LDA was investigated. It was demonstrated that for such systems there are two stable states, corresponding to two different geometries, which are separated by the potential barrier dependent on the cluster size and the density of the ionic charge distribution. The first state corresponds to a uniform charge distribution of the ions over the entire cluster volume. In the second fullerene-like stable state the positive charge is uniformly distributed over a spherical shell of a certain width.



The figures:
Total cluster energy per atom calculated within the HF for different cluster sizes at $r_s = 4$ *a.u.* (a) and for $N = 40$ within the HF and LDA (b)

• The structure, stability and annihilation of a novel finite quantum object - electron-positron droplet (EPD) - was investigated. The calculations show that electron-positron matter can exist in a metal' phase in the form of spatially compact, spherically symmetrical clusters which have large binding energies and lifetimes comparable with those of the positronium. The many-body correlations significantly contribute to the total energies and geometry of EPDs.

• The experimentally observed oblate equilibrium shapes of deposited atomic clusters were explained by simulating the interaction energy with the substrate. Minimization of the liquid-drop deformation energy of a sodium cluster allowed to obtain a wide range of equilibrium shapes: hyperdeformed and superdeformed oblate hemispheroids, hemisphere; superdeformed and hyperdeformed prolate hemispheroids. These shapes only weakly depend of the number of atoms in the cluster.

Related publications in 2009:

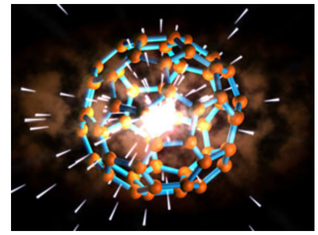
1) R. G. Polozkov, V. K. Ivanov, A. V. Verkhovtsev, A. V. Solov'yov, *Stability of metallic hollow cluster systems,* Phys. Rev. A79 (2009) 063203.

2) P.I. Yatsyshin, R.G. Polozkov, V.K. Ivanov, A.V. Solov'yov, *Structure of electron-positron clusters: Hartree-Fock approximation,* Physica Scripta 80 (2009) 048126.

3) D.N. Poenaru, R.A. Gherghescu, A.V. Solov'yov, W. Greiner, *Charged metallic clusters*, AIP Conf. Proc. 1197 (2009) 48-56 (2009).

4) D.N. Poenaru, R.A. Gherghescu, A.V. Solov'yov, W. Greiner, *Oblate equilibrium shapes of hemispheroidal atomic clusters*, Europ. Phys. Lett. 88 (2009) 23002.

5) D.M. Popova, B.N. Mavrin, A.V. Solov'yov, *Ab initio investigation of electronic and vibrational properties of ZnS and ZnSe crystals by different XC-functionals,* Int. J. Modern Phys. B23 (2009) 3845-3857.



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

Collaborators: V. Ivanov (St. Petersburg State Polytechnical University, Russia), J.-P. Connerade (Imperial College, UK).

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:

• We have demonstrated [1] that the angular distribution of photoelectrons from a strongly polarizable target (a cluster, a fullerene, a macromolecule) exposed to a laser field can deviate noticeably from the prediction of conventional dipole-photon theory due to the action of the field of alternating dipole moment induced at the residue by the laser field. The effect is sensitive to the dynamic polarizability of the residue and to its geometry, to the intensity and frequency of the laser field. Strong modifications of the photoionization process happen in vicinity of the plasmon resonance for laser fields of comparatively low intensities $10^{10} - 10^{11}$ W cm^{-2}.

• A consistent many-body theory for the description of angular resolved photoelectron spectra of metal clusters has been developed [2]. Numerical results obtained allowed us to explain the peculiarities in photoelectron angular spectra measured recently for sodium clusters in a broad range of cluster sizes.

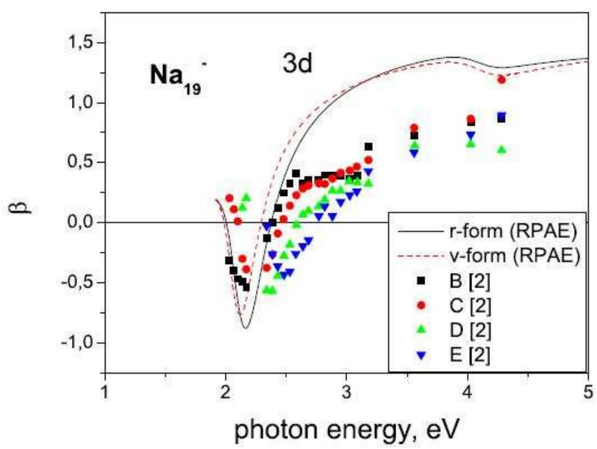


Figure: Angular asymmetry parameter for Na_{19}^{-}. Lines – quantum calculations [4], and symbols – experimental results (von Issendorf et al).

Related publications in 2009:

1) A. V. Korol, A. V. Solov'yov, *Photoionization of a strongly polarizable target,* J. Phys. B: At. Mol. Opt. Phys. 42 (2009) 015002.

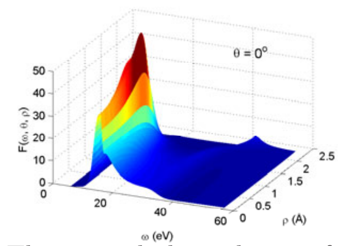
2) A. V. Solov'yov, R. G. Polozkov, V. K. Ivanov, *Many-body theory for angular resolved photoelectron spectra of metal clusters,* Phys. Rev. A submitted (2009) [arXiv:0905.0026].

2.2. Research project: 'Photo-processes in fullerenes and endohedral systems'

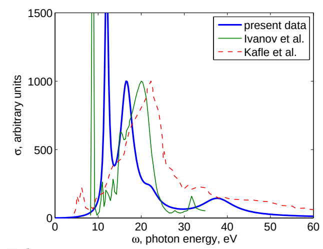
The project aims to study photo-processes (photoabsorption, bremsstrahlung, light scattering) in fullerenes and endohedral systems. Special attention is paid to the role of collective electron excitations (plasmons) and mechanisms of their relaxation.

Main results:

• Analysis has been carried out of the role of dynamical screening in the photoionization of an atom encaged in a fullerene. In vicinity of the plasmon resonance of the fullerene the dynamical screening can lead to a tremendous enhancement of the amplitude of the electromagnetic wave acting on the encapsulated object [1,2]. The result is an amplification of the photoabosorption cross section of the encapsulated species. This effect is of a general nature and will also appear for impurity atoms or molecules embedded into or attached onto a metallic cluster or a nanotube.



The spatial dependence of the dynamical screening factor for $Ar@C_{60}$ [1].



Photoionization cross section of C_{60}. Blue line – classical approach [2], black – quantum calculations [3], red – experimental results (Kafle *et al.*, *J. Phys. Soc. Japan* **77** 014302 (2008)).

• The finite thickness of the fullerene leads to the splitting of its surface plasmon into a symmetric mode and an antisymmetric mode. These manifest themselves as large peaks in the dynamical screening factor [1], (see top figure). The magnitude of this enhancement strongly depends on the nature and on the position of the confined atom. Accounting for the two types of plasmons of the fullerene (σ and π) leads to the four resonances seen in the lower figure [2]. Our simple classical model gives a good qualitative agreement with more complex calculations.

• The photoionization cross sections of C_{60} and its cations are calculated for photon energies from the ionization thresholds up to 80 eV [3]. The theoretical approach is based on the LDA, RPAE, and the jellium models. The sphere and the spherical layer jellium models are tested, with the latter providing more reliable results. Two giant resonances are found in the photoionization spectra of all fullerenes treated. Their positions and shapes are determined in agreement with the experimental data.

Related publications in 2009

1) S. Lo, A.V. Korol, A.V. Solov'yov, *Dynamical screening of an endohedral atom,* Phys. Rev. A79 (2009) 063201.

2) S. Lo, A.V. Korol, A.V. Solov'yov, *Dynamical screening of an endohedral atom,* AIP Conf. Proc. 1197 (2009) 119-133.

3) A.K. Belyaev, A.S. Tyukanov, A.I. Toropkin, V.K. Ivanov, R.G. Polozkov, A.V. Solov'yov, *Photoabsorption of C_{60} and its positive ions,* Phys. Scripta 80 (2009) 048121.

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

Collaborators: J.-P. Connerade (Imperial College, UK), S. Schramm (FIAS).

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'

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.

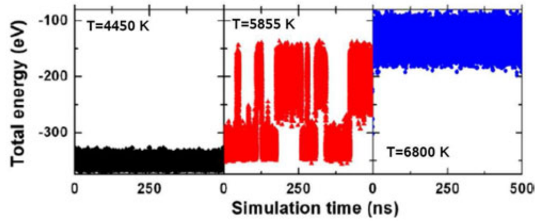
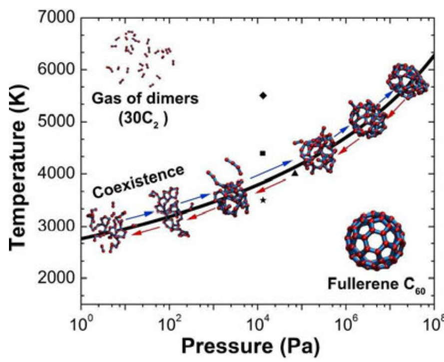


Illustration of the phase transition from the solid-like C_{60} cage state (left) to the gas of dimers and short chains, from Ref [3].

• 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.



The curve separates the region where the system can be found in either a cage (below the line) or a gaseous state (above it).

• 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 generalised temperature and pressure conditions found in arc-discharge experiments and obtained the dependence of the phase transition temperatures on pressure.

Related publications in 2009:

1) A. Hussien, A.V. Yakubovich, A.V. Solov'yov, *Studying phase transition in nanocarbon structures,* AIP Conf. Proc. 1197 (2009) 152-173.

2) A. Lyalin, A. Hussien, A.V. Solov'yov, W. Greiner, *Impurity effects on the melting of Ni clusters,* Phys. Rev. B79 (2009) 165403.

3) A. Hussien, A. Yakubovich, A.V. Solov'yov, W. Greiner, *Phase transition, formation and fragmentation of fullerenes,* Eur. Phys. J. D accepted (2009) [arXiv:0807.4435v1].

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

Main results:

We have studied the preparation and characterization of a C_{60}-based nanowire polymer, (-C_{60}TMB-)$_n$, (TMB=trimethylbenzene), which is formed when polymerization occurs in the corresponding parent nanowire via a topochemical solid-state reaction [1]. 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-TMB) 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.

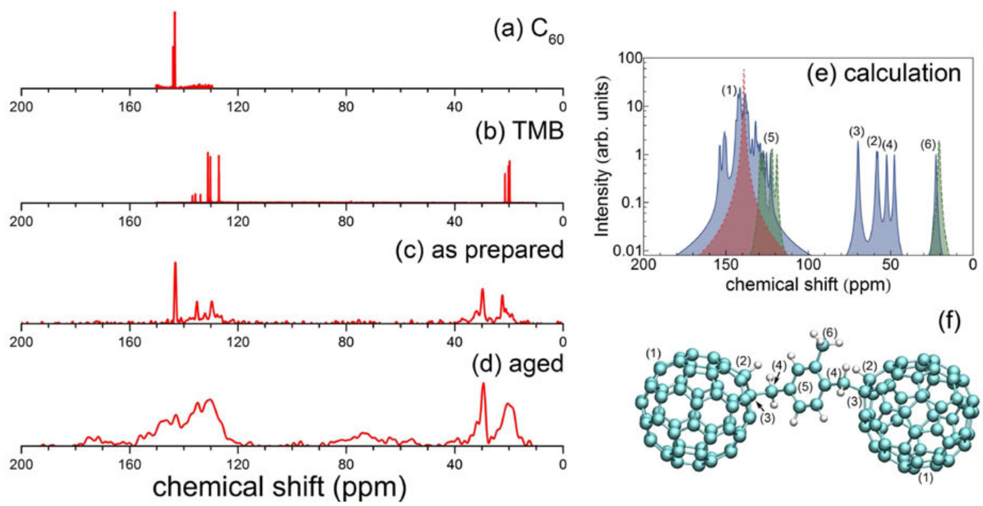


Fig. 1. Polymerization transformation in the C_{60}-based nanowire. (a)-(d): ^{13}C NMR spectrum of pure C_{60}, pure 1,2,4-TMB, as-prepared C_{60}-1,2,4-TMB adduct and the aged C_{60}-1,2,4-TMB adduct respectively. (e): calculated spectra. Solid line (blue fill), dashed line (green fill) and dotted line (red fill) show the corresponding spectra for the C_{60}-TMB-C_{60} complex as shown in (f), pure 1,2,4-TMB and pristine C_{60} respectively. The numbers labeled in (e) show the chemical shifts of the corresponding carbon atoms marked in (f).

Related publications in 2009:

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 (C_{60})-Based 1D Crystalline Nanopolymer Formed through Topochemical Transformation of the Parent Nanowire,* Phys. Rev. B submitted (2009); [arXiv:0906.2216].

