On 5 February 2003, at their meeting in Tartu
Centres of Excellence of Estonian Science
decided to act concertedly and to issue an omnibus volume
“CENTRES OF EXCELLENCE OF ESTONIAN SCIENCE. 2004”
describing the research areas of their Association

This collection is the outcome of a joint effort by Heads of all Centres

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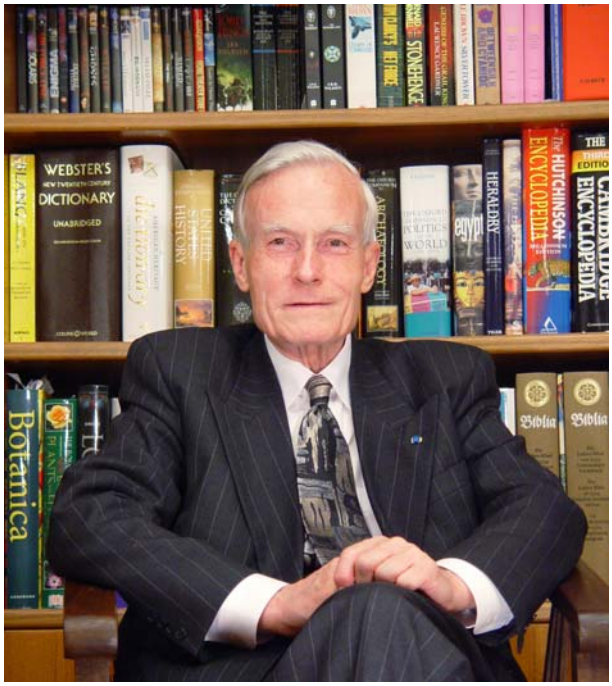
PREFACE



Academician Endel Lippmaa
Head of the Association of the Centres
of Excellence of Estonian Science

The need for theoretical erudition is frequently blatantly underrated, and mostly by those, whose resources in theoretical knowledge are somewhat sparce.

Academician Karl Schlossmann
at the inauguration ceremony
of the Estonian
Academy of Science
on 23rd October 1938

Estonia is too small a country to shape on our own the global developments and our political and technological destiny. Contemporary science and technology are both global and advance at an ever-increasing pace. The underlying momentum rests not just with some ingenious designs, but first and foremost upon breakthroughs in basic research. All real advances in basic scientific insight always find practical applications that are important for all of us. For this very reason the peak of the pyramid of knowledge forms the real basis for all novel applications, technological development and buoyant economy. The stylish multimedia, mobile communications, internet and all the modern computers and automatics would not exist at all without quantum mechanics that at first was branded as incomprehensibly contradictory, brazenly theoretical, or just irrelevant. And although no century ever repeats the past, the basic gist of progress remains the same. Some prevailing motifs of the future to come are just shaping up, such as pure hydrogen/fusion energy, global supercomputing, the molecular mechanisms of thought and consciousness, picotechnology, quantum informatics, and physics of the vacuum itself.

In order to fully understand and successfully apply the new openings and technological challenges, and for finding our own niches for their innovative development, the highest possible level of the scientists and engineers involved is needed. This cannot be achieved just by juggling the flow of monies by fund managers. All, but first of all the technology-related projects and programmes must be chosen and evaluated by fully competent and completely independent international panels. The ten centres of excellence of Estonian science were chosen along these lines. Some

applicants were site visited and profoundly evaluated by no less than six completely independent and fully external international panels. For this very reason the chosen centres of excellence combine the real scientific talent presently available in Estonia with a clear understanding of the internationally accepted ideas and priorities in science, research and development.

The current activities in the ten centres of excellence cover a wide spectrum of knowledge from vacuum to folklore. It includes the Estonian strategic guidelines in information technologies, biomedicine and biotechnology, and materials science with nanotechnology. The level of scientific ability is undisputably high and allowing real contacts and collaboration with leading research centres and companies of the world in optics and spectrometry, in high energy and condensed phase physics, in cell biology and genomics, in nonlinear dynamics and mechanics, in information technology, in quantum chemistry and solid state physics, in molecular medicine and psychophysiology, and naturally in Estonian ecology and folkloristics.

Considering the wide scientific coverage, the level of competence of the scientists involved and the guiding influence of the steering committees of world-renowned scientists in all the centres, the summary influence of the centres in providing consultations, coordination and sometimes counselling can be significant. This is particularly true in the formation of new development strategies of Estonian science and technology as well as for the pertinent educational and economy-related plans.

For all this the Centres of Excellence of Estonian Science formed at their 5th February 2003 meeting in Tartu the Association and we hope that this directory as a compilation of short descriptions of current research in progress can provide an adequate outline about some future potentialities of Estonian science.

In Tallinn 18th July 2004

Endel Lippmaa

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The Centre of Excellence for Gene and Environmental Technologies (CGET) is an institution for research and technological development carrying out cutting-edge fundamental research in molecular and cell biology and developing technological applications in the fields of gene and environmental technologies. The centre achieved the status of the Estonian National Centre of Excellence conferred by the Estonian Ministry of Education and Research in December 2001.

The centre is organized on the basis of the existing laboratories of the Institute of Molecular and Cell Biology of the University of Tartu, Tartu University's Centre for Technological Excellence (departments of Gene and Environ-

mental Technologies; (at present Tartu University's Institute of Technology) and the Institute of Zoology and Hydrobiology of Tartu University. The CGET embraces 10 research groups, the youngest of them – Bioinformatics – was created only at the beginning of 2003.

As regards research and technological development the CGET closely collaborates with the University of Tartu on teaching and training the students at both undergraduate and postgraduate levels. The centre has close relations also with the Estonian Biocentre sharing partly the same premises, equipment and library. The research groups involved in the centre publish about 50 peer-reviewed scientific articles annually. The centre recruits a research staff of 67, the number of graduate students is 115.

