NAWI-Graz Workshop

26.Juni 2009 Seifenfabrik

Programme

9:00 O.Univ.-Prof. Dr. Hans Sünkel, Rektor TU : Opening		
9:05 - 9:25 Univ.-Prof. Dr. Franz Stelzer, Vizerektor TU: „Wo steht NAWI Graz?“		
PLENARY TALKS 9:25 – 10:40		
Chair: von Grünberg (KFU)		**09:25-10:05 Gero Vogl** (Fakultät für Physik, Uni Wien) Die Mühen der Ebenen: Two-dimensional diffusion in different disciplines
		10:05-10:40 Rudolf Zechner (Institute of Molecular Biosciences, KFU Graz) The fate of fat: Breakdown of fat depots in mice and men
COFFEE BREAK 10:40 – 11:00		
MORNING SESSIONS 11:00 – 13:00		
A1 Nanoscience	**Physics, Chemistry** Chair/Organizers: Würschum (TU) Slugovc (TU)	**A1-01 11:00-11:30 Peter Zeppenfeld** (Johannes Keppler University Linz) Nanostuctures on surfaces
		A1-02 11:30-11:42 Gunter Zenkl (TU Graz) Nanoparticles for optical sensor applications
		A1-03 11:42-11:54 Stephen Berkebile (KFU Graz) Highly oriented organic molecular films
		A1-04 11:54-12:06 Alexandra Lex (University of Münster) Chemically and photochemically reactive thin siloxane layers for modification of inorganic surfaces and their application
		A1-05 12:06-12:18 Wolfram Steurer (KFU Graz) Surface dynamics phenomena of amorphous materials
		A1-06 12:18-12:30 Daniel M. Koller (KFU Graz) Organic light-emitting diodes as surface plasmon emitters
		A1-07 12:30-12:45 Andreas Trügler (KFU Graz) High-resolution surface plasmon imaging
		A1-08 12:45-13:00 Andreas Gumbsch (KFU Graz) Single-atom spectroscopy: Kondo resonance of Co adatoms on Cu(110) and Cu(110)-(2x1)O surfaces
A2 Scaling issues in earth sciences	**Earth Science** Chair/Organizers: Dietzel (TU) Hergarten (KFU)	**A2-01 11:00-11:15 Stefan Hergarten** (KFU Graz) Scaling issues in earth sciences- an overview
		A2-02 11:15-11:45 Thomas Ptak (University of Göttingen) Modeling of contaminant transport in hydraulically and hydrogeochemically heterogeneous aquifers using a sedimentological facies approach
		A2-03 11:45-12:00 Thomas Rinder (TU Graz) „Scaling“ of drainage systems –multi proxy approach for the formation of calcium carbonates in alkaline man-made environments
		A2-04 12:00-12:15 Thomas Wagner (KFU Graz) Slope-elevation relation of an orogen, a chance to decipher its stage of evolution?
		A2-05 12:15-12:30 Roland Krenn (KFU Graz) Towards understanding the dynamics of forest fires
		A2-06 12:30-12:45 Janik Deutscher (Joanneum Research) Natural hazard monitoring with differential radar interferometry
		A2-07 12:45-13:00 Heimo Truhetz (KFU Graz) Highly resolved wind climatologies under a changing climate in the alpine region and the vienna Basin
A3 Lipids and biomembranes	**Molecular Biology** Chair/Organizers: Natter (KFU) Daum (TU)	**A3-01 11:00-11:30 Laszlo Vigh** (Biological Research Centre Szeged) Stress protein response from membranes and back to membranes: lipid rafts at the crossroad
		A3-02 11:30-12:00 Johannes Nimpf (Medical University Vienna) What has the chicken egg to do with our brain?
		A3-03 12:00-12:15 Dagmar Zweytick (Akademie der Wissenschaften Graz) Small peptides-huge effect on cancer cells!
		A3-04 12:15-12:30 Maximilian Schicher (TU Graz) Functional proteomic analysis of lipolytic enzymes in human fat cells
		A3-05 12:30-12:45 Christoph Kurat (KFU Graz) Greasing the cell cycle: Cell cycle-dependent triglyceride lipolysis contributes to cell proliferation
		A3-06 12:45-13:00 Monika Oberer (KFU Graz) Structure and function of proteins in lipid metabolism
A4 Metals in biology	**Chemistry** Chair/Organizers: Mösch-Zanetti (KFU) Macheroux (TU)	**A4-01 11:00-11:34 Peter Kroneck** (University of Konstanz) Transition metals and sulfur: Nature´s perfect building blocks for efficient catalysts
		A4-02 11:34-12:08 Bernhard K. Keppler (Uni Wien) Tumor-inhibiting metal compounds from bench to bedside
		A4-03 12:08-12:21 Alice Rumpler (KFU Graz) The changing face of arsenic: valences and their consequences of toxicity
		A4-04 12:21-12:34 Karl Gruber (KFU Graz) Structure and mechanism of coenzyme B_{12}-dependent glutamate mutase
		A4-05 12:34-12:47 Pedro Traar (KFU Graz) Molybdenum and rhenium complexes in oxidation catalysis: modelling of metalloenzymes
		A4-06 12:47-13:00 Stefan Leitgeb (TU Graz) Structure-function relationships in non-heme Fe(II) dependent dioxygenases