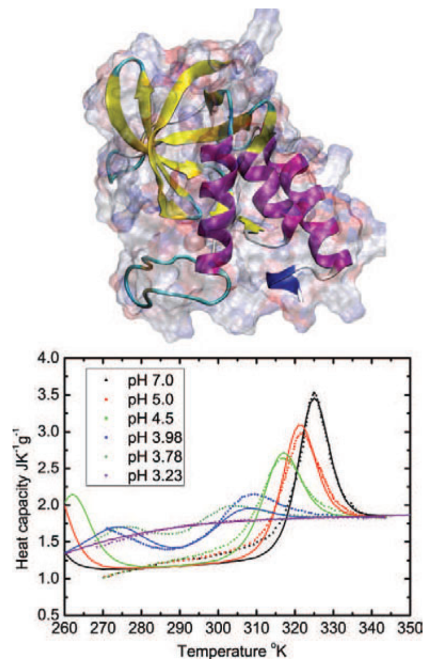
4. Research direction: 'Statistical mechanics of polypeptide and protein folding'

Collaborators: W. Greiner (FIAS).

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 understood despite numerous works devoted to this subject during the last decades. 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.

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.
- 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.



In the figure: The 3D structure of the staphylococcal nuclease protein (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 2009:

1) A.V. Yakubovich, I.A. Solov'yov, A.V. Solov'yov, W. Greiner, *Phase transitions in polypeptides: analysis of energy fluctuations,* European Phys. J. D51 (2009) 25-32.

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

3) A. Yakubovich, A.V. Solov'yov, W. Greiner, *Statistical mechanics model for protein folding,* AIP Conf. Proc. 119 (200) 186-200.

5. Research direction: 'Dynamics of biomolecules'

Collaborators: S. Volkov (Bogolyubov Institute for Theoretical Physics, Ukraine) and E. Surdutovich (Oakland University, Michigan, USA).

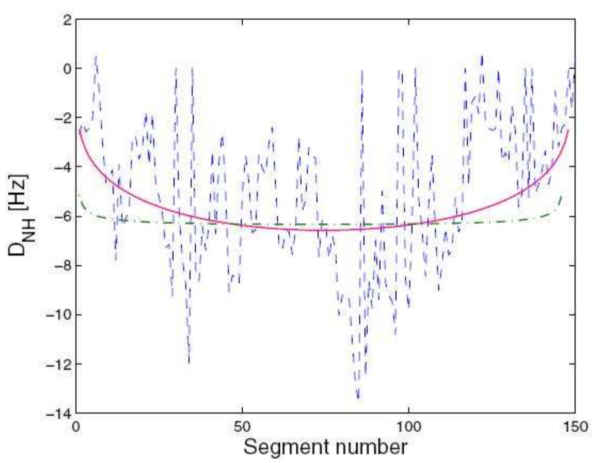
Short description: At the current level of technological and computational capabilities, methods and approaches traditionally associated with atomic and molecular physics research can now be applied to biomolecular systems, previously treated entirely using chemistry and biology techniques. We aim to elucidate essential, fundamental physical mechanisms and driving forces of various complex biomolecular processes.

Edited books and journal issues (in the year 2009):

1. A.V. Solov'yov (ed.), VI Int. Conf. on Radiation Damage in Biomolecular Systems (RADAM 2009), (Frankfurt am Main, Germany, June 30-July 05, 2009) Book of Abstracts (Printed by Goethe University, Frankfurt am Main, 2009), p. 1–168.
2. A.V. Solov'yov, M. Broyer (editors), *EPJD Topical Issue on Bio macromolecules,* European Phys. J. D51 (2009) 1–172.
3. A.V. Solov'yov, M. Broyer, *EPJD Topical Issue on Bio macromolecules,* Editorial, European Phys. J. D51 (2009) 1–3.

5.1. Research project: 'Dynamics of unfolded proteins'

Main results: A new statistical model of unfolded proteins is developed in which the stiffness of polypeptide backbone is taken into account. We used the distribution function of a semistiff protein to determine the nuclear magnetic resonance (NMR) residual dipolar couplings (RDCs) in unfolded proteins.



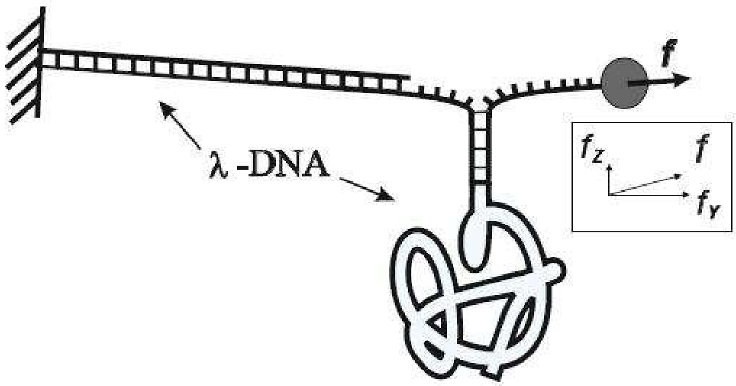
Calculated RDC profile (solid red curve) compared with the experimental one (chained blue curve) for unfolded apomyoglobin.

Related publications in 2009:

1) M. Čubrovič, O.I. Obolensky, A.V. Solov'yov, 'Semistiff polymer model of unfolded proteins and its application to NMR residual dipolar couplings', European Phys. J. D51 (2009) 41-49.

5.2. Research project: 'DNA unzipping'

Main results: The process of DNA double helix unzipping is considered as a nonlinear dynamical process due to an external force. We propose two stages for the unzipping. On the first stage the external force transforms the conformational state of the double helix and makes the unzipping possible. On the second stage the unzipping propagates along dsDNA. The boundary between the open and the closed parts of the helix moves along the chain as a step-like excitation (kink soliton).



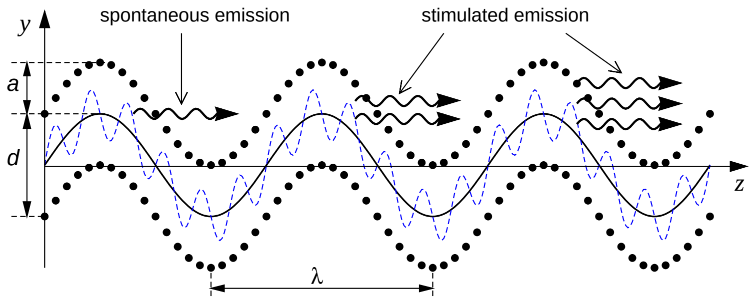
DNA unzipping by an external force studied in experiments.

Related publications in 2009:
1) S.N. Volkov, A.V. Solov'yov, *The mechanism of DNA mechanical unzipping,* European Phys. J. D54 (2009) 657-666.

6. Research direction: 'Gamma-Laser'

Collaborators: W. Greiner (FIAS), H. Backe & W. Lauth (Mainz Uni., Germany), U. Uggerhoj (Aarhus University, Denmark), S. Connell (Johannesburg University, South Africa), S. Dabagov (INFN, Italy), A. Pathak (Hyderabad University, India).

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.



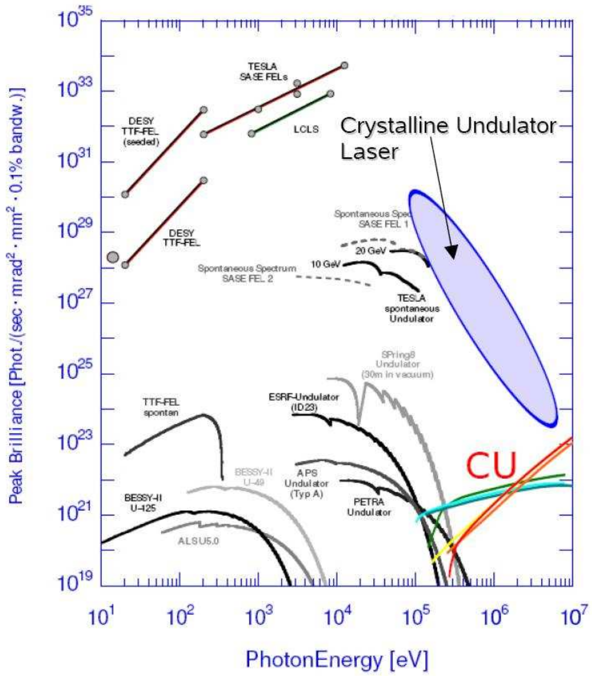
Schematic representation of spontaneous and stimulated (FEL-like type) radiation formed in a periodically bent crystal (a crystalline undulator).

Main results:

• A new scheme for amplification of coherent gamma rays is proposed. The key elements are crystalline undulators — single crystals with periodically bent crystallographic planes exposed to a high-energy beam of charged particles undergoing channeling inside the crystals. The scheme consists of two such crystals separated by a vacuum gap. The beam passes the crystals successively. The particles perform undulator motion inside the crystals following the periodic shape of the crystallographic planes. Gamma rays passing the crystals parallel to the beam get amplified due to interaction with the particles inside the crystals. The term 'gamma klystron' is proposed for the scheme because its operational principles are similar to those of the optical klystron. It is shown that the gamma ray amplification in the klystron scheme can be reached at considerably lower particle densities than in the one-crystal scheme.

• The propagation of a modulated beam of particles in a planar crystal channel is investigated. The evolution of the particle distribution is described by the Fokker-Planck type equation. Approximate analytical solution of the equation is found. It is demonstrated that the beam preserves its modulation at sufficiently large penetration depths which opens the prospect of using a crystalline undulator as a coherent source of γ-rays. This finding is a crucial milestone in developing a γ-laser.

• A peak brilliance of Crystalline Undulator based γ-Laser (CUL) is estimated. The brilliance as high as $10^{25} - 10^{26}$ Photons/(s mm^2 mrad^2 0.1% BW) can be obtained in a CUL fed by a completely modulated positron beam with current 1 kA and particle density 10^{18} cm^{-3}. This is comparable to the ordinary synchrotron radiation sources but is related to photon energies range of $\hbar\omega \sim 10^2 - 10^3$ keV unattainable to present state-of-the art devices.



• The effects of dislocations on the positron channeling in a periodically bent crystal are studied. The variation in effective potential and frequency in the different regions of dislocation affected channels is found. The wavefunctions of positrons channeled in the perfect and the dislocation affected channels are found and the channeling and dechanneling probabilities are calculated. The angular and spectral distributions of radiation intensity are calculated and compared with those of normal channeling. The calculations are carried out with varying values of dislocation density and varying undulator wavelength.

Related publications in 2009:

1) A. Kostyuk, A.V Korol, A.V. Solov'yov, W. Greiner, *A One-dimensional model of a Gamma klystron*, J. Phys. G: Nucl. Part. Phys. 36 (2009) 025107.

2) A. Kostyuk, A.V. Korol, A.V. Solov'yov and W. Greiner, *Modulated particle beam in a crystal channel,* submitted to Proceeding of SPIE (2009).

3) A. Kostyuk, A.V. Korol, A.V. Solov'yov and W. Greiner, *Stable propagation of a modulated particle beam in a bent crystal channel*, submitted to *European Physical Letters* (2009).

4) J. George, A. Pathak, A.V. Solov'yov, *Effects of dislocations on channeling radiation from a periodically bent crystal,* Journal of Physics: Condensed Matter 21 (2009)245402.

7. Research direction: 'Ion Beam Cancer Therapy'

Collaborators: E. Surdutovich (Oakland University, Michigan, USA), W. Greiner & I. Mishustin (FIAS).

Short description: The phenomena initiated by an energetic ion incident on tissue happen on many scales in time, distance, and energy. Many thorough papers have been devoted to Monte Carlo simulations of different fragments of the scenario, but they cannot include all scales together because, e.g., time scales for physical processes vary from 10^{-22} s to hours. In addition, they do not present the scenario as a hierarchy of phenomena,which is very attractive physically. Our goal is to understand the physics of beam therapy on a microscopic level and, while moving towards this goal, we present a multi-scale approach to the scenario of irradiation with ions.

Edited books and journal issues (the year 2009):

1. A.V. Solov'yov and E. Surdutovich (editors). Proceedings of 4th Int. Symp. on Atomic Cluster Collisions, (Ann Arbor, USA, July 14-18, 2009), AIP Conference proceedings 1197 (2009) pp. 1–235 (2009).

7.1. Research project: ‘Multiscale approach to IBCT’

Main results: A multiscale approach has been proposed to understand the physics related to ion-beam cancer therapy. It allows the calculation of the probability of DNA damage as a result of irradiation of tissues with energetic ions. This approach covers different scales, starting from the large scale, defined by the ion stopping, followed by a smaller scale, defined by secondary electrons and radicals, and ending with the shortest scale, defined by interactions of secondaries with the DNA. Instead of reconstructing the sequence of events using scale-dependent Monte Carlo simulations, we consider phenomena on all scales and combine them in a complete picture [1-5]. We present calculations of the probabilities of single and double strand breaks of DNA, suggest a way to further expand such calculations, and also make some estimates for glial cells exposed to radiation. The whole scope of the scientific palette is shown in Table 1.

Phenomenon	*Discipline*	*Space scale*	*Time scale*
Beam Generation	High energy Physics	m -km	
Beam transport	Radiation Physics	1-100 cm	10^{-10}-10^{-8}s
Nuclear collisions and fragmentation	Nuclear Physics	pm	10^{-22}s
Primary ionization, transport of secondaries	Atomic/Molecular Physics	1-10 nm	10^{-17}-10^{-14} s
Branching of secondaries, radicals, excited species	Chemistry	nm	10^{-14}-10^{-5} s
Local heating, heat transfer, stress	Thermo-hydrodynamics	nm	10^{-14}-10^{-9}s
Dissociative electron attachment to molecules	Quantum Chemistry	Å	10^{-15}s
Initial resulting damage effect	Biochemistry	nm	10^{-5}s
Repairing mechanisms	Molecular Biology	1-100 nm	s-min
Cellular network and interaction	Cell Biology	μm	Min
(Tumor) Cell death	Medicine	mm	min-years

Table 1. Space and time scales of the relevant phenomena.