Research sums allocated to the centre per years (in Estonian crowns: 1 Euro=15.65 Estonian crowns): 2001 – 666 500, 2002 – 666 500, 2003 – 2 150 000 2004 – 3 193 000 EEK.

Defended MSc and PhD degrees: in the launching year of the centre (2001) 11 MSc and 2 PhD degrees were defended; in 2002 the respective numbers were 12 MSc degrees and 1 PhD degree. Within the year 2003 16 MSc and 6 PhD degrees were awarded.

BIOINFORMATICS

The bioinformatics group started in February 2003. In September 2003 the group moved into new premises at Riia Street 23, Tartu.

The group has focused on the following research topics:

MODELLING OF HAPLOTYPE STRUCTURE OF THE HUMAN GENOME

Understanding the haplotype structure of the human genome is required for association studies as well as for understanding evolutionary forces shaping the genome. We develop new methods for efficient and universal informative marker (tagSNP) selection from the human genome. Understanding the structure of human genome allows to develop new methods for large-scale association studies. We are working on multipoint analysis methods that would allow whole-genome analysis in order to detect genetic basis of human diseases.

DESIGN OF DNA MICROARRAYS

DNA arrays are used for different genomics studies. Under this topic we have developed and improved algorithms for selection of primers and hybridisation probes for different types of microarrays – for example genotyping microarrays (APEX) and microarrays for detection of gene dosage (MAPH). Additionally, methods for automatic design of high quality PCR primers and automatic grouping of PCR primers have been developed. We are planning to investigate methods for designing microarrays for species identification.

MODELLING OF GENE REGULATION NETWORKS

Gene regulation is studied *in silico* by collecting and merging large datasets about gene expression, protein-protein and DNA-protein interactions. The database is used for construction and analysis of gene regulation networks. New methods for pattern discovery and fast clustering of biological data are being developed. One of the EU supported projects is aiming to study regulation of alternative splicing using pattern discovery methods.

The research on these topics is headed by Prof Maido Remm and Dr Jaak Vilo. The bioinformatics group has extensive collaboration with ot-

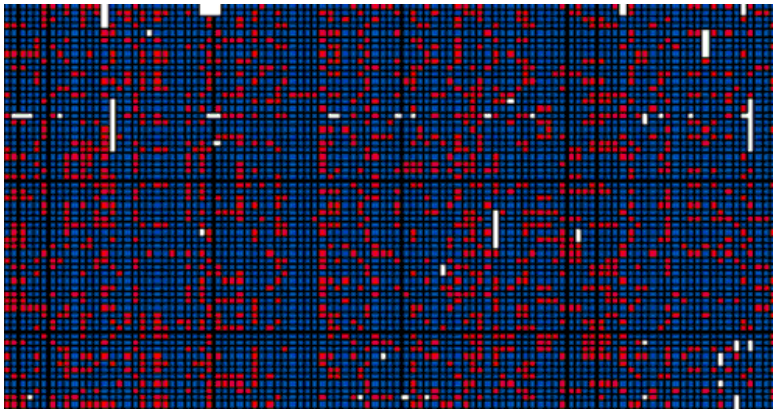

Fig. 1.
Haplotype patterns in the human chromosome 22. Individual DNA samples are in rows, different markers along chromosome 22 are shown in columns. Full dataset contained 60 rows and 1204 columns. Blue and red dots mark different alleles of analysed markers. The extent of linkage disequilibrium was analysed computationally and compared in different chromosomal regions and in different populations.
Dawson et al. (2002) Nature 418: 544.

her research groups in Europe (European Bioinformatics Institute, The Sanger Institute, München Technical University, University of Helsinki, Karolinska Institute).

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BIOCHEMISTRY

We are interested in understanding molecular processes of mitochondrial DNA metabolism in budding yeast *Saccharomyces cerevisiae*. We employ a combination of biochemical and yeast genetics tools to study the factors determining maintenance of the mitochondrial genome.

Mitochondrial DNA metabolism is not strictly controlled by the cell cycle S phase. What are the mechanisms, coordinating mitochondrial DNA synthesis and cell growth and division, is largely unknown. Mitochondrial genome of the yeast in a monomeric form is approximately 80 kb long. However, monomeric mitochondrial DNA form is present only in minor amounts. Largely the mitochondrial DNA forms a heavily branched high molecular network in which recombination has an active role to play. We are interested in understanding how is the DNA synthesis initiated in this system, what is the mechanism that ensures the approximately constant level of the mitochondrial DNA per cell and how is the branched DNA network correctly divided between the mother and emerging daughter cells.

In order to understand the role of different gene products in mitochondrial DNA metaboism, we have introduced various 2 dimensional gel analysis methods that allow us to analyze the topology of complex mixtures of mitochondial DNA molecules.

We have also purified several individual protein factors involved in mitochondrial DNA metaboism and pursued their biochemical analysis in order to better understand their role in mitohondia. Currently we are mainly focused on the role of two helicase proteins Hmi1p, and Pif1.

Research staff: prof Juhan Sedman (PhD), scientists Priit Jõers (MSc), Silja Kuusk (MSc), Tiina Sedman (MSc).

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BIOTECHNOLOGY

The main interest of the biotechnology laboratory lies in human genome structure, organization and genes responsible for complex diseases. The research is financed by a Core Grant from the Estonian Ministry of Education and Research, research grants from the Estonian Science Foundation and EC FP5 and FP6 grants.

We are working in two main research areas and two smaller subtopics led by senior scientists.