A5 Discrete mathematics and number theory	**Mathematics** Chair/Organizers: Grabner (TU) Geroldinger (KFU)	**A5-01 11:00-11:45 Alain Pagne** (Centre de Mathematiques Laurent Schwartz (CMLS) École polytechnique, Palaiseau Cedex) Additive combinatorics as an invitation to mathematics
		A5-02 12:00-12:15 Andreas Philipp (KFU Graz) Orders in algebraic number fields with half-factorial localizations
		A5-03 12:15-12:30 Andreas Reinhart (KFU Graz) *v*- ideal semigroups and divisorial lattices
		A5-04 12:30-12:45 Martin Jancevskis (TU Graz) Waring´s problem on some dense set
		A5-05 12:45-13:00 Christoph Temmel (TU Graz) Percolation on infinite graphs
LUNCH BREAK 13:00 – 14:20		
PLENARY TALKS 14:20 – 15:30		
Chair: von Grünberg (KFU)		**14:20-14:55 Gerhard Holzapfel** (Institute of Biomechanics, TU Graz) Biomechanics in the interdisciplinary context of bioengineering, biology, chemistry and medicine
		14:55-15:30 Herwig Hauser (Fakultät für Mathematik, Uni Wien) Geometry, Symmetry, Singularity
BREAK 15:30 – 16:00		
AFTERNOON SESSIONS 16:00 – 18:00		
B1 Scientific computing in science and engineering	**Mathematics** Chair/Organizers: Haase (KFU) Steinbach (TU)	**B1-01 16:00-16:40 Carsten Wolters** (University of Münster) Source analysis of epileptiform activity using high-resolution FE head modeling
		B1-02 16:40-17:00 Nagaiah Chamakuri (KFU Graz) Numerical solutions for optimal control of reaction-diffusion systems in cardiac electrophysiology
		B1-03 17:00-17:20 Sarah Engleder, Peter Urthaler (TU Graz) Fast boundary element methods in wave propagation problems
		B1-04 17:20-17:40 Aurel Neic (KFU Graz) Using the parallel toolbox in applications
		B1-05 17:40-18:00 Christoph Augustin, Markus Windisch (TU Graz) Parallelized domain decomposition methods for applications in biomechanics and acoustics
B2 System biology and metabolic networks	**Molecular Biology** Chair/Organizers: Nidetzky(TU) Schwab (TU)	**B2-01 16:00-16:40 Matthias Reuss** (Uni Stuttgart) Stochastic simulations of 4D-spatial temporal dynamics of molecule movements in biosystems
		B2-02 16:40-17:00 Jürgen Zanghellini (TU Graz) On the use and abuse of fat for life-quantitative modeling of triglyceride homeostasis in yeast
		B2-03 17:00-17:20 Franz Hartner (TU Graz) Utilising the methanol metabolism of the yeast pichia pastoris for cofactor regeneration during biotransformations
		B2-04 17:20-17:40 Mario Klimacek (TU Graz) Metabolite profiling and flux control analysis in the optimization of microbial bioprocesses
		B2-05 17:40-18:00 Stephan Pabinger (TU Graz) Metabolic model of penicillium chrysogenum
B3 Biocatalysis and bioorganic chemistry	**Chemistry** Chair/Organizers: Faber (KFU) Kroutil (KFU)	**B3-01 16:00 – 16:30 Ulf Hanefeld** (TU Delft) Heterogeneous catalysts and enzymes for the synthesis of cyanohydrins
		B3-02 16:30 – 17:00 Andreas Schmid (TU Dortmund) The use of oxidoreductases for biocatalytic oxyfunctionalization
		B3-03 17:00 – 17:15 Christiane Gödl (TU Graz) Sweet temptation. from structure-function relationships of disaccharide phosphorylases to application in synthesis
		B3-04 17:15 – 17:30 Grit Straganz (TU Graz) Towards novel oxygenase-type reactions catalyzed by the atypical, 3-His ligated, nonheme Fe(II) centre
		B3-05 17:30 – 17:45 Silvia M. Glück (KFU Graz) New approach for racemisation based on „catalytic promiscuity“
		B3-06 17:45 – 18:00 Klaus Zangger (KFU Graz) NMR protein structure determination using paramagnetic restraints
B4 Quantum physics in the femto- and nano-world	**Physics** Chair/Organizers: Gattringer (KFU) Von der Linden (TU)	**B4-01 16:00-16:40 Uwe-Jens Wiese** (University Bern) From quantum spins to emergent field theories
		B4-02 16:40-17:00 Martina Blank (KFU Graz) Quarks and gluons: functional approaches
		B4-03 17:00-17:20 Daniel Mohler (KFU Graz) Quarks and gluons on a space-time grid
		B4-04 17:20-17:40 Ralf Gamillscheg (TU Graz) Strongly correlated materials: effects and simulations
		B4-05 17:40-18:00 Hannes Allmaier (TU Graz) Electron correlations in spintronic materials
B5 Polymer science	**Central Polymer Lab** Chair/Organizers : Stelzer (TU)	**B5-01 16:00-16:30 Franz Stelzer (**TU Graz) Polymeric materials- from laboratory to technological applications
		B5-02 16:30-17:00 Otto Glatter (KFU Graz) Isasomes in thermo-reversible polysaccharide hydrogels
		B5-03 17:00-17:25 Rupert Kargl (KFU Graz) Properties and utilisation of cellulose model surfaces from ionic liquid solutions
		B5-04 17:25-17:45 Eugen Maier (TU Graz) Hybrid photovoltaic cells via a novel direct route
		B5-05 17:45-18:00 Robert Saf (TU Graz) CePoL updates
FREE BEER & BBQ 18:00		

Plenary Talks

09:25-10:05
Die Mühen der Ebenen:
Two-dimensional diffusion in different disciplines
Gero Vogl
Fakultät für Physik, Uni Wien

We firstly study atom diffusion in the two-dimensional space of very thin surface layers; synchrotron radiation in grazing incidence enables the observation of this stochastic motion ("random walk"). Secondly we try to apply the principle of random walk to the dispersion of plants and men in the two-dimensional space of earth's surface

10:05-10:40
The fate of fat: Breakdown of fat depots in mice and men
Rudolf Zechner
Institute of Molecular Biosciences, KFU Graz

14:20-14:55
Biomechanics in the interdisciplinary context of bioengineering, biology, chemistry and medicine
Gerhard Holzapfel
Institute of Biomechanics, Center of Biomedical Engineering
TU Graz

Mechanics regulates biological processes at the molecular, cellular, tissue, organ, and organism levels. Biomechanics has the goal to better explain phenomena in bioengineering, biology, chemistry and medicine, and hence to improve, for example, diagnostic methods, therapeutic interventions, medical devices and tissue engineering. By means of several examples the presentation will show the importance of biomechanics to quantify the mechanical environment in health, disease, or injury. Using medical imaging, powerful computers, experimental data and mechanics, computational models serve the basis for the "virtual patient".