Related publications in 2009:

1) A. V. Solov’yov, E. Surdutovich, E. Scifoni, I. Mishustin, W. Greiner, ‘Physics of ion beam cancer therapy: a multi-scale approach’, Phys. Rev. E79 (2009) 011909.

2) E. Surdutovich, A.V. Solov’yov, *A physical palette for the ion-beam cancer therapy, Europhysicsnews* **40** 21-24 (2009).

3) E. Surdutovich, E. Scifoni, A. V. Solov’yov, *Ion-beam cancer therapy: news about a multiscale approach to radiation damage,* Mutation Research, submitted (2009).

4) E. Surdutovich, E. Scifoni, A. V. Solov’yov, *A multiscale approach to the physics of radiation damage,* AIP Conf. Proc. 1197 (2009) 209-218.

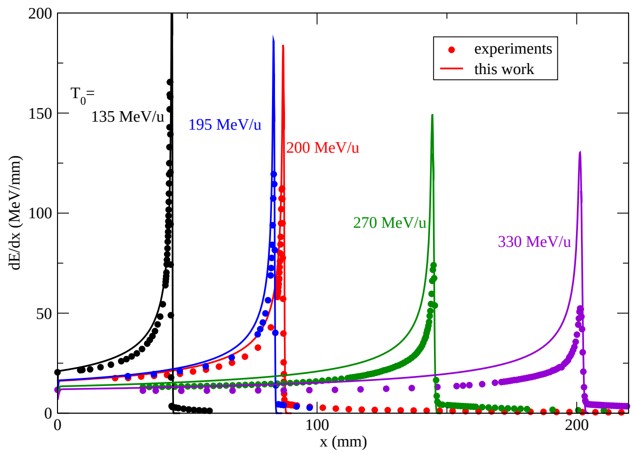
5) E. Surdutovich, A. V. Solov’yov, *Suggested temporal study of DNA repair after radiation damage,* Radiation Research, submitted (2009).

7.2. Research project: 'Secondary electrons production in tissue-like medium'

The project aims at the development of theoretical approaches and numerical tools for efficient calculation of the spectrum of abundancies and energy distribution of secondary electrons produced during a passage of fast ions through a tissue-like medium.

Main results:

• A new parametric model has been set up for secondary electrons production in water. The obtained parameterization can be used also for a fast calculation of the position of the Bragg peak for a given energy of the projectile with a therapeutically accepted precision (see on figure). An advantage of such parameterization is its universality for different applications and its analyticity, which makes all calculations fast.



Linear energy deposition for carbon ions for different initial energies: our model (lines) compared to experiments from GSI (dots)

• For higher ion energies, the dielectric response approach, previously tested for protons, and herein applied for heavier ions, is shown to be successful in describing the details of secondary electron spectra profiles. We compare two approaches and show that they can be used for different values of secondary electron energies.

Related publications in 2009:

1) E. Surdutovich, O.I. Obolensky, E. Scifoni, I. Pshenichnov, I. Mishustin, A.V. Solov'yov and W. Greiner, *Ion-induced electron production in tissue-like media and DNA damage mechanisms,* European Phys. J. D51 (2009) 63-71.

2) E. Scifoni, E. Surdutovich, A. V. Solov'yov, *Spectra of secondary electrons generated in water by energetic ions,* Phys. Rev. E, submitted (2009).

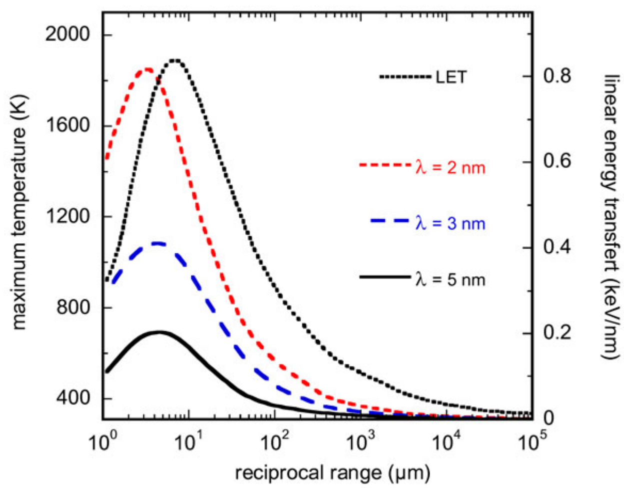
3) E. Surdutovich, E. Scifoni, A. V. Solov'yov, *Ion-beam cancer therapy: news about a multiscale approach to radiation damage,* Mutation Research, submitted, (2009).

4) E. Scifoni, E. Surdutovich, A. V. Solov'yov, *Stopping Power and Secondary Electrons in Ion Beam Cancer Therapy,* AIP Conf. Proc. 1197 (2009) 217-228.

7.3. Research project: 'Inelastic thermal spike model'

Main results: The inelastic thermal spike model is developed and applied in relation to high-energy $^{12}C^{6+}$ beams (hundreds of MeV/u) used for cancer therapy. The heat transfer has been calculated in the vicinity of the incident-ion track. It is shown that there is a very large temperature increase in the vicinity of ion tracks near the Bragg peak during the time interval from 10^{-15} to 10^{-9} s after the ion's passage as well as an increase in pressure, as large as tens of MPa. These effects suggest a possibility of thermo-mechanical pathways to disruption of irradiated DNA.

The figure illustrates the profile of the maximum temperature of water reached during the heat transfer, depending on the distance along the ion's track for 500-MeV/u C ions. The highest temperatures are observed near the Bragg peak, which is about 30 cm deep, where the ion's energy is less than 25 MeV/u, and has a width of about 1 mm. The figure shows that the maximum temperature may be as large as 1900 K for a more probable electron-phonon mean free path $\lambda = 2$ nm and 700 K for a less probable $\lambda = 5$ nm.



Maximum temperature versus reciprocal range for 500-MeV/u carbon ions. The linear energy transfer (LET) is plotted as well [1].

Relatedc publications in 2009:

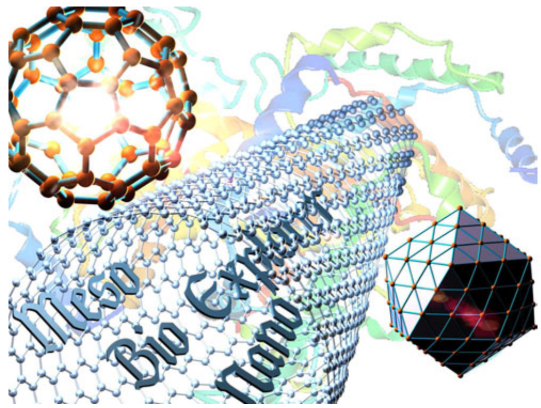
1) M. Toulemonde, E. Surdutovich, A.V. Solov'yov, *Temperature and pressure spikes in ion-beam cancer therapy*, Phys. Rev. E80 (2009) 031913.

8. Research direction: 'Software development'

Collaborators: S. Schramm (FIAS), H. Backe & W. Laut (Univ. Mainz, Germany), V. Ivanov (St. Petersburg State Polytechnical Univ., Russia).

8.1. Research project: 'The MBN Explorer'

Meso-Bio-Nano Explorer (MBN Explorer) is a software package being developed in the group for the last 5 years. Nowadays, it is a powerful tool capable to describe molecular systems at different levels of details. The software package is primarily designed to perform molecular dynamics simulations and optimizations of various complex systems. MBN Explorer treats the motion of particles within the formalism of classical mechanics. There are two principal types of objects which can be defined in the program: a point particle interacting with the system by a defined potential and a rigid body - a set of the particles with the fixed geometry.



An illustration of a hypothetical Meso-Bio-Nano system - a challenging task for MBN Explorer.

MBN Explorer provides user the possibility to specify the interactions within the system using a large variety of pairwise and many-body potentials, to combine and develop new potentials by summation or multiplication of the embedded ones. One important class of potentials that is treated with MBN Explorer worth to be mentioned separately. This is the so-called potential of Molecular Mechanics which is widely used for the description of bio-macro-molecules and polymers. In this potential the interactions within the system are assigned according to a predefined topology of the molecule.

The code of MBN Explorer is written in a way that it can be easily extended for treatment of new types of systems with new potentials. This feature of the code allows one to apply MBN Explorer for a great variety of the tasks. The universality of the software package is not compromised with its performance. The speed of the single-processor calculations using MBN Explorer is compatible with the speed of other contemporary software packages being developed worldwide, e.g. NAMD or CHARMM. Nowadays, the code is being extensively developed in order to perform efficient multiprocessor calculations on CPU and GPU clusters.

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.

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

The project aims at an extension of the MBN Explorer code for GPU-based calculations, to explore the advantages and behavior of a new calculation models, because it promises to provide faster calculation times.

Main results:

All atom molecular dynamic simulations are a 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 the available computing 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.

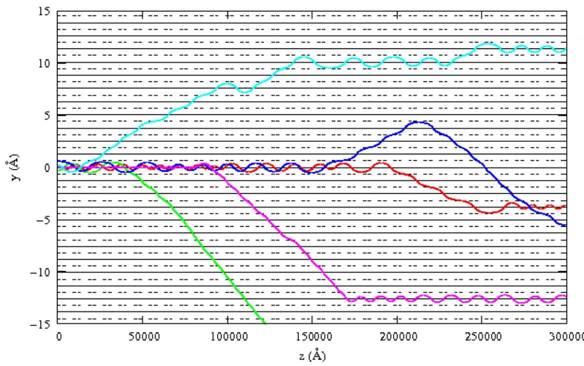
The computing power of the Center for Scientific Computing (CSC) of the Goethe University Frankfurt, which currently operate computer clusters consisting of 300 modern computers, is $\sim$ 20 Tflops/s. On the other hand, the computer power of the computer cluster in the FIAS, consisting of 16 Tesla supercomputers based on the Compute Unified Device Architecture (CUDA) developed by NVIDIA [www.nvidia.com], is $\sim$ 60 Tflops/s. That difference promises to provide fasters and cheaper calculations with the usage of CUDA GPUs supercomputers.

Therefore, we have extended the molecular dynamics part of the MBN Explorer code in order to perform calculations on graphical processors. The "CUDA-branch" of the MBN Explorer includes a specific force field for the modeling of the carbon base materials. Up to now the stability of the carbon nanotubes on the Ni_{309} cluster has been investigated. Nowadays, with that force field we investigate of the carbon nanotubes growth process on the catalytic particle (Ni_{309} cluster).

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

The FORTRAN 95 code will be used for a comprehensive numerical study of the channeling of ultrarelativistic particles and the properties of radiation from a crystalline undulator. Currently the algorithm is being constructed 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 radiative damping force, the transition between axial and planar channeling, the rechanneling effect as well as the influence of the temperature on the channeling process. The algorithm will be combined with another one that allowes to calculate spectral-angular distriburion 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 crystals. It allows to vary a number of parameters: the energy of the projectile, the type and size of the crystal and its orientation relative to the beam direction. Examples of simulated trajectories demonstraiting dechanneling and rechanneling phenomena are shown in the figure.



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

The package of codes is under construction for numerical description of spherically symmetric metallic clusters, fullerenes and various endohedral systems. Ground and excited states are calculates within the jellium model approach using the Hartree-Fock approximation and the Local Density Approximation. It will allow one to compute:

• electronic wave functions of the ground state, single-electron energy and total energy of the system;

• wave functions of discrete and continuum excited states, energy spectrum of discrete excitations and the scattering phaseshifts;

• cross sections of photoabsorption and the angular distribution of photoelectrons within single-electron approaches (Hartree-Fock and LDA) as well as the Random Phase Approximation (RPA) and the Random Phase Approximation with Exchange (RPAE).

Related publications in 2009:

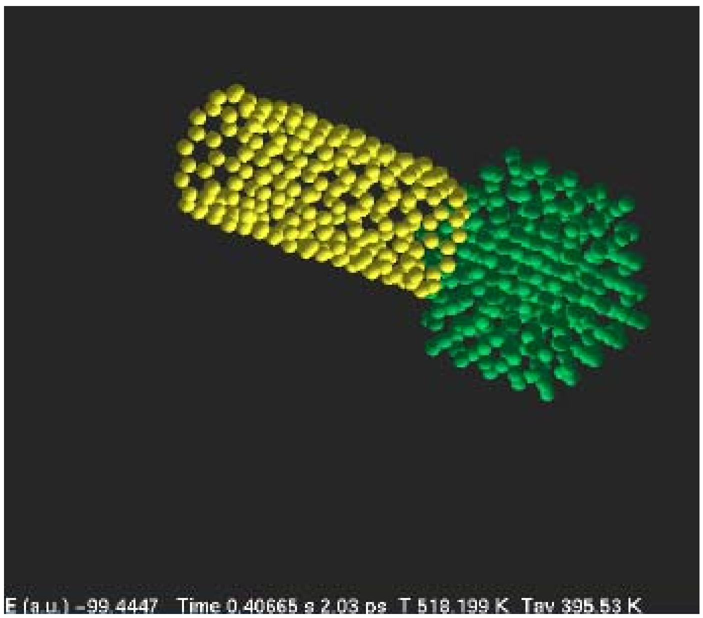
1) A. V. Verkhovtsev, R. G. Polozkov, V. K. Ivanov, A. V. Solov'yov, *Stability of metallic hollow cluster systems,* Phys. Scripta 80 (2009) 048104.