GENE ANALYSIS TECHNOLOGY group – (Prof Andes Metspalu, MD, PhD and Assoc. Prof Ants Kurg, PhD) is developing a new high throughput genotyping technology (APEX) that enables to analyze up to 30 000 SNPs per individual. There are also other applications, like the determination of gene copy number, etc. The research activity involves the development of a new microarray fluorescence detector together with our partners in Estla and Asper Biotech. We have received a new gene analysis instrument GeniomOne (FeBit, Germany) to implement the new microarray technology enabling *in situ* oligo synthesis.

HUMAN GENOME ANALYSIS – (Prof Andres Metspalu MD, PhD) aims to conduct studies on haplotype structure in the human genome and compare it with different populations in Europe and elsewhere. The main goal is to find SNP markers for high throughput association studies (incl. longevity, obesity, depression) and pharmacogenomic analysis. The group is also working with some new human genes (e.g. HUBERT) trying to find their function.

Smaller topics:

- Proteomics – Dr Siiri Altraja, PhD, is analysing proteins associated with airway remodelling.
- Molecular diagnostics – project is led by Dr Andres Salumets, PhD. The main goal is to develop new gene tests, noninvasive methods for prenatal DNA analysis incl. the isolation and analysis of fetal cells from maternal blood.

In addition to the abovementioned projects the biotechnology group has a close collaboration with an independently financed (by The Wellcome Trust) research unit led by an associate professor Maris Laan, PhD. The unit is working with several new population genetics projects which main objective is to understand the formation of the linkage disequilibrium in the human genome.

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EVOLUTIONARY BIOLOGY

The research carried out at our group tries to give answers to a range of very general questions, at the heart of which lies the understanding of the foundation and richness of the human genetic pool. We thereby study the demographic processes that accompanied the exodus of anatomically modern humans from Africa. As geneticists we predominantly investigate the global variability of human maternal and paternal lineages, human mtDNA and Y-chromosome, that is. We analyze the genes of native people from all the inhabited continents – from Estonians and other Europeans, ethnic groups of Siberia, Hindus and Chinese to Sub-Saharan Africans, Australian Aborigines and Native Americans of South America.

The phylogenetic reconstruction of gene trees and the derived dating (coalescence time) of the branching points give us the experimental data, interpretation of what is interdisciplinary – in-volving integrated knowledge on archaeology and history in general, nature of stochastic processses, topology, linguistics, paleoanthropology and paleoclimatology, etc.

Inherently, this kind of research can only be successful in tight contact and direct collaboration with scientists all over the world representing most different disciplines.

In the end of 2003 our group consists of seven researchers and lecturers, five PhD students and seven masters students. About 10 undergraduates are currently obtaining their first experimental and theoretical skills at our lab. Above that, there is a constant flow of 3–6 young guest researchers from various countries which include for instance Tuvinians, French, Portuguese, Jakuts, Croatians, Israelis, Swiss and Russians.

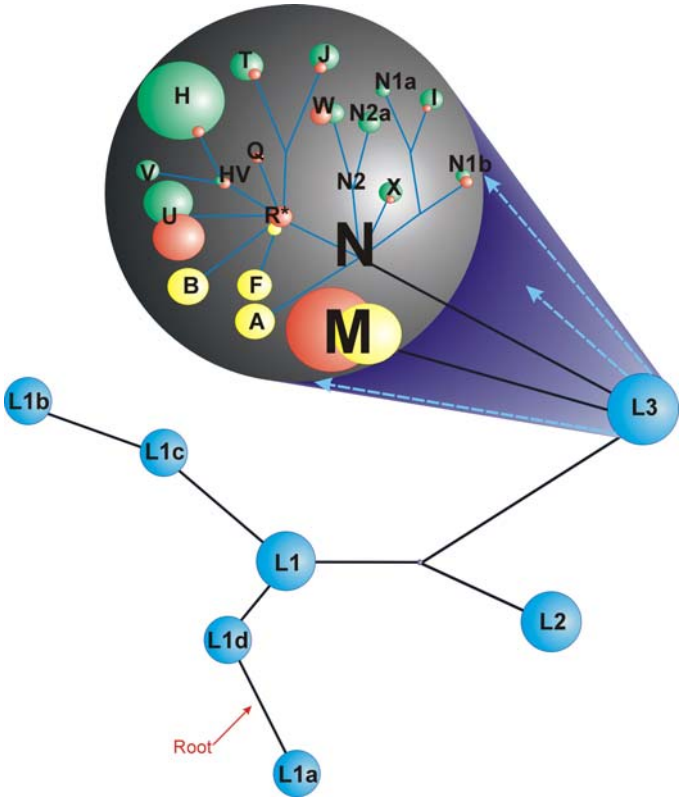

Fig. 2.
Depicts the general backbone of the global human mtDNA tree(adapted from Kivisild et al. 1999). Colours of spheres indicate population groups as follows: blue – Africans; yellow – east Asians and native Americans; red – Indians and green – western Eurasians. The diameter of the sphere depicts the relative frequency of the haplogroup. Note that all non-African lineages arise from two lineages M and N which in turn branch from a single African mtDNA cluster.

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FUNCTIONAL GENOMICS

RESEARCH AREA

The application of molecular biology has been a major technological advance which enables long-standing questions to be revisited with greater powers of resolution.

This approach involves the generation of new mutants in the mouse germline by homologous recombination in embryonic stem cells to mutate candidate genes. Our main focus is on transcription factors (e.g. GATA2 and GATA3) and their target genes which are involved in the development of the urogenital- and nervous system.