14:55-15:30
Geometry, symmetry, singularity
Herwig Hauser
Fakultät für Mathematik, Uni Wien

Take a polynomial in three variables, e.g. $P(x,y,z) = x^2 + z^2 - y^3(1-y)^3$. In general it is extremely difficult to determine the shape and geometry of the set F of all solutions of the equation P = 0. This set F is a surface in Euclidean three-space. In the simplest cases it looks like a paraboloid or the surface of a cone. But in general, computer programs tend to depict it incorrectly. In the lecture, we will present several (correct) visualizations of surfaces. This will allow us to describe typical geometric phenomena like symmetry and singularities. As such solution sets are ubiquitous in physics, chemistry and industry (not only in mathematics), their understanding is instrumental in various concrete applications.

Morning Sessions

A1 Nanoscience

organized by: Roland Würschum (TU)
Christian Slugovc (TU)

A1-01

Nanostuctures on surfaces
Peter Zeppenfeld
Institute of Experimental Physics, Atomic Physics and Surface Science Johannes Keppler University Linz

I will report on the fabrication and characterization of nanostructures from a surface science perspective. The physical mechanisms leading to ordering and pattern formation at surfaces will be illuminated and examples of nanostructured surfaces and their use as templates for subsequent growth of thin metal and organic films are presented.

A1-02

Nanoparticles for optical sensor applications
Gunter Zenkl
Institute for Chemistry and Technology of Materials, TU Graz

By bringing receptors combined with optical signalling units into the nanometer scale, new ways for the sensing of various analytes are paved.

A1-03

Highly oriented organic molecular films
Stephen Berkebile
Institute of Physics, KFU Graz

With appropriate choice of substrate and growth conditions, well-ordered and oriented monolayer and 'single' crystalline films of conjugated organic molecules can be grown – a prerequisite for unambiguous experimental electronic band structure determination with angle-resolved ultraviolet photoemission spectroscopy and the study of the growth of organic heterostructures with a defined orientation.

A1-04

Chemically and photochemically reactive thin siloxane layers for modification of inorganic surfaces and their application
Alexandra Lex
Institute of Chemistry and Technology of Materials, TU Graz
Institute of Physical Chemistry University of Münster

Organic thin film transistors (OTFTs) modified with chemically reactive interfacial layers between the gate dielectric and the semiconducting polymer show a strong dependence of the electric characteristics on the presents of amines rendering them highly promising for chemical probes and sensors.

A1-05

Surface dynamics phenomena of amorphous materials
Wolfram Steurer
Institute of Experimental Physics, TU Graz
Institute of Physics, KFU Graz

Investigations of the vibrational dynamics of amorphous materials by surface-sensitive methods have revealed a wealth of new physics recently. The discovery of the surface boson peak in silica glass and a novel gap-filling in the surface vibrational density-of-states of amorphous selenium are two examples which will be presented in this contribution.

A1-06

Organic light-emitting diodes as surface plasmon emitters
Daniel M. Koller
Institute of Physics, KFU Graz

Surface plasmons are coupled hybrid modes of light and electrons at dielectric/metal interfaces, which can be spatially confined beyond the diffraction limit of light. The here demonstrated combination of surface plasmons and organic light-emitting diodes enabled the development of a nano-optical light source, which is potentially interesting for nano-photonic devices.

A1-07

High-resolution surface plasmon imaging
Andreas Trügler
Institute of Physics, KFU Graz

Energy filtered transmission electron microscopy (EFTEM) is emerging as a novel characterization tool in plasmonics. In this talk, I will present our numerical approach for simulating EFTEM maps of metallic nanoparticles, and will demonstrate that EFTEM allows to directly monitor surface plasmons with nanometer resolution. Our results are in perfect agreement with experimental data of the FELMI centre, TU Graz.

A1-08

Single-atom spectroscopy: Kondo resonance of Co adatoms on Cu(110) and Cu(110)-(2x1)O surfaces
Andreas Gumbsch
Institute of Physics, KFU Graz

We have applied scanning tunneling spectroscopy (STS) in a cryogenic 5 K scanning tunneling microscope to probe the interaction of single cobalt atoms with the Cu (110) and the oxygen-reconstructed Cu (110)-(2x1) O surfaces. The interaction of the conduction electrons of the substrate with the magnetic impurity atoms via spinexchange causes Kondo resonances in the STS spectra.

A2 Scaling issues in earth sciences

organized by: Martin Dietzel (TU)
Stefan Hergarten (KFU)

A2-01

Scaling issues in earth sciences- an overview
Stefan Hergarten
Institute of Earth Sciences, KFU Graz

Spatial and temporal scaling problems are ubiquitous in all fields of earth sciences. Available data originate from point measurements, laboratory experiments or observations on the outcrop scale, while many questions address regional or even continental scales. Concerning time, similar problems arise as many process show intermittent activity. Similarly, in modeling the physics and chemistry behind the phenomena seem to be clear only at small scales.

A2-02

Modeling of contaminant transport in hydraulically and hydrogeochemically heterogeneous aquifers using a sedimentological facies approach
Thomas Ptak
Geosciences Center, Universität Göttingen

It is well known that aquifer structural properties and the resulting heterogeneous distribution of hydraulic conductivity and porosity significantly control groundwater flow and spreading of solutes. In addition, physico-chemical aquifer heterogeneity influences the interaction of reactive solutes with the aquifer material, and may tend to enhance tailing of reactive solutes. To consider both types of heterogeneity, a reactive solute transport modeling approach was developed, allowing for a sedimentological facies-based upscaling of small-scale laboratory measurements to field scale.