Growing of Carbon Nanotubes

Collaborators: Stefan Schramm[1,2], V. Dick[3], A. Yakubovich[1], S. Lo[3], Dr. I. Solov'yov[1], Prof. Dr. A. Solv'yov[1]

[1] FIAS, [2] Center for Scientific Computing (CSC), [3] FIGSS

In a newly started project we study the growth of carbon nanotubes on catalytic metal clusters. The molecular-dynamics simulations are performed with effective force fields for the various atoms. The code was implemented on GPU graphics processors which led to a speed-up of the simulation by a factor of more than 100 depending on the system size. As a test standard metal cluster melting could be reproduced in this approach. The same ansatz is being used for studying the fragmentation of buckyball-buckyball collisions. As the computational GPU framework is largely problem-independent this approach will be used for many related problems in the future.



Snapshot of a simulation of the dynamics of a carbon nanotube on a Ni Cluster.

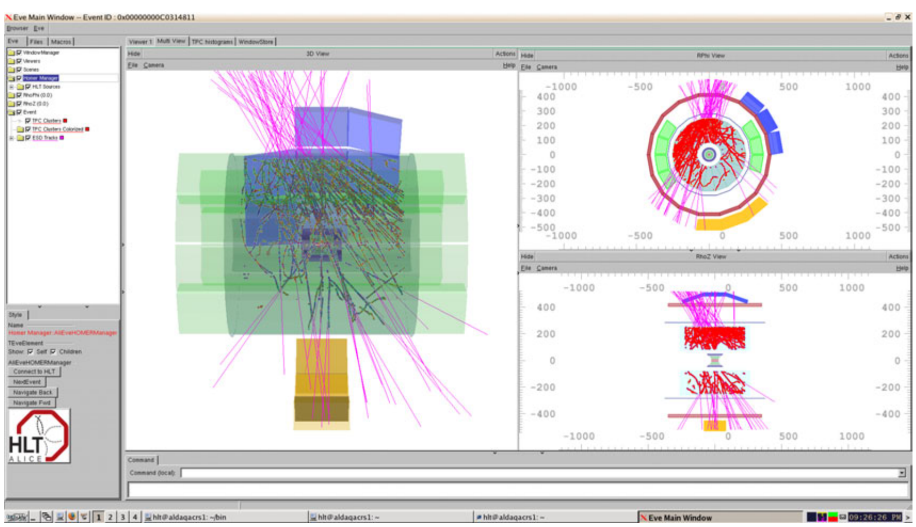
4.5 Scientific Computing, Information Technology

ALICE High Level Trigger

Collaborators: Thorsten Alt, Sergey Gorbunov, Sebastian Kalcher, Volker Lindenstruth, Jörg Peschek, Dr. Timm Steinbeck, Jochen Thäder

The ALICE High Level Trigger is designed to reduce the data rate of the ALICE experiment (A Large Ion Collider Experiment) at CERN from 25 GB/s to 1.25 GB/s. For this a large cluster has been built, that is designed for up to 1000 nodes. On this cluster the data from the collisions (events) is reconstructed online, with event processing rates of more than 1 kHz. In addition to the decision which parts of the on-line data will be saved to permanent storage for later analysis, the HLT also provides the reconstructed data for a quasi-live online display. The first stage of processing can be performed already in FPGAs on special purpose PCI-X receiver cards, that receive the data via optical links from the detectors. The further processing tasks are performed by software on the cluster nodes, with a flexible and robust software framework distributing the data among the different processing tasks on the cluster nodes. One of the main points of attention for the reconstruction has been placed on the track recognition in the TPC, ALICE's largest detector. The fast online tracking algorithm and its capability to be executed on GPU for acceleration are discussed in a separate contribution. The figure shows a measured cosmic particle inside the detector 60m under ground.

The HLT has proven itself already for more than one year in productive use during the commissioning of the ALICE experiment. Examples of its use include a lossless online compression of data by a factor of 15 at a rate of 800 events per second event processing capabilities of up to 2.1 kHz or 160 MB/s. For extended periods of time the HLT is already being used in detector tests using cosmic radiation, to select only events with tracks in the detector. Here the online display of the reconstructed tracks has also proven to be a useful tool. For the future further enhancements and performance improvements of the HLT software are foreseen together with additional cluster nodes and the integration of a high-performance system area network for a more efficient intra cluster-communication.



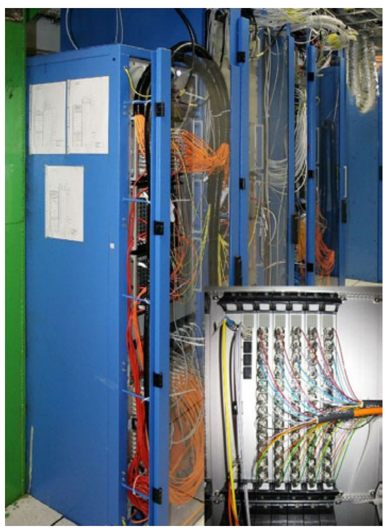
ALICE TRD Trigger

Collaborators: Volker Lindenstruth, Venelin Angelov, Jan de Cuveland, Felix Rettig, Stefan Kirsch, Dirk Hutter

The Transition Radiation Detector (TRD) is a sub-detector of the ALICE Experiment, contributing to particle identification, tracking, and trigger by implementing more than 1.2 million analog channels. The TRD trigger is setup to select one particle out of 16000 within less than 6 microseconds while performing a full track reconstruction. It implements a hierarchy of TRAP processing chips and a global tracking unit.

The TRAP chip performs digitization, filtering and processing of the analog signals from the detector. The track segments (tracklets) found and the zero-suppressed raw data are sent via a readout-tree and 1080 2.5 Gb/s optical links to the GTU. The whole detector utilizes 65,000 TRAP chips, implementing 4 CPU Cores each.

The GTU is the central part of the TRD read-out and trigger system. Consisting of 109 FPGA-based nodes, the GTU performs an online reconstruction of each TRD event, analyzing up to 20,000 track segments. It provides a L1 trigger contribution to ALICE less than 6.5 ţs after the interaction and implements high-speed multi-event buffering of TRD raw data. The development and production of the hardware of the GTU is completed. The system is installed at CERN and in operation since 2007. The correct interplay with the ALICE Data Acquisition System (DAQ) and the Central Trigger Processor (CTP) have been verified. A trigger on cosmic events delivered by the GTU allows to gather calibration and alignment data efficiently. More complex trigger schemes like a trigger on di-lepton pairs with predefined momentum or on high-energy jets are under development for the upcoming start of the LHC.



Related publications in 2009:

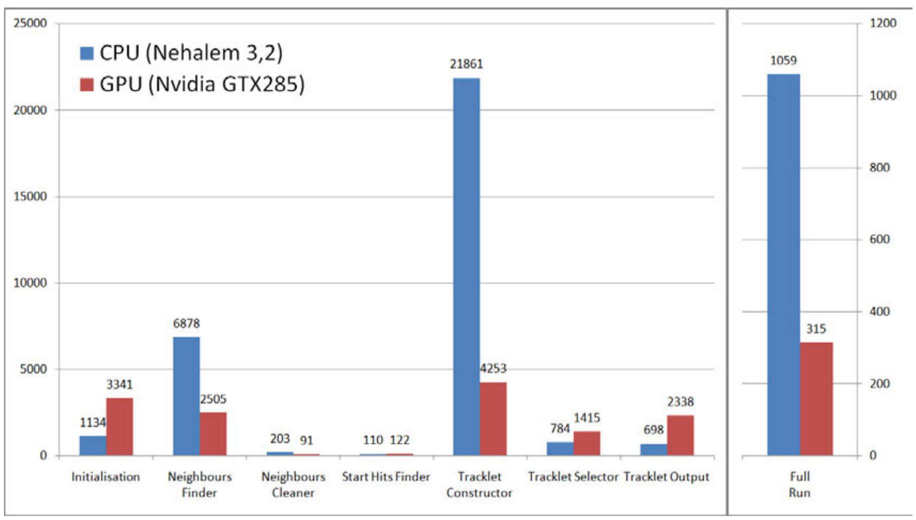
Jan de Cuveland, *A Track Reconstructing Low-latency Trigger Processor for High-energy Physics*, Dissertation, Heidelberg, 2009

V. Angelov, V. Lindenstruth, *The educational processor SWEET-16*, Prepared for 19-th International Conference on Field Programmable Logic and Applications FPL09, ISBN 978-1-4244-3892-1, p. 555–559.

Alice TPC Online Tracker

Collaborators: Sergey Gorbunov, Matthias Kretz, David Rohr, Volker Lindenstruth

The ALICE Experiment is one of four LHC experiments. Itt's event reconstruction, in particular of Pb-Pb Collisions, requires substantial computational power (thousands of processors). During the last years commercial off the shelf graphics hardware became more and more powerful and support for running general purpose code in high level languages has greatly improved. To benefit from this development the tracker for the Alice HLT has been adopted to be able to run on NVIDIA GPUs using the CUDA framework. Major challenges hereby have been an efficient usage of the several memory types available on the GPU as well as a good overall utilization of the GPU's many processors by dynamically scheduling tasks among them. Several memory optimizations could also be applied to the CPU code resulting in about half the execution time. In benchmarks using data of simulated central Pb-Pb collisions a Geforce GTX 285 outperforms a state of the art Intel Nehalem Prozessor (3,2 GHZ) utilizing 8 threads by a factor of about 3.3. Output of the GPU tracker was proven to exactly match the CPU tracker's results. The recent version is included in the HLT framework and is currently tested in the HLT cluster at CERN.



The figure shows the relative performance of the CPU in comparison to the GPU for the different processing steps during the event reconstruction

Fast Cellular Automaton tracker for ALICE High Level Trigger

Collaborators: Sergey Gorbunov, Matthias Kretz, David Rohr, Volker Lindenstruth

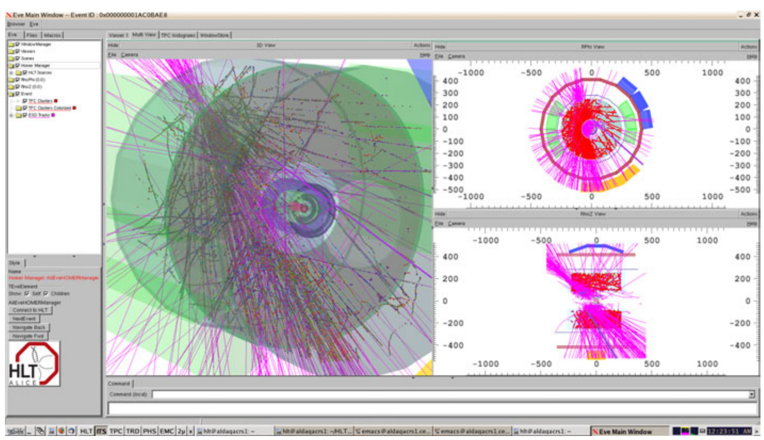
The core of the event reconstruction in ALICE is the reconstruction of particle trajectories (tracking) in TPC detector, the main tracking detector of the experiment. For this propose a fast on-line algorithm has been developed. It reconstructs all types of data including physics events, cosmics and special calibration events.

The algorithm combines a Cellular Automaton method [1], which is used for a fast pattern recognition, and the Kalman filter method [2], which performs a fit of found trajectories and the final track selection. The algorithm has proved its high performance (99.9% for the proton-proton events and 95.8% for the central Pb-Pb collisions) in comparison with the off-line reconstruction (99.9% and 95.8% correspondingly). In addition to the the high efficiency, the on-line reconstruction is an order of magnitude faster than the off-line analysis: 19.6ms(pp) or 17.6s(PbPb central) in comparison with 66.0ms or 160.1s for the off-line.

An important feature of the algorithm is an ability to use GPU hardware accelerators, giving another order of magnitude speed-up for the on-line data processing. The GPU accelerators allow to perform a fast reconstruction of heavy ion collisions where a track density is very high.

The first GPU implementation of the algorithm was developed for the NVIDIA graphic card. In addition, the algorithm was adopted for the upcoming Intel Larrabee graphic card. For this propose the code has been vectorized [3] , implying a detailed investigation of the SIMD instructions and development of general vector classes.

The GPU tracker is integrated to the High Level Trigger framework and will be used for the on-line data processing in the ALICE experiment.



A cosmic shower, reconstructed in HLT

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Lattice QCD with distributed GPUs

Collaborators: Volker Lindenstruth, Frithjof Karsch, Matthias Bach, Wolfgang Söldnerr, Olaf Kaczmarek, Christian Schmidt, Piotr Bialas

Lattice QCD today is one of the big computational challanges. As a brute force solution to QCD it allows to study quark gluon plasma in areas where perturbative methods fail. For the evaluation of the equation of state a rational hybrid monte carlo method is used.

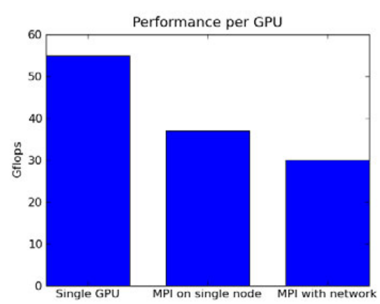
Up till now Lattice QCD calculations are often performend on specialized hardware like the apeNEXT or extremely large systems like the BlueGene. Those system are special, in that the single nodes are rather slow, but communication between the nodes is extremely efficient. However production of and access to this systems is expensive.