Transcription factor GATA3 plays essential role in multiple developmental processes. We have demonstrated a novel role for GATA3 during early steps of kidney and genital tract embryogenesis. GATA3 is expressed in the Wolffian duct-derived epithelia, and in GATA3-deficient ($GATA3^{-/-}$) mouse embryos, the Wolffian duct is misguided during its caudal elongation (Fig. 3). cDNA microarray hybridisation experiments were performed with the RNA extracted from the wild type and $GATA3^{-/-}$ embryos. As a result we identified over 100 genes that were differentially expressed in the wild type and $GATA3^{-/-}$ mouse embryos.

Mutant mice were constructed where into ric-8 locus reporter gene lacZ was inserted. Ric-8 (synembryn) was detected in CNS at different developmental stages.

Several Pax2+/-Pax8+/- mice double-mutants were constructed, which male and female animals were non-fertile due to their urogenital abnormalities. There were also successfully created new transgenic mice for Cre/loxP-mediated mutagenesis.

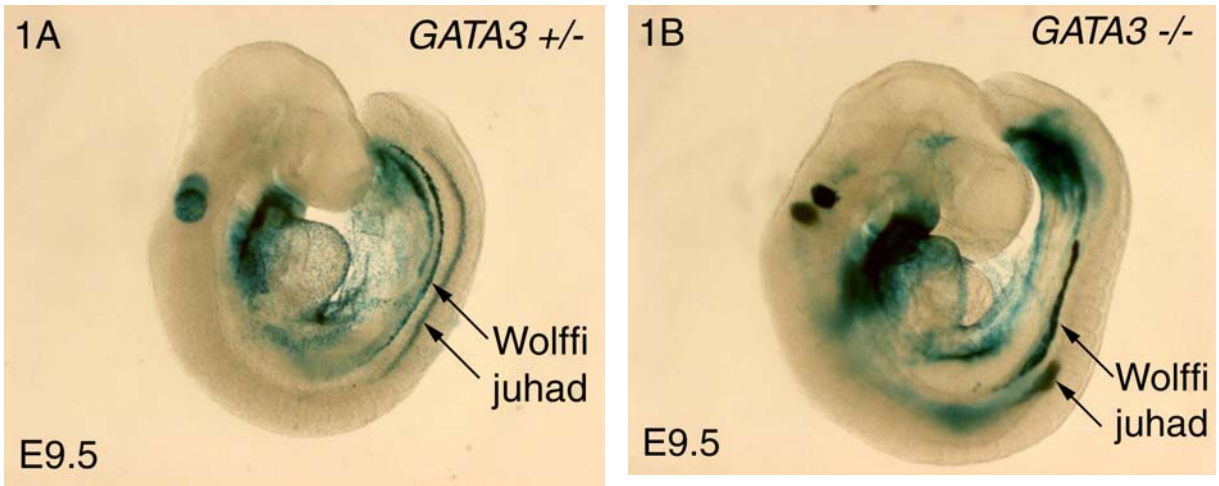

Fig. 3.
(A)The Wolffian duct, marked by lacZ expression, is actively extending caudally in E9.5 GATA3 heterozygotes (arrows). (B) In E9.5 $GATA3^{-/-}$ mutants, extension of the Wolffian duct has terminated.

The "knock-outs" of different genes frequently die early in embryogenesis. The problem can be resolved by using cell-penetrating peptides, as cargo for PNA into the cells. These complexes are also very useful to combine classical "knock outs" and "knock-downs" with PNA to down-regulate simultaneously several genes.

The research staff consists of Prof Alar Karis, PhD; Prof Jüri Kärner, PhD, DSc; senior scientist Illar Pata, PhD; senior scientist Margus Pooga, PhD; associate Prof Raivo Raid, PhD. In addition 2 scientists, 6 PhD students, MSc and undergraduate students are involved in the work of our group.

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GENETICS

MOLECULAR MECHANISMS OF GENE REGULATION AND GENETIC DIVERSITY IN CHANGING THE ENVIRONMENTAL CONDITIONS (supervisor Prof Ain Heinaru)

The main subject of the present project is to verify the ecological impact of genetically characterized and engineered bacteria on biodegradation and bioremediation of organic contaminants in the environment. Laboratory and field experiments were carried out in order to test the effect of phytoremediation and bioaugmentation for remediation of organic pollutants in semi-coke. For bioaugmentation experiment the set of bacteria consisting of three biodegradative strains isolated from nearby area was selected. Several molecular microbiological methods including PCR-DGGE were used to assess and compare the microbial community structure and diversity as well as the presence and diversity of biodegradative genes in collected samples. The dominant bacterial species based on 16S rDNA sequences in semi-coke samples were also identified. These analyses revealed that semi-coke microbial community is characterized by few dominant populations and possesses low diversity. The phytoremediation increased the number of bacteria and diversity of microbial community in semi-coke. In plots with plants dominated two different multicomponent phenol hydroxylases (LmPH) belonging to low- and moderate K_s kinetics groups indicating more active biodegradation of phenolic compounds. Bioaugmentation increased biodegradation intensity of oil products up to 50% compared to untreated controls. We also assessed microbial community structure of sediments from water bodies polluted by semi-coke dump area leachate. We also continued research of catabolic pathways determining the sequential decomposition of phenolic compounds in mixed substrate cultivations in pseudomonads. In Estonia we have isolated the bacterium *Achromobacter xylosoxidans subsp. Denitrificans* strain EST4002 containing a plasmid pEST4011 which encodes genes for degradation of 2,4-dichlorophenoxy-acetic acid. The total nucleotide sequence of the 76623 bp plasmid pEST4011 has been determined.

Research staff: scientists Eva Heinaru, Jaak Truu, Ene Talpsep, Eve Vedler, Signe Viggor, 2 PhD studens and several graduate and post-graduate students.