A2-03

„Scaling“ of drainage systems –multi proxy approach for the formation of calcium carbonates in alkaline man-made environments
Thomas Rinder
Institute of Applied Geosciences, TU Graz

Clogging of tunnel drainage systems is cost-intensive due to maintenance action. Reaction mechanisms can be deciphered by a multi proxy approach (e.g. Sr/Ca and Mg/Ca ratios, pH, stable isotope distribution). Accordingly, environmental conditions during primary CaCO3 formation may be reconstructed and CaCO3 precipitation as well as degree of cement-water interaction can be monitored. Upscaling of in-situ experimental results in the Koralmtunnel provides modelling tools for ongoing overall sinter formation within the whole drainage system in order to consider necessary retaliatory action.

A2-04

Slope-elevation relation of an orogen, a chance to decipher its stage of evolution?
Thomas Wagner
Institute of Earth Sciences, KFU Graz

Slope-elevation distributions for particular drainage areas show the actual stage of development for an active orogen. Analytical solutions of an uplifting orogen and its decay by surface erosion perfectly fit the observed data (extracted from digital elevation models). This consistency suggest young (5Ma) additional topographic build up of the Alps, thereby provoking general geological believe.

A2-05

Towards understanding the dynamics of forest fires
Roland Krenn
Institute of Earth Sciences, KFU Graz

The signatures of self-organized critical phenomena are ubiquitous in nature and include, i.e., tumor growth, solar flares, earthquakes, superconducting vortices, and forest fires. Placing the emphasis on simulations of a self-organized critical cellular automaton model, we show that lightning-induced and manmade forest fires cannot be treated separately in wildfire modeling, hazard assessment and forest management.

A2-06

Natural hazard monitoring with differential radar interferometry
Janik Deutscher
Institute of Digital Image Processing, Joanneum Research

In the past decades, the space-geodetic technique of differential radar interferometry has enabled earth scientists to monitor earth deformation processes remotely, repeatedly and at larger scales as is possible with ground based geodetic methods. In our study we aim at exploiting the potential of new radar satellites (e.g. TerraSAR-X) together with time-series of older data sets, for monitoring and assessing various geologic and glaciological deformation processes in areas at risk of natural hazards in the Alps and in Iceland.

A2-07

Highly resolved wind climatologies under a changing climate in the alpine region and the vienna basin
Heimo Truhetz
Wegener Center for Climate and Global Change and Institute for Geophysics, Astrophysics, and Meteorology, KFU Graz

A hybrid dynamic/diagnostic climate modelling approach has been developed and applied for the periods 1981-1990 and 2041-2050 (IPCC scenario IS92a) to estimate climate change effects on near-surface wind in the Alpine region (10 km grid spacing) and the Vienna Basin (200 m grid spacing). Model errors, climate change signals, and effects of error correction are presented.

A3 Lipids and biomembranes

organized by: Klaus Natter (KFU)
Günther Daum (TU)

A3-01

Stress protein response from membranes and back to membranes: lipid rafts at the crossroad
Laszlo Vigh
Head of the Molecular Stress Biology Group
Institute of Biochemistry, Szeged

Similar to heat stress, isothermal perturbations of membranes can also modulate the expression of stress-protein molecular chaperones. Lipid molecular species involved in the activation of stress-signaling pathways is delineated. Membrane associated stress- proteins control major attributes of membranes. These principals can yield pharmaceutical agents that have the potential of major therapeutic benefit to number of disease states.

A3-02

What has the chicken egg to do with our brain?
Johannes Nimpf
Max F. Perutz Laboratories, Inst. of Medical Biochemistry
Med Uni Wien

During mammalian brain development the formation of the laminated structure of the forebrain is mediated by the receptor-mediated reelin-signaling pathway. In egg laying species like the chicken, the development of the egg is dependent on receptor-mediated yolk deposition in the growing oocyte. Surprisingly, both processes are mediated by the same protein the VLDL receptor.

A3-03

Small peptides-huge effect on cancer cells!
Dagmar Zweytick
Institute of Biophysics and Nanosystems Research
Austrian Academy of Sciences

In our project we copy and enforce a weapon against cancer cells in the form of small cationic peptides that are important components of the innate immune system of all species. To enhance its natural antitumor properties the membrane-active part (LF11) of lactoferricin is taken as a parent peptide.

A3-04

Functional proteomic analysis of lipolytic enzymes in human fat cells
Maximilian Schicher
Institute of Biochemistry, TU Graz

We report on the identification of lipid hydrolysing enzymes in human fat cells using a functional proteomics approach.
For this purpose, cultured human fat cells were incubated with a fluorescent inhibitor specifically binding to the active site of the target enzymes. After protein separation by gel electrophoresis, the fluorescent protein spots were cut out and identified by mass spectroscopy. Results from comparative studies showed that fat cells of different origin expressed tissue specific enzyme patterns.

A3-05

Greasing the cell cycle: Cell cycle-dependent triglyceride lipolysis contributes to cell proliferation
Christoph Kurat
Department of Molecular Biosciences, KFU Graz

Recovery from quiescence and cell cycle entry go along with a rapid mobilization of storage lipids in budding yeast. Recently, we found out that triglyceride degradation is cell cycle regulated. Absence of lipolysis results in a delay in cell cycle entry, pointing at a crucial role for lipid homeostasis during this process.

A3-06

Structure and function of proteins in lipid metabolism
Monika Oberer
Institut für Molekulare Biowissenschaften, KFU Graz

Changes in the energy status of an organism require the hydrolysis of stored triacylglycerols from adipose tissue. This reaction called lipolysis is performed by specific lipases (ATGL, HSL, MGL) and an activator protein (CGI-58). We investigate the structure-function relationship of these important metabolic proteins with biochemical and biophysical methods.