In recent years multi and many core architectures have involved, continuing an increase in single node compute power even though the race for higher clock speeds as come to a halt. Today such architectures are available in GPUs, providing an excellent ratio between arithmetical power and costs. Therefore GPUs provide an interesting platform for lattice QCD calculations.

In a first step we have been able to implement a GPU based conjugate gradient solver for calculations with staggered fermions. This solver is the most expensive step in Lattice QCD calculations. Our solver achieves a performance of $\simeq$ 55 Gflops on one NVIDIA Tesla C1060. A multi GPU version has been implemented which scales over multiple GPUs in a single system. This performance has only been possible by heavily optimizing the memory access patterns of the algorithm, which in its current implementation now saturates the memory bandwidth of the GPUs.

As with increasing arithmetical power of a single node the penalties of communication increasingly limit the overall performance of the algorithm. Therefore we are studying different methods in partitioning the problem and organizing the communication in ways to optimize overall algorithm performance. Key points to reach that goal are to minimize communication and parallelize communication and calculations as far as possible.

In addition work is ongoing in implementing a full rational hybrid monte carlo algorithm. This implementation is based on a full rational hybrid monte carlo code existing for the apeNEXT, but due to the different nature of the hardware major parts of it have to be rewritten to work efficiently. Having the rational hybrid monte carlo will allow physical results to be calculated using the fast GPU based Lattice QCD code.



FAIR Computing - Planning for the FAIR Green-IT Cube

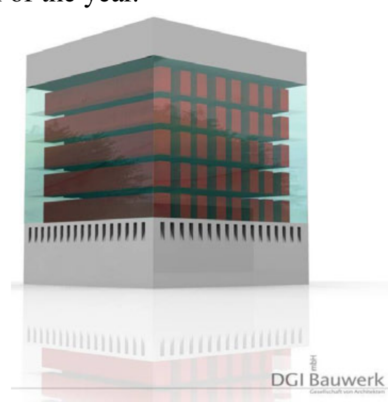
Collaborators: Volker Lindenstruth, Horst Stöcker

The planning for the new FAIR and GSI data center has started. It uses a 3D steel structure, much like a high rack warehouse. The choice of an open multi floor system allows for shorter interconnect lengths, which grows only with the third root of the system size as compared to the square root for 2D false floor architectures. The racks reside on steel double T-Bars. The pitch of a rack row can be customized to fit the rack depth. The floor of a story is covered with floor tyles, also residing on the same double T-bars without extra cost. The T-bars have standard mounting holes for the power and cooling water distribution along side of the double T-bars. They also serve as support for the cable trays. The T-bars implement holes to allow cables being routed in transverse direction. Appropriate cable trays are installed. This architecture completely avoids false floors by implementing the ceiling of the lower floor as the false floor of the story above at no extra cost, while providing convenient access.

The computers are mounted in 19” racks, which implement a heat exchanger at its back door. Therefore the warm air of the computers travels only a few centimetres before it is being cooled back down to ambient temperature. The advantage of this system is the use of air for cooling only inside the racks. The rack autonomously cools its own heat without leaking hot air to the outside. Therefore there is basically no limit to the packing density of racks in this architecture.

One disadvantage of using cooling water is the risk of spills, which is increased by the use of an open, multi story architecture. The planned Green-IT system operates the cooling piping below atmospheric pressure. This requires each floor to implement independent pressure controls due to the barometric pressure differences. Appropriately large piping cross sections are required, especially inside the chillers. In order to optimise the efficiency of the heat usage heat pumps are avoided by operating the data center at high ambient temperatures. First estimates show, that it is possible to operate at ambient temperatures of 30^0C. This temperature is high enough in order to allow the usage of the cooling water directly for heating, if floor and wall heating is implemented, which is being planned for the new buildings. The higher cooling water temperature also grants a higher cooling efficiency, allowing to use free cooling during a large fraction of the year.

The figure shows a sketch of the planned building. It’s dimensions are $26x26m^2$ cross section. The ground floor implements a height of 5m, allowing the operation any of possibly air cooled equipment, such as tape robots. The following 5 layers of 2,5m height each implement a minimum of 150 racks per layer. The top floor is used for the cooling equipment. The minimum cooling power foreseen is 3MW with an upgrade option to at least 6MW. The total height of the building is about 23m. The estimated cooling overhead is 10% (PUE=1,1).



V. Lindenstruth, H. Stöcker: *Method and apparatus for 3D green IT*, Patent submitted to DPMA, 7. July 2008

A manycore hybrid UrQMD

Collaborators: Marcus Bleicher[1], Volker Lindenstruth[2], Hannah Petersen[1], Jochen Gerhard[2], Jan Steinheimer[1]

[1]Institut für Theoretische Physik, Frankfurt, [2]FIAS

A major aim of the FAIR project planned near GSI at Darmstadt is the exploration of baryonic matter at ultra high densities similar to the interior of Neutron stars. Here on expects to observe a multitude of phenomena, most notably, the restoration of chiral symmetry, the transition to a color deconfined state of matter and the crossing of the critical point of QCD. Dynamical simulations of heavy ion interactions at relativistic energies are important to link the observed final state of particles to the properties of the matter created in these collisions. The evolution of the energy and particle densities can be calculated by solving the Boltzmann-equation or the corresponding dissipative hydrodynamic equations.

The simulations code UrQMD, of the institute for theoretical physics, has been lately enhanced by a hydro-phase. After collision, a hydro-phase is computed by the SHASTA algorithm. Due this calculations more accurate modeling is guaranteed. To underlay actual experiments, a vast collection of hereby created events are needed to build reliable statistics.

Unfortunately, a simple parallel execution of classical hydro-code shows massive slow downs, which become even worse, if one augments the number of time-steps to be computed. Therefore parts of the code were analyzed and ported to C++, enabling the usage of hardware accelerators like GPGPUs. The transition to fully single-precision central routines was realized, without a significant loss of precision in final results. Currently we experiment with OpenMP and SSE, which shall be used widely in a new version of the hybrid code. Enabling hereby a speedup on modern systems, which without redesign is dissipated. In future, large parts of the computation shall be running on GPGPUs. First step is the full installation of hydro-phase on GPGPU systems.

NeuRA: The Neuron Reconstruction Algorithm

Philip Broser, Alexander Heusel, Daniel Jungblut, Gillian Queisser, Sebastian Reiter, Roland Schulte, Christine Voßen, Gabriel Wittum

In recent years, novel microscopy methods have been developed allowing for a never imagined precision in detection of microstructure of the brain. Confocal and multi-photon microscopy have become a principal technique for high-resolution fluorescence imaging in biological tissues because it provides intrinsic optical sectioning and exceptional depth penetration. Thus, 3D fluorescence images of neurons including their entire dendritic morphology can be obtained within their native environment. To use this new knowledge in modeling, novel algorithms for extracting morphology information are necessary.

Automatic reconstruction allows the fast, high-throughput determination of characteristic anatomical features, for instance the dendritic branching pattern of neuronal cells, unlike standard manual reconstruction techniques, which are time-consuming and highly dependent on the experience of the anatomist. In vitro methods also suffer from scaling problems due to shrinkage in fixed tissue. Automatic reconstruction will help to establish large databases of neuronal morphologies for modelling of cellular and network signal processing.

In order to address this issue, we designed a software tool NeuRA, which allows the automatic reconstruction of neuronal morphology (Broser et al. 2004). To accomplish the task of automatic reconstruction, NeuRA provides the four main components:
1. Inertia based filter for the native image data
2. Segmentation of the data
3. Reconstruction of the branching pattern
4. Export of the data in common file format.

In practice, the signal-to-noise ratio in such data can be low, especially when dendrites in deeper layers of the cortex are imaged in vivo. Typically, discontinuities in the fluorescence signal from thin dendrites are encountered, as well as a noisy fluorescence background not originating from the labelled neuron, and the combination of these difficulties strongly requires a suitable pre-processing of the data before reconstruction.

To address the problem of noise, we use a novel inertia-based filter for 3D volume data which enhances the signal-to-noise ratio while conserving the original dimensions of the structural elements and closing gaps in the structure (Broser et al 2004). The key idea is to use structural information in the original image data - the local moments of inertia - to control the strength and direction of diffusion filtering locally. In the case of a dendrite, which can be locally approximated as a one-dimensional tube, diffusion filtering is effectively applied only parallel to the axis of the tube, but not perpendicular to it. Thus, noise is averaged out along the local axis of the dendrite, but dendritic diameters are not affected.

The second release of NeuRA, *NeuRA 2,* supports multiple GPUs. Since 2-photon and confocal microscopy significantly improved within the last years, three dimensional microscope images of neuron cells with a resolution of 2048x2048x400 are available now. To process these large data, NeuRA 2 uses the massively parallel architecture of state-of-the-art graphic processing units (GPUs) and is able to distribute the data among multiple GPUs at single computers or computer clusters, allowing to process images of a size of up to several GBytes in a few minutes. To accomplish the four substeps above, in NeuRA 2 additional algorithms have been incorporated to give the user more possiblities. In particular, a multi-scale enhancement filter has been implemented.

The object-oriented software design of NeuRA strictly encapsulates data access, data processing and workflow control, allowing the fast processing of large images as well as the easy extension with other image processing operators. NeuRA 2 automatically checks the available GPUs and divides the input image in suitable overlapping subimages of a size suited for the single GPUs. Linear interpolation in the overlap regions, when reassembling the single subimages, guarantee continuous output images. The NeuRA 2 user interface allows a comfortable reconstruction of the data, including a preview mode to adapt the parameters of the image processing operators on the fly.

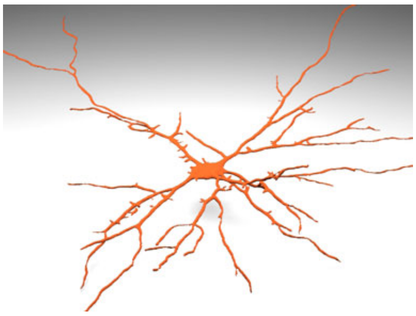


Figure 1. Reconstruction of a neuron cell

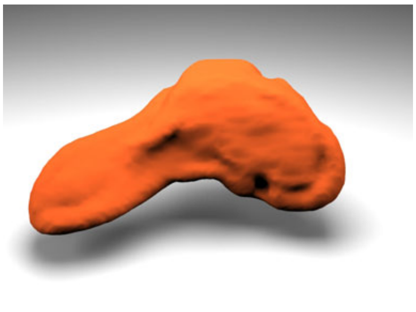


Figure 2. Presynaptic bouton

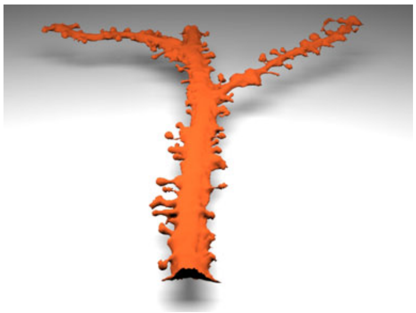


Figure 3. Dendrite segment with spines

Using general noice reduction and segmentation methods rather than model-based techniques, NeuRA 2 is not limited to reconstruct neuron cells (Figure 1). It can also be used to generate surface meshes from archaeological (Figure 5; Jungblut et al 2009b) or medical computer tomography images (Figure 6), as well as nuclei (Queisser et al 2008) or other neurobiological microscopy images, like presynaptic boutons (Figure 2) or dendrite segments with spines (Figure 3).

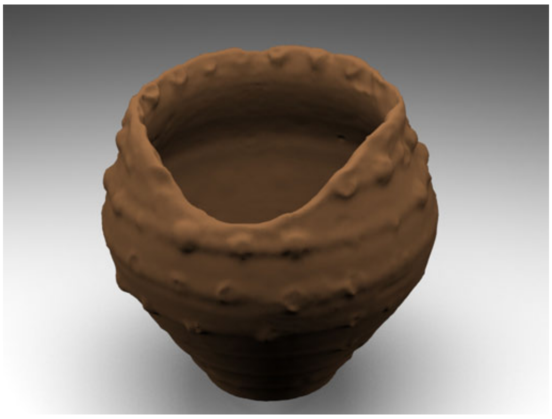


Figure 5. Reconstruction of a ceramic vase

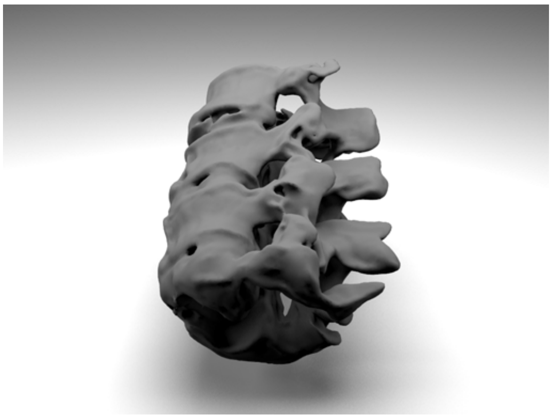


Figure 6. Reconstruction of a cervical spine

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Modelling the Nuclear Calcium Code

Gillian Queisser, Gabriel Wittum

Calcium regulates virtually all cellular responses in the mammalian brain. Many biochemical processes in the cell involved in learning, memory formation as well as cell survival and death, are regulated by calcium (Bading 2000, Milner 1998, West 2002). Especially when investigating neurodegenerative deseases like Alzheimer's or Parkinson's disease the calcium code plays a central role. Signalling from synapses to nucleus through calcium waves and the subsequent relay of information to the nucleus that activates transcriptional events was of special interest in a project together with the Bading lab at the IZN in Heidelberg.