PHYSIOLOGICAL AND GENETIC ADAPTATION OF PSEUDOMONADS TO A NEW ENVIRONMENT (supervisor Assoc. Prof Maia Kivisaar)

In nature microbes are constantly exposed to variable and stressful environments and this leads to rapid adaptation of microbial populations to new environments. The adaptation of bacteria may either be physiological which is short-term strategy or genetic which generates new variants in populations resulting in micro-

bial diversity. An idea that molecular mechanisms controlling mutation dynamics may have evolved to increase the rate of mutation under the environmental stress has stimulated intense scientific debate.

We are studying molecular bases of mutagenic processes in *Pseudomonas* bacteria by concentrating on mechanisms that allow genetic adaptation of microbial populations under the environmental stress. Our results provide evidence that stress-induced transposition can be genetically programmed strategy to enhance genetic adaptation of microbial populations under harsh environmental conditions. We have found that transposition of Tn*3* family transposon Tn*4652* (originated from TOL plasmid pWW0) is exclusively stationary-phase-specific event, regulated by DNA-bending protein Integration Host Factor (IHF) and stationary-phase sigma factor σ^S (Ilves et al., 2001). Additionally, transposition of Tn*4652* is regulated by some, yet unknown signals, mediated by two-component signal transduction system ColRS. Our current studies are focused on further characterisation of stress-induced regulatory network controlling frequency of transposition in *P. putida*.

Results of our recently published study suggest that mutation processes in cells that have been starving for a short period are not entirely compatible with those for a prolonged starvation. It appeared that the spectrum of stationary-phase mutations among early-arising mutants differed from that of late-arising ones. Point mutations occurring in stressed cells can be stimulated by mechanisms that possibly involve increased mutation rates (induction of error-prone DNA polymerases, inefficiency of DNA repair systems). We have observed an increase in a frequency of occurrence of certain type of mutations (1-bp deletions but not base substitutions or other deletions) in bacterial populations that have been starved for a long period. The increase in a frequency of such mutations became apparent only in starving *P. putida* cells carrying functional error-prone DNA polymerase pol IV. Study of involvement of other DNA polymerases on stress-induced mutagenesis in *Pseudomonas* is currently in progress. We are also going to study the efficiency of major DNA repair pathways (MMR, GO, NER) in *Pseudomonas* under stressful conditions.

One part of our research is focused on studies of physiological adaptation of bacteria to different growth conditions. We are investigating molecular mechanisms which control transcription of genes encoding phenol and benzoate degradation pathways in *P. putida*. We have shown that growth media composition strongly influences expression of phenol degradation pathway: transcription of the pathway-encoding genes is repressed in rich-medium-grown bacteria but rapidly induced under stressful conditions. Our next studies in this field are focused on research how a metabolic status of cells would affect the activity of enzymes influencing cellular amount of inducer of the operons and how the transport of phenolic compounds is regulated.

This work is supported by grants from the Estonian Science Foundation and by Howard Hughes Medical Institute (HHMI) International Research Scholars Program grant. The research staff consists of associate Prof Maia Kivisaar (PhD); senior scientist Rita Hõrak (PhD); 3 scientists Andres Tover (MSc), Riho Teras (MSc) and Heili Ilves (MSc); PhD student Signe Saumaa (MSc); 3 MSc and 9 undergraduate students.

STUDY OF NOVEL BIOTECHNOLOGICALLY APPLICABLE PROMOTERS AND GLUCOSE REPRESSION IN METHYLOTROPHIC YEASTS (supervisor Assoc. Prof Tiina Alamäe)

Methylotrophic yeasts *Hansenula polymorpha, Pichia pastoris* ja *Candida boidinii* are used as hosts for the heterologous expression of various genes producing biotechnologically important products such as vaccines, enzymes etc. Expression cassettes mostly use strong and regulated promoters of methanol-specific genes. We have studied molecular biology and biochemistry of the utilization of disaccharides in *H. polymorpha*. We have cloned and sequenced the maltase gene of this yeast and have shown that its promoter has very promising properties from the aspect of biotechnology. According to our data the promoter of the maltase gene of *H. polymorpha* can potentially be used in expression cassettes to be tested in different hosts. We will go on with the study of the promoter to specify conditions allowing maximum expression from the promoter and compare its strength and regulation with those of some other promoters. We are also interested in glucose repression mechanisms in *H. polymorpha*. We have shown that glucose signaling in *H. polymorpha*, although mediated by glucose-phosphorylating enzymes, should be different from that described in baker's yeast.

Research staff: Tiina Alamäe, PhD (group leader), Helen Udras (PhD student).

REGULATION OF VIRULENCE FACTORS EXPRESSION IN BACTERIAL PATHOGEN ERWINIA CAROTOVORA
(supervisor Assoc. Prof Andres Mäe)

We are studying the interaction between the nonspecific bacterial phytopathogen *Erwinia carotovora* and host plant. It has a wide host range, attacking a number of plant species if the conditions are favorable. The virulence of this pathogen is dependent on the production of a large arsenal of plant cell wall-degrading enzymes also called virulence factors. Many of the virulence factors appear to play dual role in Erwinia-plant interaction: in addition to being virulence factors they also induce plant defence responses. The importance of plant cell wall-degrading enzymes production to the virulence of *Erwinia carotovora* and its very tight regulation encouraged us to look for novel virulence factors and for the possible interaction between the different regulatory systems controlling their expression. The resistance to pathogen infection is usually characterized by very rapid activation of defence genes in plant cell. The focus of this initiative will be on characterization of the unknown virulence factors of *Erwinia carotovora*, characterization of their regulation and their role in induction plant defence response. To be able to devise new strategies for the control of plant pathogens and to develop disease resistant crop plants, understanding of the molecular mechanisms of plant-pathogen interaction is a prerequisite. For these studies *Erwinia*-plant interaction provides an excellent model system for studies of plant response to nonspecific pathogens.