A4 Metals in biology

organized by: Nadia Mösch-Zanetti (KFU)
Peter Macheroux (TU)

A4-01

Transition metals and sulfur: Nature´s perfect building blocks for efficient catalysts
Peter Kroneck
Department of Biology, Universität Konstanz

Numerous biological processes depend on transition metals (e.g. Fe, Cu, Mo) coordinated to sulfur ligands. Prime examples are the iron-sulfur clusters, the type 1 Cu electron transfer center, and Mo (or W) bound to the dithiolene moiety of molybdopterin. This lecture will cover structural and functional aspects of this important class of metal sites.

A4-02

Tumor-inhibiting metal compounds from bench to bedside
Bernhard K. Keppler
Institute of Inorganic Chemistry, Uni Wien

Beside the well-established role of platinum in cancer therapy, other metals such as ruthenium, gallium and lanthanides open up new avenues by offering different activity profiles and mechanisms of action. Complexes with biologically active ligands and tumor-targeting strategies are being studied in order to maximize the impact on cancer cells.

A4-03

The changing face of arsenic: valences and their consequences of toxicity
Alice Rumpler
Institute of Chemistry/Analytical Chemistry, KFU Graz

Arsenic is an element with a reputation – enhanced by Agatha Christie – as a powerful poison. But even if you don't have enemies, there's a good chance that you will come face to face with arsenic regularly in your daily life. In this talk, the current status of arsenic will be discussed, with special emphasize on its toxicity induced by the transition of oxidation-states. Moreover, it will be elucidated, if health-conscious people need to be frightened that they might meet a similar fate to the victims in Agatha Christie's detective stories or if Paracelsus' declaration is imperative: The dose makes the poison!

A4-04

Structure and mechanism of coenzyme B_{12}-dependent glutamate mutase
Karl Gruber
Institute of Molecular Biosciences, KFU Graz

Coenzyme B_{12} dependent enzymes catalyze various rearrangement reactions involving high energy radicals as intermediates. We specifically determined and analyzed crystal structures of glutamate mutase from *Clostridium cochlearium*, which catalyzes the interconversion of (S)-glutamate and (2S,3S)-3-methylaspartate, in order to elucidate the mechanism of cofactor activation and of substrate rearrangement.

A4-05

Molybdenum and rhenium complexes in oxidation catalysis: modelling of metalloenzymes
Pedro Traar
Institute of Chemistry/Inorganic Chemistry, KFU Graz

Transition metal complexes play an important role as integral part of catalysts in both biological and technical processes. In nature a particular class of enzymes containing molybdenum is known to transfer an oxygen atom from a substrate to another. The synthesis of molybdenum and rhenium model complexes using organic ligands should mimic these metalloenzymes and are investigated towards their catalytic activity in oxygen transfer reaction (OAT). The talk will give an overview about synthetically prepared molybdenum and rhenium complexes and their possible use in catalytic reactions.

A4-06

Structure-function relationships in non-heme Fe(II) dependent dioxygenases
Stefan Leitgeb
Institute of Biotechnology, TU Graz

Non-heme Fe(II) dependent dioxygenases share a highly conserved active site structure despite catalyzing oxidative transformations of a broad range of different substrates. Dke1 promotes the oxidative cleavage of β-diketone structures and was used a model system for the investigation of structure-function relationships within this class of enzymes.

A5 Discrete mathematics and number theory

organized by: Peter Grabner (TU)
Alfred Geroldinger (KFU)

A5-01

Additive combinatorics as an invitation to mathematics
Alain Pagne
Centre de Mathematiques Laurent Schwartz (CMLS)
École polytechnique, Palaiseau Cedex

The aim of this talk is to offer a mathematical trip to the audience. With such a trip, we would like to demonstrate the central position of additive combinatorics in mathematics with the help of two kinds of examples. First, when additive combinatorics is used as an efficient tool. Second, when it is a user of techniques from other mathematical fields. Well, as will clearly appear, this typology is only an excuse to display nice additive mathematics.

A5-02

Orders in algebraic number fields with half-factorial localizations
Andreas Philipp
Institut für Mathematik und wissenschaftlichen Rechnen, KFU Graz

The maximal order O_K of an algebraic number field is a Dedekind domain, and its arithmetic is completely determined by its Picard group $Pic(O_K)$. In particular, O_K is factorial if and only if its Picard group is trivial. In contrast, non-principal orders are not integrally closed, hence they are never factorial, and their arithmetic depends not only on their Picard group but also on the localizations at singular primes. A non-principal order O with $|Pic(O)| \geq 3$ inherits many arithmetical properties from the maximal order. In contrast, only little is known about the arithmetic of non-principal orders whose Picard group has at most two elements, even if all localizations are half-factorial. In this case, using special saturated submonoids as tools, we are able to give a quite explicit description of various arithmetical invariants such as the elasticity $\rho(O)$, the minimum distance $\min\Delta(O)$, and the catenary degree $\mathsf{c}(O)$. In particular, we prove that $\rho(O) \in \{1, 3/2, 2\}$ and $\min\Delta(O) \leq 1$.

A5-03

***v*- ideal semigroups and divisorial lattices**
Andreas Reinhart
Institut für Mathematik und wissenschaftlichen Rechnen, KFU Graz

For an integral domain R with quotient field K, let $(K^\times)$ denote the group of nonzero fractional principal ideals, $F^\bullet(R)$ be the semigroup of non-zero fractional ideals (equipped with the usual multiplication of ideals) and $F_v^\bullet(R)$ be the semigroup of nonzero fractional divisorial ideals (equipped with the v-multiplication). Let $F(R)^\times$ resp. $F_v(R)^\times$ be the corresponding subgroups of invertible fractional ideals resp. v-invertible fractional divisorial ideals. While the Picard group $F(R)^\times/(K^\times)$

and the divisor class group $F_v(R)^\times/(K^\times)$ are well established classical objects in commutative algebra, the corresponding ideal class semigroups $F^\bullet(R)/(K^\times)$ and $F_v^\bullet(R)/(K^\times)$ have been studied only recently in ring theory. The deviation of their semigroup structure from being a group can be described in terms of the ideal semigroup itself, and thus we investigate the ideal semigroups $F^\bullet(R)$ and $F_v^\bullet(R)$. In particular, we look for conditions on R under which these ideal semigroups are not too far from being a group (for example, whether they are almost complete or π-regular). Our main focus is upon the hitherto not investigated v-ideal semigroups and the corresponding divisorial lattices. One typical result (which in fact follows from a more general theorem) is as follows: If T is a subring of an algebraic number field and if L is a quotient field of T, then $F_v^\bullet(T)$ and $F_v^\bullet(T)/(L^\times)$ are almost complete and π-regular semigroups.