Electron microscopy studies in hippocampal rat tissue carried out at the lab revealed novel features of the nuclear membrane morphology (Wittmann et al., to appear). While current text book depictions show the nucleus to have a spherical form, these electron micrographs showed infolded membrane formations of both nuclear membranes (Figure 1, left).

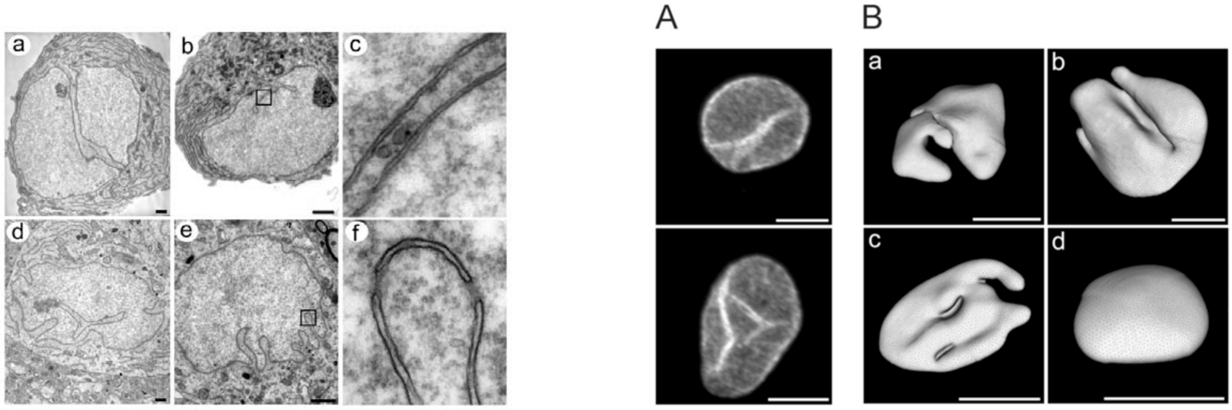

Figure 1: Left: Electron microscopy slices through various hippocampal nuclei (a,b,d,e). The micrographs show infolded envelope formations of both nuclear membranes (c). As seen in f, the infoldings contain nuclear pore complexes as entry points for cytosolic calcium. Right: Confocal slices of two different nuclei (A). This data is used to reconstruct nuclei in 3-d (B). The 3-d reconstructions show the formations of nuclei ranging from highly infolded to nearly spherical.

To assess the realistic morphologies of hippocampal nuclei and to investigate the influence of the diverse structures on nuclear calcium signalling, we used NeuRA (Queisser et al. 2008) to reconstruct the nuclear membrane surface from confocal microscopy recordings (Figure 1, right). As a first result one could ascertain, that the hippocampal area contains a large quantity of highly infolded nuclei, where the nuclear envelope divides nuclei into microdomains. Furthermore, measuring surface and volume of infolded and spherical nuclei showed that all nuclei are nearly equal in their volume but infolded nuclei have an approx. 20% larger surface than spherical ones (Wittmann et al., in press). This surface increase is proportional to the increase in nuclear pore complexes (NPCs) on the membrane through which cytosol can freely diffuse into the nucleus. This observation, and the visible compartimentalisation of nuclei led us to investigate the morphological effect on nuclear calcium signalling.

Therefore we developed a mathematical model describing calcium diffusion in the nucleus, calcium entry through NPCs including the realistic 3-d morphology. The discrete representation of the PDE-based biophysical model is solved using the simulation platform uG. Information stored in calcium signals is mainly coded in amplitude and frequency. We therefore investigated these parameters w. r. t. various nuclear morphologies. Figure 2 shows the differences in calcium amplitude within single nuclei, w. r. t. compartment size. Due to changes in the number of NPCs and differences in diffusion distances, small compartments elicit higher calcium amplitudes than large compartments. This can have a substantial impact on the biochemical events downstream of calcium and therefore affect gene transcription in the cell. Furthermore, infolded nuclei show visible differences in resolving high frequency calcium signals compared to spherical nuclei and large compartments respectively.

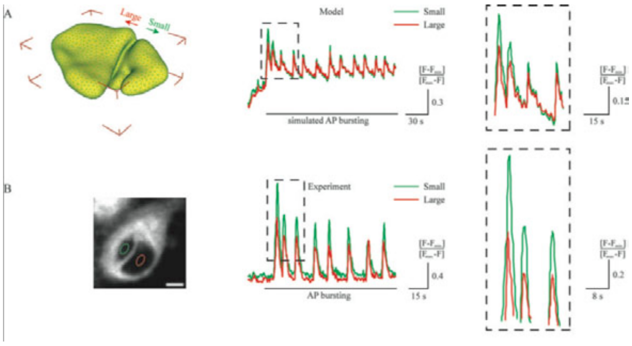

Figure 2: Measuring the calcium signal in two unequal nuclear compartments shows, that smaller compartments elicit higher calcium amplitudes in model simulations (top) and experimental calcium imaging (bottom). This shift in amplitude can have effects on biochemical, transcription related processes.

Figure 3 shows that given a 5 Hz stimulus to the cell, small compartments are more adept at resolving this frequency than large compartments. We therefore ascertain, that hippocampal neurons fall into categories of "frequency resolvers" and "frequency integrators". The effects of nuclear morphology on amplitude and frequency seen in simulations, were then verified in experimental settings (see Figures 3 & 4).

In an attempt to evaluate the effect of these changes in the nuclear calcium on events closely related to transcription, the phosphorylation degree of the protein histone h3, involved in gene transcription and chromosomal reorganisation, was related to the degree of nuclear infolding. As a result, experiments show, that with increasing degree of nuclear infolding the degree of histone h3 phosphorylation increases as well (see Figure 4). We could therefore show a novel feature of nuclear calcium signalling. The structures of hippocampal nuclei are highly dynamic and show nuclear plasticity upon recurrent cellular activity. The capability of a neuron to adapt its organelle's morphology adds an extra layer of complexity to subcellular information processing, and could therefore be necessary in higher brain function.

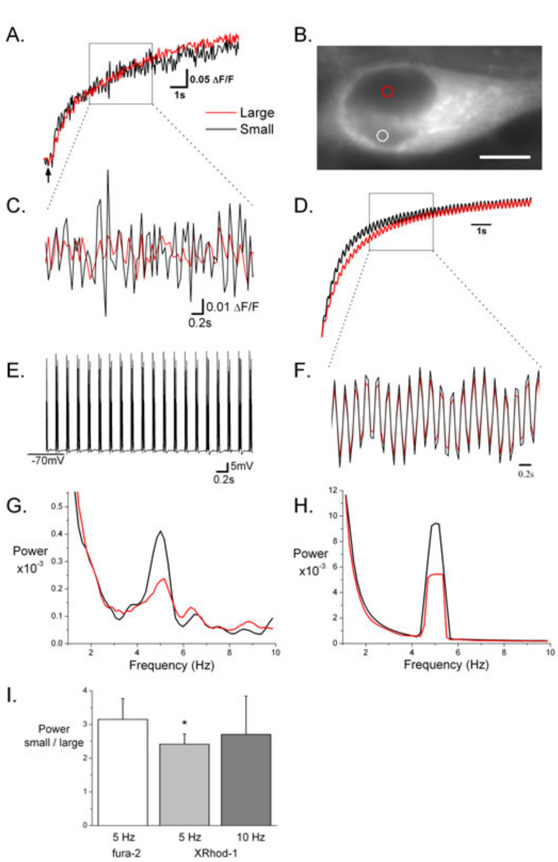

Figure 3: Stimulating an infolded nucleus (A, E, D) with unequal sized compartments (B) shows, that smaller compartments are more adept at resolving the high-frequency signal (C, F). Both power plots in experiment (G, I) and model (H) show a stronger 5 Hz resolution in the small compartment.

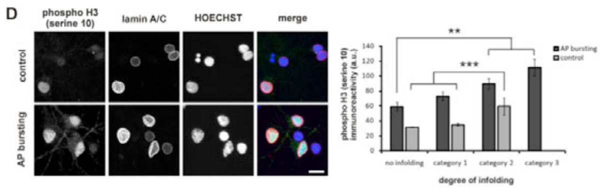

Figure 4: Measurements of histone H3 phosphorylation in respect to degree of nuclear infolding (ranging from weakly to strongly infolded). Phosphorylation degree increases proportionally with the degree of infolding.

Remark: All images are taken from Ref. Wittmann et al..

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Electric Signalling in Neurons

Konstantinos Xylouris, Gabriel Wittum

The brain is a tremendously complex network of small entities called neurons. Thus, in order to understand how it stores, processes, and creates new thoughts, it is crucial to figure out how these units do actually work. The neuron builds up a potential difference over its membrane due to the surrounding ionic liquids. If this potential difference, the membrane potential, changes from its resting value and exceeds a certain threshold, this locally created excitement, the action potential, starts travelling throughout the neuron. Now, there are different influences which play an important role in the generation, travelling and form of these action potentials. One very vital leverage is the morphology. Others are the channel distributions on the membrane and the intracellular and extracellular potential. Furthermore, the modelling of the extracellular potential can provide an essential means to study the activity of a living brain.

In order to capture all of these factors, we generalised the three-dimensional passive model from (Voßen et al. 2006) to an active one by incorporating the Hodgkin-Huxley dynamics (Hodgkin and Huxley 1952).

So far, compartment models have been developed based on one-dimensional cable equations (Rall 1962) which take into account some morphological features with the help of parameters like the radius or length of a specific neuronal part. Nevertheless, one unrealistic assumption of this model is that the extracellular potential is zero. In order to overcome this characteristic Gold et al. (2006) suggested to couple the cable equation with a three-dimensional potential model.

Here, we follow a new approach, with which the extracellular potential and the membrane potential can be simulated at once, taking into account the full morphology of a neuron.

The model is based on the first principle of the balance law of charges. Because there are no free charges in the intracellular and extracellular space, the potential obeys the Laplace equation in these spaces. Across the membrane, however, there are two membrane fluxes, the capacitory and Hodgkin-Huxley flux, which are balanced with fluxes arriving at and departing from the membrane (Figure 1):

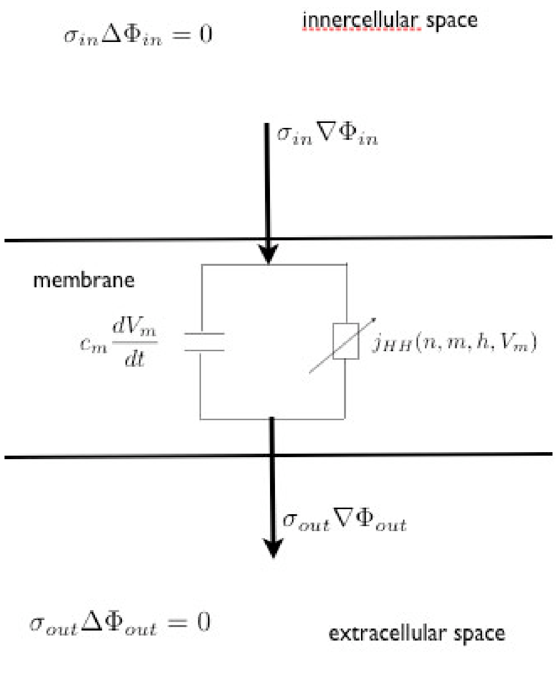

Figure 1. Pattern on which the model is derived

$$\int_{\partial B} \sigma \nabla \Phi dS(x) = 0$$

$$\int_{\Gamma \cap B} c_m \frac{dV_m}{dt} + j_{HH} dS(x) =$$

$$\frac{1}{2}\left\{ \int_{\partial B \cap \Omega_{in}} \sigma_{in} \nabla \Phi_{in} \cdot n dS(x) - \int_{\partial B \cap \Omega_{out}} \sigma_{out} \nabla \Phi_{out} \cdot n dS(x) \right\}$$

$$+\text{Hodgkin-Huxley-Equations}$$

Figure 2. 3D-Model equations to be solved

All in all, we come up with five non linearly coupled integro-differential equations (Fig. 2), which are discretised with finite volumes in the space and implicit methods in the time. The arising linear system of equations has been implemented and solved using uG (Bastian and Wittum 1994, Lang and Wittum 2005). On the basis of a reconstruced real neuron a computational geometry could be retrieved. The simulation carried out on this geometry is depicted in (Figure 3). Thereby a current was injected leading to an action potential which travels throughout the given structure.