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MICROBIOLOGY AND VIROLOGY

The research group which has gathered around the Department of Microbiology and Virology, Institute of Molecular and Cell Biology, Tartu University has been focused on the study of the life cycles of different viruses. Specifically, the animal and human papillomaviruses, Epstein-Barr virus, Semliki Forest Virus (SFV), Hepatitis C Virus and Human Immunodeficiency Virus type 1 (HIV1) have been studied extensively. We have mainly studied the molecular mechanisms of the replication of the viral genomes during the different phases of the life cycle.

We have identified the molecular mechanism of partitioning and segregation of the episomal genomes of the papillomaviruses. This biological function is provided by the viral E2 protein ability for mitotic chromatin attachment and tethering of the viral genomes to the mitotic chromatin. This results in the co-segregation of the viral genomes with the cellular chromosomes into the daughter cells.

Analysis of the papillomavirus replication revealed that tumour suppressor protein p53 is involved in the regulation of the papillomavirus amplificational replication at the initial stages of the establishment of infection.

The studies of the SFV replication machinery led to several significant results. First, the mechanism of SFV polyprotein processing and biogenesis of functional SFV NA replicase complex was studied in detail (article and attached figure). It was demonstrated that the well coordinated and timely regulated processing pathway is the only way of formation of the functional structures.

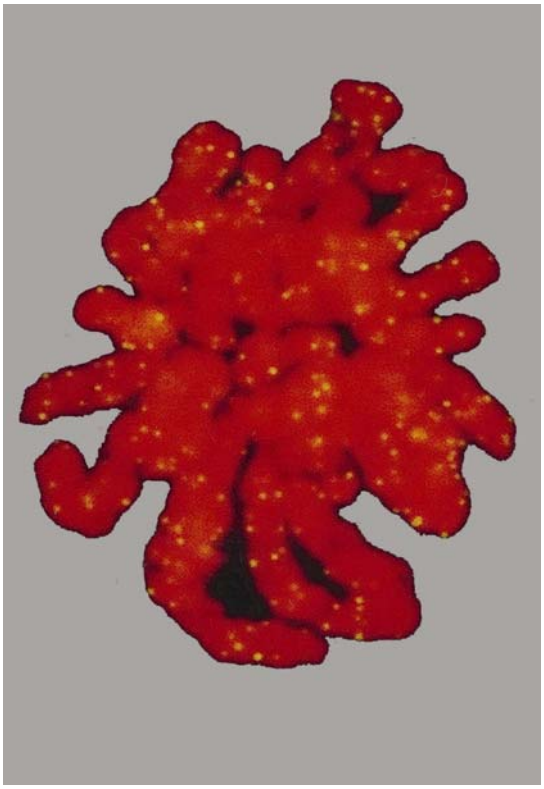

Fig. 4.
JVI 1262-03**.** Localisation of Bovine Papillomavirus type 1 (BPV1) E2 protein on the mitotic chromosomes in CHOBgl40 cell line constitutively expressing E1 and E2 proteins and maintaining extrachromosomally BPV1 URR containing plasmid. E2 is visualized by immunofluorescence analysis and appears as yellow dots on the background of propidium iodide counterstained mitotic chromosomes (red).

Second, number of ts-mutations, affecting SFV replication were mapped in SFV genome. The biological effects of these mutations on SFV replication and functions of SFV encoded proteins are under investigation.

Third, studies of the enzymatic activities of SFV encoded non-structural protein led to identification of different mechanisms how the enzymatic activity is regulated. This, in turn, leads to construction of the multifunctional expression systems based on these elements.

INTERNATIONAL GRANTS

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EU 5-th Framework grant "Semliki Forest virus based therapeutic systems".

The Wellcome Trust Senior Research Fellowship "Alphavirus genomes as models and tools for studies of RNA replication, virus-cell interactions and virus induced pathogenesis of positive strand RNA viruses".

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MOLECULAR BIOLOGY

Biosynthesis, degradatation of nucleic acids and proteins as biological macromolecules and regulation of these processes is studied both in eukaryotic and procaryotic systems. The field is fundamental science. The group lead by Dr Jaanus Remme is involved in studying protein biosynthesis. Main objects are bacterial ribosome, r-proteins and rRNAs, and the genetic code. Main problems are ribosome biogenesis, in particlur ribosome assembly and ribosomal rationale for the universal genetic code. The group of Dr Tõnis Örd studies molecular mechanisms of programmed cell death in neural cell lines. In particluar, functioning of caspases, a group of specific proteases.

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ANTIBIOTICS (supervisor senior researcher Tanel Tenson)

Our laboratory is studying the mechanisms of action of antibiotics. Three research directions are ongoing or will be started in the near future.

Firstly, we try to elucidate the exact biochemical mechanism of action of several ribosome targeted antibiotics. We concentrate mainly on macrolides (from which erythromycin is the most well-known example), evernimicin and chloramphenicol. We study how these antibiotics affect the ribosome and therefore inhibit

protein synthesis. In addition, we investigate how inhibition of protein synthesis influences other physiological processes in the bacterial cell. To study the mechanisms of action of antibiotics we need to know better the basic principles of protein biosynthesis. Therefore we have studied initiation of prokaryotic translation.

Our second research direction that will be started at the beginning of 2004 will involve studies on the reasons why some antibiotics are bactericidal (kill the bacterial cell) and some bacteriostatic (inhibit cell growth).

The third direction that will be started at the end of 2004 includes studies on the role of antibiotics and other microbial secondary metabolites in the natural environment.