A5-04

Waring´s problem on some dense set
Martin Jancevskis
Institut für Analysis und Computational Number Theory,
TU Graz

Let N be an integer. For some given $s,k \in \mathbb{N}$, Waring's Problem asks for the solvability of $N = x_1^k + \ldots + x_s^k$ in integers $x_1,\ldots,x_s$. First, we want to give a brief overview on the history of Waring's Problem and the Hardy–Littlewood method. Secondly, we want to introduce recent developments on Waring's Problem. In particular, we assume the variables x_i to be an element of certain sieve sequences and to fulfill some digital restrictions.

A5-05

Percolation on infinite graphs
Christoph Temmel
Institut für Mathematische Strukturtheorie, TU Graz

We motivate percolation with some real world models and then turn to the mathematical model. The main discussion will be centered on phenomena like phase transitions and their relationship with the structure of the underlying graph. Furthermore some other aspects like the distribution of large clusters, finite approximations and more complicated models are presented.

Afternoon Sessions

B1 Scientific computing in science and engineering

organized by: Gundolf Haase (KFU)
Olaf Steinbach (TU)

B1-01

Source analysis of epileptiform activity using high-resolution FE head modeling
Carsten Wolters
Institute for Biomagnetism and Biosignalanalysis, University of Münster
Bioelectric source reconstruction in the human brain from scalp Electro- and Magneto- encephalography (EEG/MEG) signals is sensitive to head volume conductor properties, i.e., tissue geometries and conductivities. A mathematical dipole is widely used as the model of the primary current source. Since the inverse problem is not uniquely solvable, different classes of approaches exist and will be presented, which are based on different a-priori knowledge. All inverse methods are based on solutions to the corresponding forward problem, i.e., the simulation of the electric potential and the magnetic flux at the head surface for a dipole in the cortex sheet of the human brain. A successful application of the presented approaches to the fields of presurgical epilepsy diagnosis will be finally discussed.

B1-02

Numerical solutions for optimal control of reaction-diffusion systems in cardiac electrophysiology
Nagaiah Chamakuri
Institut für Mathematik und wissenschaftlichen Rechnen
KFU Graz

A numerical approach to solving the optimality systems corresponding to optimal control problems governed by the bidomain equations, one of the most complete descriptions of the cardiac bioelectric activity at the tissue and organ level, is presented. They consist of a system of elliptic partial differential equations coupled with a nonlinear parabolic equation of reaction-diffusion type, where the reaction term, modeling ionic transport is described by a set of ODEs.

B1-03

Fast boundary element methods in wave propagation problems
Sarah Engleder, Peter Urthaler
Institut für Numerische Mathematik, TU Graz

The propagation of waves in porous media, acoustic waves and electromagnetic waves can be simulated using the boundary element method. In engineering applications fast methods are used, which speed up the computation time and reduce storage costs significantly. In this talk the basic ideas of these methods are presented.

B1-04

Using the parallel toolbox in applications
Aurel Neic
Institut für Mathematik und wissenschaftliches Rechnen,
KFU Graz

The parallel toolbox contains an interface for parallel algorithms as well as multilevel parallel iterative solvers for discretized PDEs. The basic concepts of data distribution and realization are presented and the functionalities of the toolbox are explained. We focus on performance comparisons and performance gain achieved in engineering and medical applications.

B1-05

Parallelized domain decomposition methods for applications in biomechanics and acoustics
Christoph Augustin, Markus Windisch
Institut für Numerische Mathematik, TU Graz

A fast way to treat complex algorithms is the strategy of parallel computing. One way to achieve such a parallelization are domain decomposition methods. In this talk we present the main ideas of these methods and their application to problems in the fields of biomechanics and acoustics.

B2 Systems biology and metabolic networks

organized by: Bernd Nidetzky (TU)
Helmut Schwab (TU)

B2-01

Stochastic simulations of 4D-spatial temporal dynamics of molecule movements in biosystems

Matthias Reuss
Institut für Bioverfahrenstechnik, Uni Stuttgart

Spatial temporal distribution of biomolecules is an important issue for a wide range of systems. The numerical approach presented in this lecture is based on the stochastic simulation of the random walk of single molecules and probalistic modeling of reactions beween different molecule species. The examples chosen vary primarily in scale and architecture of the biosystem of interest. Signal transduction processes and endocytosis are selected to illustrate the molecular traffic inside individual cells in which diffusion processes are considerably hindered by the cytoskeleton. Alternatively vectorial transport processes via motor proteins are taken into account. A substantially more complex and challenging architecture needs to be considered for the movement of drug molecules in cancer tissues, because of different transport mechanisms in the vascular system and the interstitial space. Independendent from the specialities of the architecture of the biosystem under consideration the biological reactions are modeled in a probalistic manner.

B2-02

On the use and abuse of fat for life- quantitative modeling of triglyceride homeostasis in yeast

Jürgen Zanghellini
Institut für Genomik und Bioinformatik, TU Graz

It is well known that the accumulation of excess body fat has adverse affects. However, fat depots are not always evil. Using the example of yeast, we will present a quantitative, mathematical model and show that stored excess fat provides a major advantage for a rapid initiation of cellular growth.