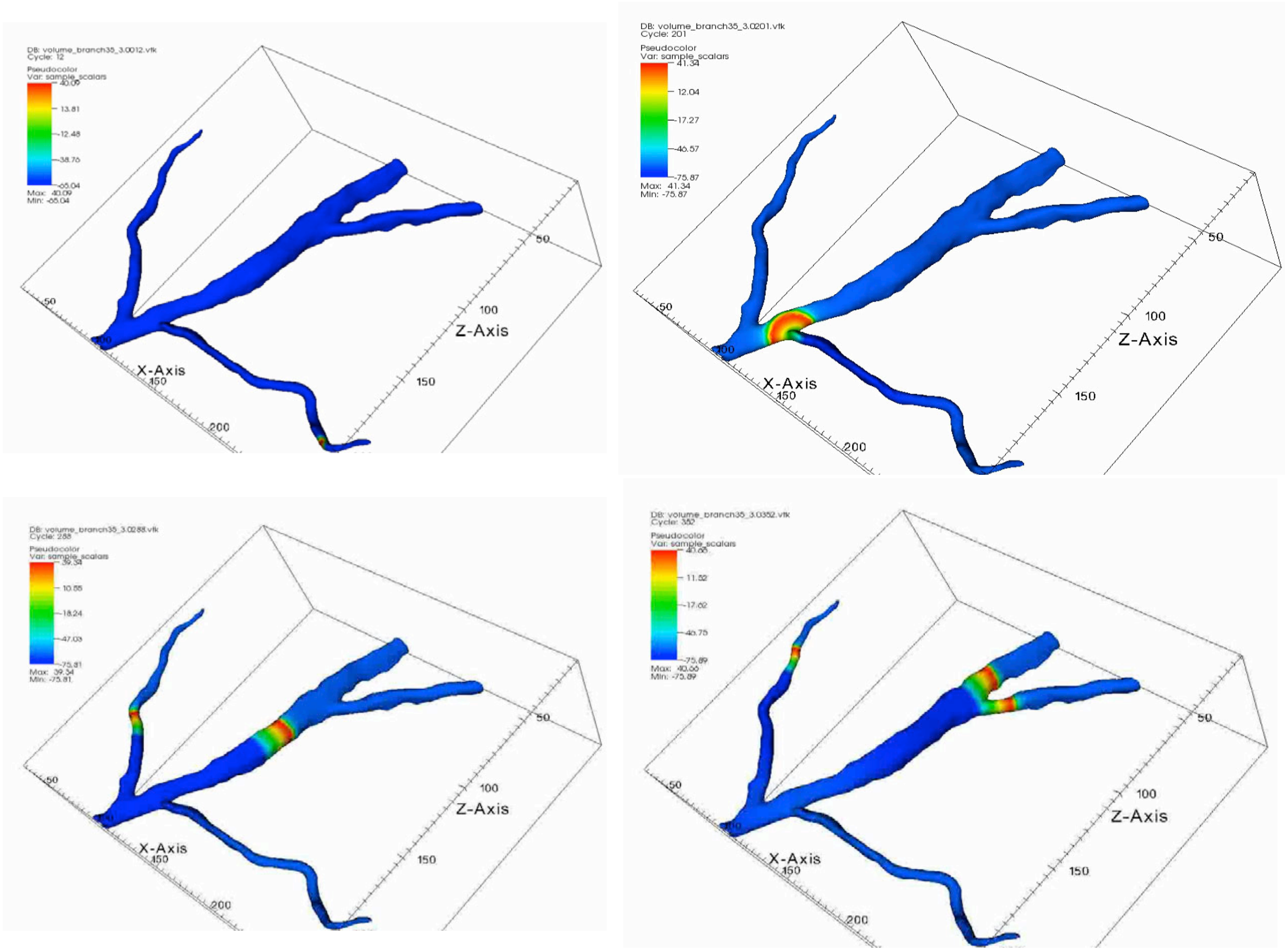

Figure 3. Spike propagation on a small part of a reconstructed real neuron

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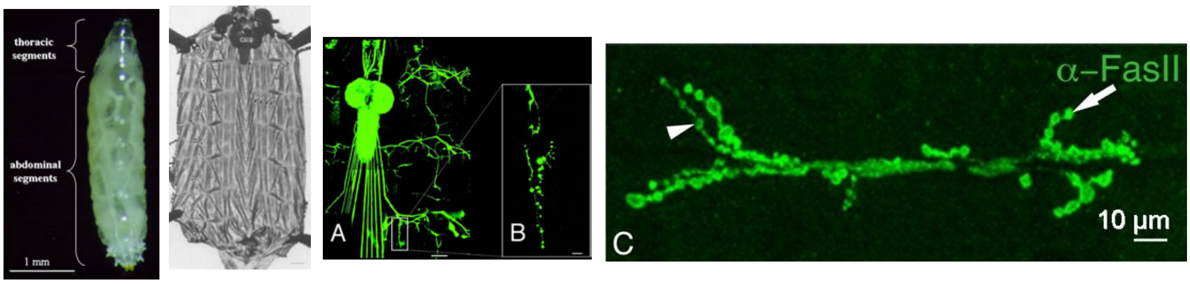
Development and Functionality of Elementary Networks

Markus M. Knodel, Dan Bucher, Daniel Jungblut, Gillian Queisser, Christoph Schuster, Gabriel Wittum

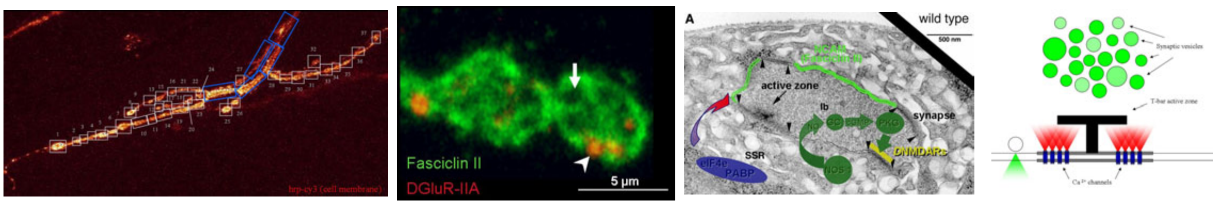
An important challenge in neuroscience is understanding how networks of neurons are processing information. Synapses are junctions between cells and thus play an essential role in cellular information processing, however, detailed quantitative and mathematical models of the underlying physiologic processes occuring at synaptic active zones are lacking. We are developing mathematical models of synaptic vesicle dynamics at a well characterised model synapse, the Drosophila larval neuromuscular junction (Kidokoro et al. 2004). The synapse's simplicity, accessibility to various electrophysiological recording and imaging techniques, and the genetic malleability which is intrinsic to the Drosophila system make it ideal for computational and mathematical studies.The Drosophila larva is shown in Figure 1, starting from the larva itself, the opened version with the muscles, the stained nerve system up to the neuromuscular junction NMJ.



Larva Muscles Stained CNS Stained Neuromuscular Junction

Figure 1. Larva, its muscles and the central nervous system, NMJ in another scale shown

Once we consider the NMJ in detail, one finds that it consists of a lot of big synaptic boutons of which each one harbours several synapses. The boutons are filled with vesicles which on their own are filled with neurotransmitter, in our case glutamate. The vesicles of each bouton get shared by different synapses. When an action potential arrives at the synapse, the vesicles may fuse with the membrane. Some synapses harbour a so-called T bar, others not. A reductionists scheme starting from the bouton chain down to single boutons and finally synapses and vesicels is shown in Figure 2.



NMJ 2 boutons Scheme of bouton Synapses, T bar

Figure 2. A reductionist approach

We have employed this reductionist approach and started by modelling single presynaptic boutons. Synaptic vesicles can be divided into different pools however a quantitative understanding of their dynamics at the Drosophila neuromuscular junction is lacking (Rizzoli and Betz 2005). We performed biologically realistic simulations of high and low release probability boutons (Lnenicka and Keshishian 2000) using partial differential equations (PDE) taking into account not only the evolution in time but also the spatial structure in two and three space dimensions.

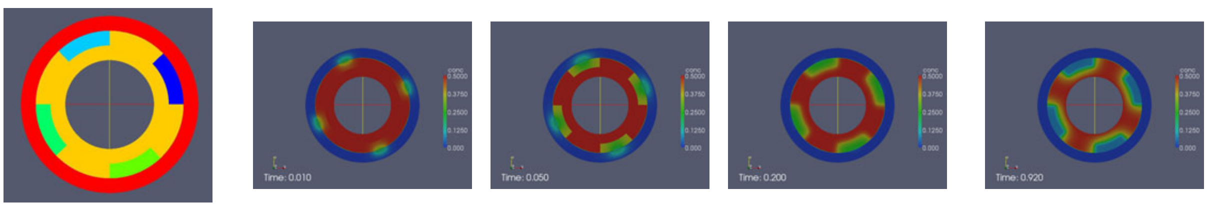


Figure 3. Bouton model and Time evolution of integrated bouton model, exocytosis of glutamate into cleft

PDEs are solved using *uG*. Numerical calculations are done on parallel computers allowing for fast calculations using different parameters in order to asess the biological feasibility of different models. In preliminary simulations, we modeled vesicle dynamics as a diffusion process (Yeung et al. 2007) describing exocytosis as Neumann streams at synaptic active zones. The initial results obtained with these models are consistent with experimental data. This work is still in progress.

The regions of a bouton within a simple integrated model are shown in Figure 3, first picture. We identify the ready-for-release-pool and the synapses (yellow and blue/green) as the presynaptic part, wheras the red surface repsresents the synaptic cleft. Simulations based on this geometry are shown in Figure 3, wheras we show comparisons between the measured outstream and content within the cleft and the Evoked Post Synaptic Potentials (EPSP) as measured within the experiment. Models in 2 and 3D using realistic parameters are in particular subject of this project. In Figure 4, we show a 3D simulation.

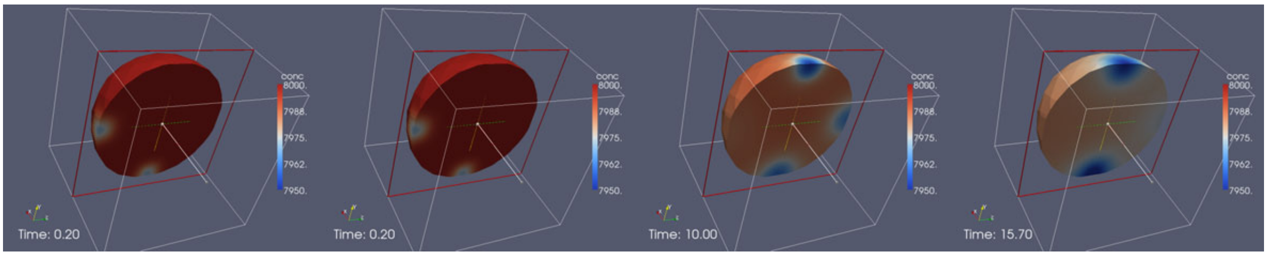


Figure 4. A three dimensional model of vesicle dynamics within the presynaptic boutons

The next step will consist of the calculation on reconstructed (using NeuRA) realistic geometries. A single bouton and a chain we see in Figure 5.

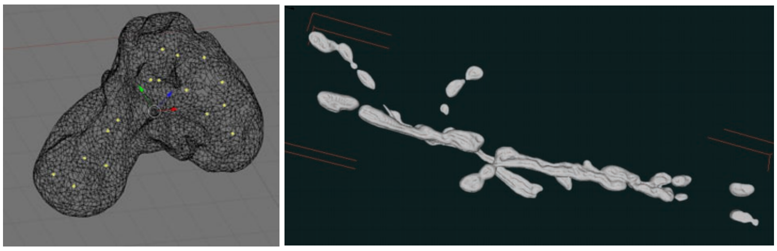


Figure 5. Reconstructed boutons and chain

Finally, we modelled Calcium in the presence of a T bar and without it in order to understand the consequences of this biological barrier. In Figure 6 we show comparisons of Ca influx.

Further refinements are currently being implemented, including simulations

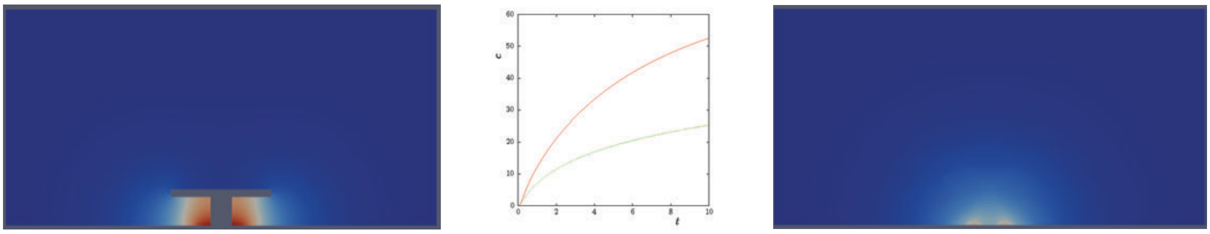


Figure 6. Calcium influx with T bar and without

using morphologically realistic geometries which were generated from confocal scans of the neuromuscular junction using NeuRA. Other parameters such as glutamate diffusion and reuptake dynamics, as well as postsynaptic receptor kinetics are intended to be incorporated in the future.

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NeuArch, NeuClass: Neuron Data Management and Classification Tools

Markus Dreier, Holger Heumann, Gillian Queisser, Gabriel Wittum

In the age of technological leaps in the neuroscientific world, a multitude of research areas, computational tools, mathematical models and data-aquiring methods have emerged and are rapidly increasing. Not only is data mass exploding, but also different data types and research approaches account for large diversification of data and tools. At the G-CSC ongoing research of an interdisciplinary nature brought about the need for organised and automatic data & tool structuring. Furthermore, we see a central data & tools management as an optimal means for scientific knowledge exchange, especially in decentralised research projects.