The research directions are led by Tanel Tenson (biochemistry of ribosome targeted antibiotics), Niilo Kaldalu (the bactericidal and bacteriostatic effects) and Veljo Kisand (ecological aspects of antibiotics).

We have active collaboration with the laboratory of prof. Måns Ehrenberg at Uppsala University (Sweden). The research is funded by The Wellcome Trust, the Estonian Targeted Financing and the Estonian Science Foundation.

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CELL BIOLOGY

The cell biology group headed by Prof Toivo Maimets was founded in 1990. From the very start the main focus of the research carried on in this group concentrated on the the tumor suppressor protein p53. This protein lies in the very centre of the cell proliferation regulating pathways and the gene encoding it is mutated in over one half of the human tumors. In addition, several regulative mechanisms have been shown to inhibit the function of the p53 protein in tumors harboring normal p53 genes.

From the very beginning the transcription activation function of p53, which is considered the main biochemical property of this protein has been one of the main topics addressed in this group. In particular, regulation of this activity by the oligomeri-

zation of the p53 protein has been intensively studied.

Another topic intensively addressed in the cell biology group is the regulation of p53 activities by DNA damage. p53 is an important part of the DNA-damage sensing mechanism in the cell. In response to the DNA damage p53 becomes activated and induces or facilitates inhibition of cell cycle progression and induction of programmed cell death – apoptosis. Passage of damaged DNA containing multiple mutations and other lesions from one cell generation to another is an important mechanism of carcinogenesis. The effect of different DNA damaging agents as well as the effect of different dosage of DNA damage on p53 has been studied in the cell biology group.

The introduction of a new powerful technique – flow cytometry – into this group has made it possible to address the regulation of p53 transcriptional activation properties on a single cell level. This has led to novel understanding of transactivation by p53 – namely that p53 can function both in graded "rheostat" and in binary "on/off switch" manner.

Along with studies of the transactivation properties of p53, addressing the pathways of its activation by oncogenes has emerged as a new promising field of research in this group. In particular, the connections between p53 and a leucocytic marker CD43 are intensively studied. CD43 is thought to participate in the early stages of carcinogenesis and is activating the p53 response. This work is conducted in close collaboration with prof. G. Hansson's group in the University of Göteborg. Recently a new project was launched to study the interaction between p53 and its negative regulator Mdm2 using novel FRET (Fluorescence Resonance Enenergy Transfer) technique.

Along with the p53 research two more topics are addressed in the cell biology group. The role of TGF-β in carcinogenesis and functions of integrins in human thrombocytes are the new research areas introduced into this group recently.

The research staff consists of Prof Toivo Maimets, associate Prof Sulev Ingerpuu, senior scientist Dina Lepik, postdoctoral student Ade Kallas and scientists Viljar Jaks, Lilian Kadaja, Arvi Jõers (7 PhD); 2 PhD students Anu Sikut, Kärt Padar and scientist (4 MSc); 3 MSc students. In addition 12 undergraduate students are preparing their thesis under supervision of the cell biology group's staff.

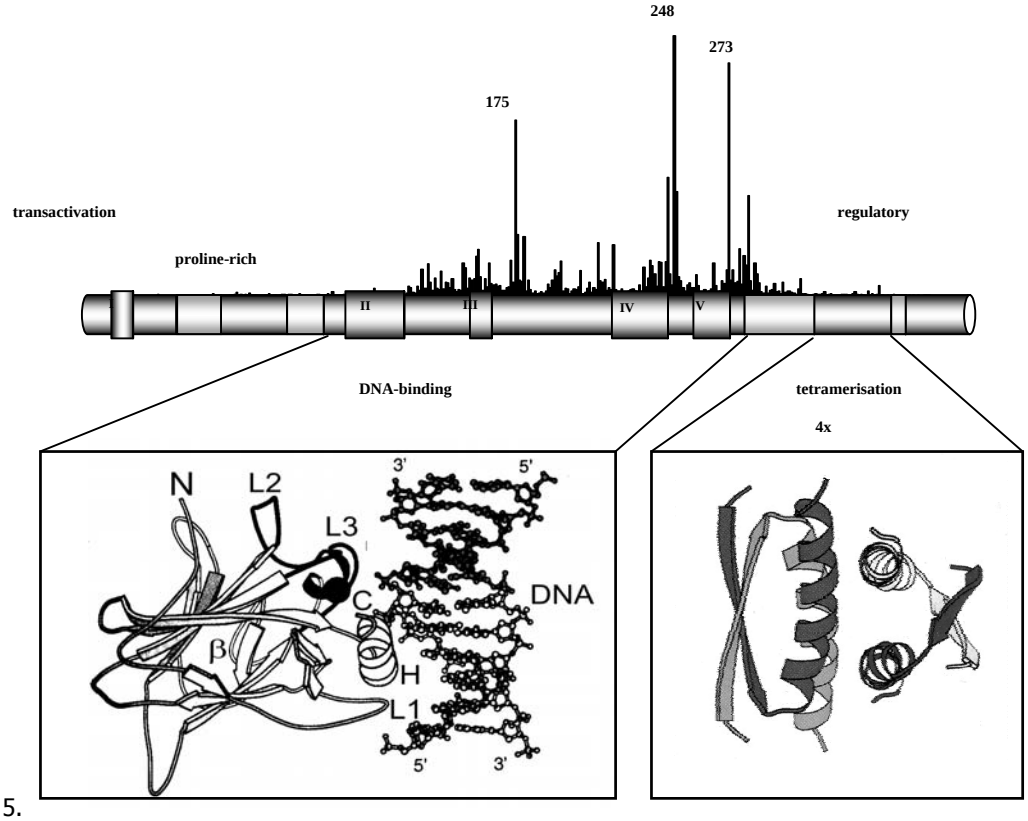

Fig. 5.
Tumor suppressor protein p53 is capable of tetramerization (by forming dimer of dimers; right insert) and specific binding to DNA (left insert) activating thereby transcription from its target genes. Majority of the mutations occurring in human cancers are localised into the DNA-binding region of p53, mainly in the evolutionally conserved domains II-V, where the most frequently affected codons are 175, 248 and 273.