B2-03

Utilising the methanol metobolism of the yeast pichia pastoris for cofactor regeneration during biotransformations

Franz Hartner
Institute of Molecular Biotechnology, TU Graz
Beate Pscheidt, Kirsten Schroer, Klaus P. Luef, Anton Glieder

Efficient regeneration of cofactors like NADH is necessary for a viable industrial biocatalytic reduction process. Here, we present a NADH regeneration process for bioreductions based on the Pichia pastoris methanol utilisation pathway. Pathway variants with improved NADH regeneration rates were predicted using a simple kinetic model. Subsequently we confirmed the validity of the model experimentally with a set of recombinant P. pastoris strains.

B2-04

Metabolite profiling and flux control analysis in the optimization of microbial bioprocesses

Mario Klimacek
Institute of Biotechnology and Biochemical Engineering, TU Graz

A systematic integral approach which combines quantitative metabolomics with kinetic enzyme models to determine in vivo enzymatic action is presented by means of the yeast xylose pathway engineered in Saccharomyces cerevisiae. Together with comprehensive metabolite profiling, in vivo coenzyme utilization of xylose reductase and potential bottlenecks in the xylose to ethanol conversion could be successfully identified.

B2-05

Metabolic model of penicillium chrysogenum

Stephan Pabinger
Institute of Genomics and Bioinformatics, TU Graz

A genome-scale metabolic model of the mold Penicillium Chrysogenum will be extremely useful for developing strategies to increase the production of penicillin. By combining the annotated genome sequence, available literature and established models of related organisms a catalog of all metabolic reactions is created. This catalog can be used to interpret transcription data, identify regulatory features and improve the gene annotation.

B3 Biocatalysis and bioorganic chemistry

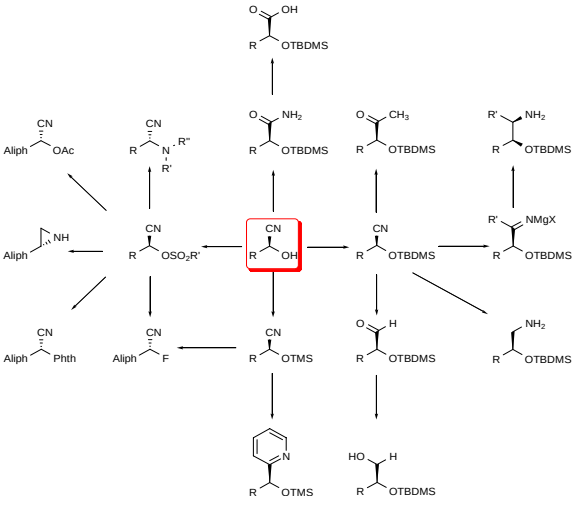
organized by: Kurt Faber (KFU)
Wolfgang Kroutil (KFU)

B3-01

Heterogeneous catalysts and enzymes for the synthesis of cyanohydrins

Ulf Hanefeld
Department of Biotechnology, Biocatalysis & Organic Chemistry, TU Delft

Cyanohydrins are versatile building blocks in Organic Chemistry. Their catalytic synthesis applying heterogenous catalysts and enzymes will be discussed. Due to their rather low stability cyanohydrins should be converted or protected immediately. New approaches and strategies for the successful application of catalysts will be demonstrated.



B3-02

The use of oxidoreductases for biocatalytic oxyfunctionalization

Andreas Schmid, Bruno Bühler, Katja Bühler, Lars M. Blank
Larboratory of Chemical Biotechnology, Faculty of Biochemical and Chemical Engineering, TU Dortmund

Oxidoreductases catalyze a large variety of selective oxyfunctionalization reactions, which are important in industrial organic synthesis but difficult to achieve by chemical means. Examples showing high productivities for alcohol, epoxide, aldehyde, and acid synthesis and critical factors in the application of these complex enzyme systems will be discussed.

B3-03

Sweet temptation. From structure-function relationships of disaccharide phosphorylases to application in synthesis

Christiane Gödl, Thornthan Sawangwan and Bernd Nidetzky
Institute of Biotechnology and Biochemical Engineering,
TU Graz

In terms of annual tons of product, the largest enzymatic processes used in industry are transformations of carbohydrates. Rate accelerations on the order of 10^{15}-fold and ability to distinguish between multiple hydroxyl groups on the substrate are special hallmarks of enzyme catalysis in the conversion of sugars.
Structure-function relationship studies and potential applications in biocatalytic synthesis of a special group of carbohydrate-processing enzymes, the disaccharide phosphorylases, are presented.

B3-04

Towards novel oxygenase-type reactions catalyzed by the atypical, 3-His ligated, nonheme Fe(II) centre

Grit Straganz
Institute of Biotechnology and Biochemical Engineering,
TU Graz

The impressive synthetic-catalytic potential of metal dependent nonheme Fe (II) oxygenases makes them a promising resource for biocatalysts and poses the question, how new reactivities can be created. Here we report the discovery and engineering of novel reaction pathways by taking advantage of the intrinsic promiscuity of the monomuclear nonheme Fe(II) centre.

B3-05

New approach for racemisation based on „catalytic promiscuity“

S.M. Glück[a,b], A. Bodlenner[a,b], B.M. Nestl[a,b], C.C. Gruber[a], N. Baudendistel[c], B. Hauer[c], W. Kroutil[a], K. Faber[a]
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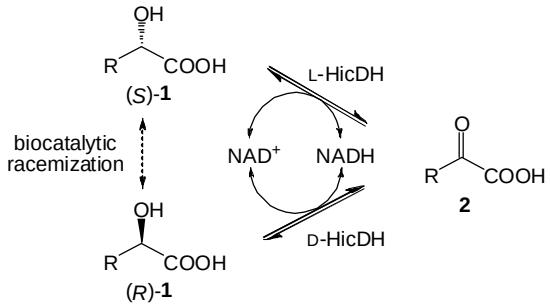
[c]BASF AG, GVF/E-B9, D-67056 Ludwigshafen, Germany

Biocatalytic Racemisation is a powerful tool and the key to dynamic resolution by recycling the non-reacting enantiomer in kinetic resolution processes. A novel approach based on the 'catalytic promiscuity' of enzymes was developed. This concept was successfully applied for the racemisation of α-hydroxycarboxylic acids employing a matching pair of stereocomplementary α-hydroxyisocaproate dehydrogenases (L- and D-HicDH).