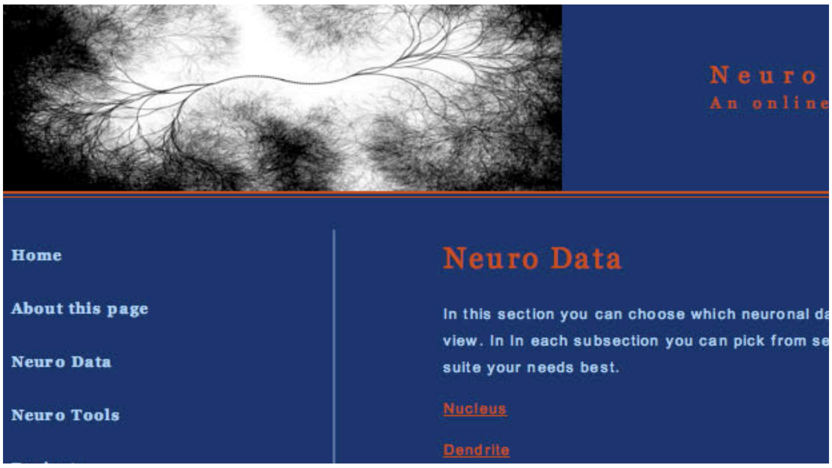

Figure 1. Screenshot of the NeuArch interface

Many databases have emerged in the field of neuroscience and computational neuroscience. Adding a G-CSC-based Neuron Data & Tools Management, will provide a platform for in-house development and data aquisition for broad use in the neuroscientific world.

The *NeuArch* database is developed with the established Ruby on Rails scripting language, a web application framework language with which many large database interfaces are developed nowadays. Ruby on Rails is directly tied into MySQL databasing. The abstract, layered description of the database-structure is shown in Fig. 1.

The database has two main objectives. For one, it will offer public access to all data which the owners have agreed to make public. Hence, it will offer a central way to offer and distribute data to the broader community. Special attention is given to the way data is acquired, processed and stored, so that comparability of data is guaranteed.

Second, the database shall have structured layers of private and semi-private data access. That way, data can be shared within single projects or groups, closed to the public. This will lighten the data exchange process in interdisciplinary project work, which most of the time requires frequent exchange of large data. An Alert and Information system layer will provide the database user with updates on project work and data, new publications and general information.

Private and secured layers are furthermore a strong incentive for researchers to use the database and upload their data. Not only is the researcher's workload minimised by automated data-storage but is their data accessible over longer time-periods than in the common lab set-up (think of a PhD-student finishing his/her thesis, burning most of his data on DVD and leaving for a new job).

The realisation of such a database with Ruby on Rails is a combination of pure programming and the use of various and well tested plugins. The security of the database is an inevitable subject, which the programmer must face. The Administrator needs to have an all-access account so he can handle database support. Project-specific accounts have to be created with different user permissions. With this variety of access possibilities the database needs to be shielded against security risks, which are taken care of by the environment used.

Various data types will be stored on the database. The necessary tools for working with the available data are either downloadable via the mainpage of the database, or via links to the different sources. The Users can communicate over scientific projects via database wikis and upload all their sources in short time, to receive quick feedback. The database itself provides progress to the scientific projects, as it is reachable from all over the world and data can be exchanged and discussed quickly.

In addition to the automatic reconstruction of neuron morphologies by *NeuRA*, a new tool has been developed for the automatic classification of cells, *NeuClass*. This is a typical entry point of data into the database. Thus we developed a new approach for the classification of neuron cells.

The shape of neuronal cells strongly resembles botanical trees or roots of plants. To analyze and compare these complex three-dimensional structures it is important to develop suitable methods. In (Heumann and Wittum 2009) we review the so called tree-edit-distance known from theoretical computer science and use this distance to define dissimilarity measures for neuronal cells. This measure intrinsically respects the tree-shape. It compares only those parts of two dendritic trees that have similar position in the whole tree. Therefore it can be interpreted as a generalization of methods using vector valued measures. Moreover, we show that our new measure, together with cluster analysis, is a suitable method for analyzing three-dimensional shape of hippocampal and cortical cells.

The corresponding tool NeuClass has been applied to many experimental data available. Fig. 2 shows such a classfication obtained by NeuClass.

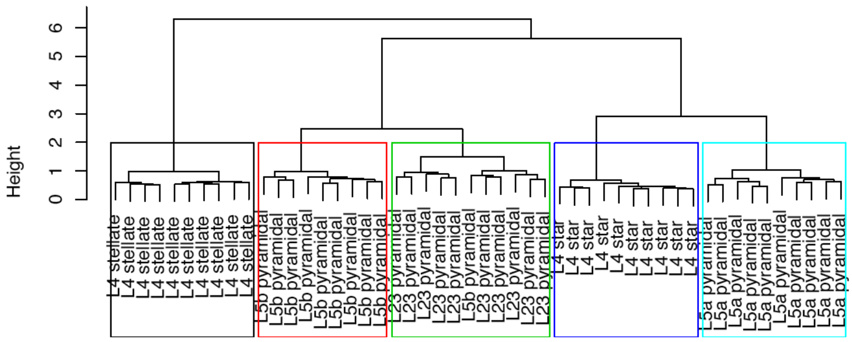

Figure 2: The tree-edit distance discriminates well between the different cell types.

The algorithm performed nicely. In spite of the fact that complexity of the tree-edit distance algorithm used is not optimal, all the computations from (Heumann and Wittum 2009) were performed in at most a few minutes. On larger datasets it may be useful to parallelize the algorithm which is straightforward. Besides complexity issues, it should further be investigated using more cell datasets, what parameters should be used for charaterization of cells.

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NeuGen: A tool for the generation of realistic morphology of cortical neurons and neural networks in 3D

Jens Eberhard, Alexander Wanner, Sergei Wolf, Gillian Queisser, Gabriel Wittum

In the past decade, computer simulations of cellular behaviour of single neurons or small networks of neurons with an accurate dendritic and axonal morphology have become increasingly common. The complex morphology of the neurons is usually taken from experimental data resulting in anatomically precise compartmental models. The complex geometric morphology is important for the understanding of the neuronal integration, see (Schaefer et al. 2003).

The reconstruction of anatomically precise compartmental models of neurons from experiments either manually or automatically with the help of reconstruction software is rather tedious and time-consuming. Depending on dye and recording technique such a reconstruction is only feasible for one or a few neurons at a time. Hence, a software program that is able to generate three-dimensional (3D) synthetic neuron geometries and neural networks and which is based on experimental findings is an invaluable tool.

We created the software package NeuGen (Eberhard et al. 2006) for the generation of realistic neurons and neural networks in 3D. NeuGen provides an easy way to construct not only single cells but also complex networks with a large number of neurons. The networks are interconnected by synapses. These synapses are created at axonal locations determined by a geometrical function of the distance to the dendrites of all other neurons.

NeuGen implements a straightforward algorithm which utilises forward stepping rules. Further each neuron type builds an independent class in NeuGen. The algorithm directly maps anatomical fingerprints of the different neuron types onto a coordinate-based description for the three-dimensional neuron geometry. Therefore NeuGen uses statistical distributions based on morphological parameters given by realistic data and some basic compartmental model elements.

NeuGen is intended to generate neural networks as cortical columns connecting layer 5 (L5) and layer 4 (L4) with layer 2/3 (L2/3) in the cortex; see figure 1 (middle) for the layers. It provides the generation of L2/3 pyramidal cells, L5 A and L5 B pyramidal cells, L4 star pyramidal cells, and L4 stellate neurons. The different cell types are automatically located in their associated layers.

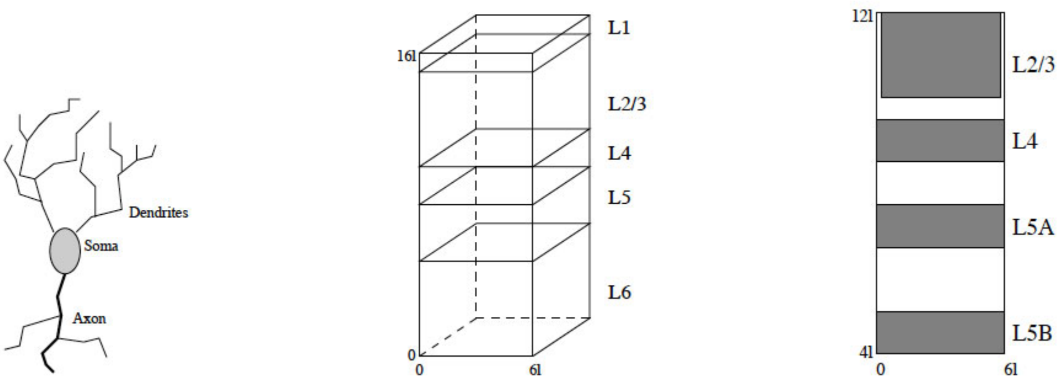

Figure 1. Sketch of a neuron with soma, dendrites, and axon (left). Schematic representation of a cortical column with its layers denoted by layer 1 (L1), layer 2/3 (L2/3), layer 4 (L4), layer 5 (L5), and layer 6 (L6), and its dimensions where $l = 100\mu m$ (middle). Bounding boxes for the locations of the somata used by Neu-Gen for the generated cells. The boxes are illustrated by the shaded areas within the cortical column (right).

It uses parameter distributions derived from experimental anatomical data to construct synthetic neurons of different morphological classes. Within each class, the statistically constrained implementation of the algorithm produces non-identical neurons. The generated cells resemble the morphological classes of real neurons from which the morphological parameters were extracted. To illustrate the capabilities of NeuGen, Figures 2-3 show various results of generated neurons and networks. A graphical user interface allows neuronal network generation without programming.

NeuGen can output ".hoc" format for compartmental simulation. The neuronal structures can be converted into files for 3D surface generation with the software package NeuTria. NeuTria is a flexible tool for surface generation of realistic morphology of neurons and neuronal networks in three dimensions. This allows the implementation of highly detailled biophysical models on realistically generated 3-d-morphologies.

Figure 2. Four different L2/3 pyramidal cells with 8 dendrites starting from the soma (yellow). The cells show the terminal tuft being characteristic for the apical dendrite. The axonal tree is coloured in blue.

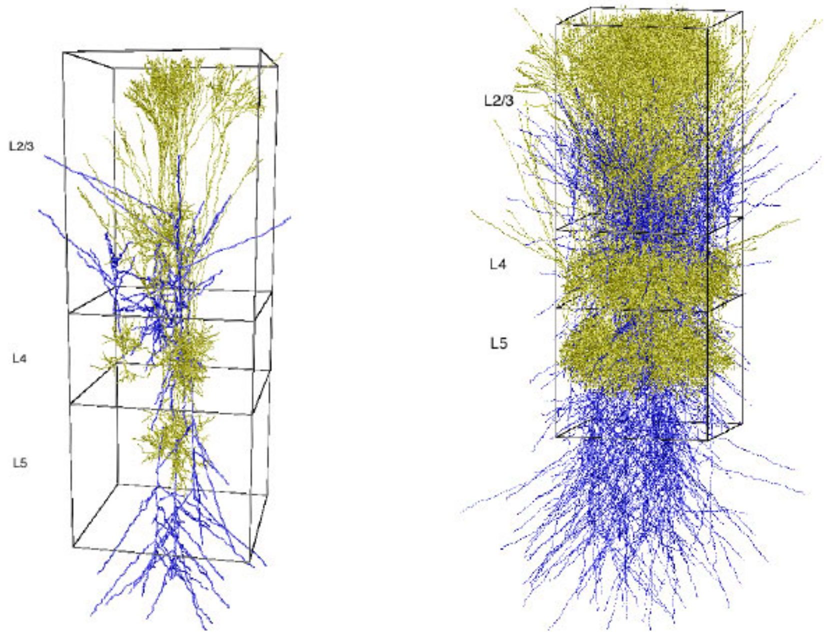

Figure 3. Left: A generated network for a cortical column with 10 cells. The net consists of three L4 stellate neurons, two L4 star pyramidal cells, three L2/3 pyramidal cells, and two L5 A pyramidal neurons. All neurons have 9 dendrites starting from the soma. Right: A generated network for a cortical column with 150 cells. The net consists of 40 L4 stellate neurons, 30 L4 star pyramidal cells, 40 L2/3 pyramidal cells, and 40 L5 A pyramidal neurons. The neurons have 9 dendrites starting from the soma. The boundaries of the cortical column are indicated by the boxes.

The next step will be the deployment of detailed neuronal morphologies for the hippocampus. The main cells of the rat hippocampus are CA1 and CA3 pyramidal cells. The experimental anatomical data of these morphological classes are available in morphology databases, e. g. NeuroMorpho, Southampton Database, as well as in the existing literature.

NeuGen can read and visualise the data, which are in SWC, hoc, NeuroML any other common formats. It is necessary to extract the parameters like number of dendrites, diameters and branching angles to construct synthetic neurons. The mass of data in a realistic model is time-consuming and requires computational effort. NeuGen uses efficient algorithms in order to reduce this computational effort.

NeuGen includes an own simulation package, called NeuSim (Wanner, 2007). NeuSim simulates compartmental models on geometries generated by NeuGen on massively parallel computers.

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5. Cumulative List of Publications

Cumulative listing of journal articles and conference proceedings published in the year 2009 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 2009

[1] 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." 2009. arXiv:0911.5430 [hep-ex].

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