HicDH = α-Hydroxyisocaproate Dehydrogenase

B3-06

NMR protein structure determination using paramagnetic restraints

Klaus Zangger
Department of Chemistry, Organic & Bioorganic Chemistry, KFU Graz

NMR spectroscopy has developed into one of the principal methods in structural biology for determinations of the three-dimensional structure of proteins. Currently proteins from various sources are investigated in the BioNMR group at the IfC: bacterial toxins and antitoxins, proteins involved in bacterial conjugation, allergens or an S-layer protein.

B4 Quantum physics in the femto- and nano-world

organized by: Christof Gattringer (KFU)
Wolfgang von der Linden (TU)

B4-01

From quantum spins to emergent field theories

Uwe-Jens Wiese
Institut für theoretische Physik, University Bern

The collective condensed matter physics of discrete quantum spins gives rise to effective continuous classical fields whose dynamics resembles those of particle physics. Using efficient cluster algorithms the physical properties of quantum spin systems can be calculated using Monte Carlo simulations. They agree quantitatively with analytic effective field theory predictions.

B4-02

Quarks and gluons: functional approaches

Martina Blank
Institut für Physik, KFU Graz

Quarks and gluons are fundamental constituents of matter which build up all strongly interacting particles. It will be described how specialized mathematical and numerical techniques, so-called "functional approaches", are applied to the strong interaction to describe physics at the femtometer scale.

B4-03

Quarks and gluons on a space-time grid
Daniel Mohler
Institut für Physik, KFU Graz

Although the fundamental equations that describe quarks and gluons are known, the properties of matter that emerge from these equations are not understood in all detail. A modern approach to some of the unsolved problems is to replace continuous space-time by a 4-dimensional grid, a formulation which also allows for numerical simulations. Recent results from this approach are presented.

B4-04

Strongly correlated materials: effects and simulations
Ralf Gamillscheg
Institut für Theoretische Physik - Computational Physics, TU Graz

So-called strongly correlated materials show very interesting phenomena like superconductivity and unconventional phase transitions. Other related systems are coupled photonic cavities, which exhibit novel quantum effects of light. In this talk some examples of physical properties of these materials and computational methods will be presented.

B4-05

Electron correlations in spintronic materials
Hannes Allmaier
Institut für Theoretische Physik - Computational Physics, TU Graz

Future state of the art devices like quantum computers or spin-field effect transistors are developed and built using the fundamental aspect of spintronics, that is that not only the charge but also the spin of the active materials is manipulated. In many cases these favourable properties come at a cost being inherent electron correlation effects that pose new problems. In this talk an introduction in this fascinating area of physics will be given.

B5 Polymer science

organized by: Franz Stelzer (TU)

B5-01

Polymeric materials- from laboratory to technological applications
Franz Stelzer
Institute für chemische Technologie von Materialien
TU Graz

B5-02

Isasomes in thermo-reversible polysaccharide hydrogels
Otto Glatter (a)
M. Tomšic (a,b), C. Kulkarni (a),
S. Guillot (a,c), L. Sagalowicz, (d), M. E. Leser (d)

(a) University of Graz, Department of Chemistry, Austria
(b) University of Ljubljana, Faculty of Chemistry and Chemical Technology,
Slovenia.
(c) Centre de Recherche sur la Matière Divisée, Université d'Orléans, France.
(d) Nestlé Research Center, Department of Food Science, Switzerland.

Self-assembled thermo-gelling emulsions were developed by blending internally self-assembled particles (ISAsomes) with thermo-reversible polysaccharide hydrogels of methylcellulose (MC), k-carrageenan (KC), and their 1:1 mixture.
In this way the hierarchical structure of ISAsome samples was successfully promoted yielding a highly stable colloidal systems allowing for a simple temperature tuning of the sample appearance(gel/sol) as well as the internal self-assembled structure.

B5-03

Properties and utilisation of cellulose model surfaces from ionic liquid solutions
Rupert Kargl
Department of Chemistry
KFU Graz

Cellulose model surfaces with a thicknesses in the nanometer-range where prepared from solutions in the ionic liquid ethylmethylimidazolium acetate (EMIMAc). The films where characterized according to their thickness, surface roughness, elemental composition and swelling behavior. Beside the characterization, a proof of principle study for the utilization of the films as a sensor support was performed.

B5-04

Hybrid photovoltaic cells via a novel direct route
Eugen Maier
Institute for Chemistry and Technology of Materials
TU Graz
Eugen Maier (a), Thomas Rath (a), Alejandro de Santis (a), Michael Edler (a), Achim Fischereder (a), Christopher Fradler (a), Wernfried Haas (c), Ferdinand Hofer (c), Gernot Mauthner (b), Sonja Larissegger (a), Dorith Meischler (a), Andreas Pein (a), Robert Saf (a), Roman Trattnig (b) Franz Stelzer (a), Emil List (b) and Gregor Trimmel (a)

(a) Institute for Chemistry and Technology of Materials (ICTM),Graz University of Technology, (b) NanoTecCenter Weiz Forschungsgesellschaft mbH, A-
(c) Institute for Electron Microscopy of the TU Graz (FELMI),

Within the field of plastic photovoltaics, hybrid solar cells are an interesting alternative to p. e. fullerene based devices, as photon harvesting also occurs in the acceptor phase.
In this contribution a novel method to obtain semiconducting organic – inorganic nanostructured composite layers is presented. As prepared blends are utilized as active layers in hybrid photovoltaic devices.

B5-05

CePoL updates
Robert Saf
Institute für chemische Technologie von Materialien, TU Graz