This group is participating in two different EU 5th Framework programmes and is closely collaborating with groups in Helsinki and Göteborg Universities and Karolinska Institute.

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PLANT PHYSIOLOGY

In the group of plant physiology we investigate processes that determine the rate of leaf photosynthesis and its adjustment to external conditions. We use preferentially intact leaves as objects, in order to avoid artifacts from preparation. The approaches are mainly kinetic, where the external conditions are changed (e.g. light intensity, CO_2 and O_2 concentration, temperature etc.) and the responses of photosynthesis to these changes recorded. Gas exchange of CO_2 uptake, O_2 and water vapor evolution and optical signals of chlorophyll fluorescence and leaf absorptance at different wavelengths are measured. Not only steady state but also transient processes are analyzed. The whole methodology is based on self-elaborated unique apparatus. The apparatus and its parts are produced on request for other laboratories (e.g. Connecticut Agricultural Experiment Station, USA; Washington State University, Pullman, WA, USA; Umeå University, Sweden; Australian National University, Canberra).

An outstanding scientific problem is the understanding what determines the rate and capacity of the photosynthetic machinery. In large scale, the photosynthetic process may be divided into two: 1) processes of photon absorption and transformation of excitation energy into chemical energy; 2) processes participating in CO_2 uptake, fixation and reduction.

Photons are absorbed by Chl-containing antenna systems surrounding photochemical reaction centers. About 200 Chls are connected with each center. Each of them can absorb a photon, but the excitation must be transferred to the reaction center where photochemical charge separation takes place. The excitation is transported by resonance processes, but with an efficiency of less than 100%. In addition to inevitable physical processes of excitation loss, plants have developed regulatory non-photochemical excitation quenching which is activated under excess light in order to avoid uncontrolled, destructive redox processes. The exact mechanism of this type of non-photochemical quenching is unknown. One of our most interesting approaches in this field is spectral measurements, how the non-photochemical quenching depends on the wavelength of light. This work has become possible thanks to close cooperation between our laboratory and the Institute of Physics, using lasers with adjustable wavelength. Preliminary results indicate that far-red excitation (>700 nm) is quenched to a lesser extent than red. A parallel attractive problem is, how well a longwavelength photon (>680 nm) can cause photochemistry in a PSII center adjusted to 680 nm.

An important adjustment procedure of photosynthesis to varying environment is the regulation of the density (number) of photochemical centres. The two photosystems operate in sequence, PSII is splitting water and O_2 is evolved, while PSI helps to transfer these electrons to the mechanism of CO_2 reduction. We have developed two new methods for de-

An apparatus for the investigation of leaf photosynthesis using gas exchange and optical methods.

termination of the number of photochemical reaction centres. By illuminating a leaf with a very strong and short (10 μs xenon) flash all PSII centres become excited and the number of PSII centres can be determined from the amount of O_2 evolved per flash. O_2 does not evolve from PSI, but the redox changes related to electron transfer through PSI can be monitored as changes in leaf absorptance at 820 nm wavelength. Unfortunately, the 820 nm absorptance is a complex signal consiting of no less than three components. We have succeeded to deconvolute the complex signal and to separate the component describing only PSI. Now the 820 nm signal can be used for the measurement of PSI density in intact leaves and for investigation of electron transport through PSI. This achievement served a basis for following chain of logic binding the light reactions of photosynthesis to the CO_2 assimilation system.

The rate of CO_2 assimilation is determined by physical and chemical processes. Physical factors are mainly diffusion processes transporting CO_2 from external air to the active site of the CO_2 binding enzyme, Rubisco. We have developed methods for determination of the diffusion resistance on the pathway of CO_2 and found that the diffusion resistance forms about 10–30 % of the total resistance, dependent on the developmental stage of the leaf. The main resistance is of chemical character, being caused by kinetic properties of Rubisco, the CO_2 binding enzyme. Further on we succeeded in determining the actual activity of Rubisco in an intact leaf. We were surprised to find that the average turnover rate k_{cat} of an active site is slower in the leaf than it is in extracted Rubisco preparations. This was interpreted to show that in a leaf Rubisco is only partially activated. Correlating the Rubisco activity with PSI content we found a strong proportionality, with about 2 Rubisco molecules activated per PSI complex. Here we can further speculate that Rubisco is activated by the way of forming a complex with PSI via its activase. If this happens to be so then PSI is a kernel of the photosynthetic machinery that governs the light and dark reactions. The power of leaf photosynthetic machinery is proportional to PSI density. Optical methods elaborated by us allow convenently measure PSI density and use this parameter for diagnosing the state of the photosynthetic machinery in leaves.

We have already applied the above-described methods for the diagnosis of the photosynthetic machinery in birch trees gowing under elevated CO_2 and ozone concentration in open-top chambers (these are the two most important atmospheric pollutants along with SO_2). We have also investigated the development of the photosynthetic machinery in young leaves and its adjustment to illumination conditions in a dense forest canopy. Mathematical modelling of photosynthesis is widely used for the interpretation of the experimental results. A general biological problem that arises from these measurements is how the balance between the expression of Rubisco protein and the component proteins of PSI is controlled. What is the biological sense in synthesising a big amount of Rubisco and keeping it only partially active? Is Rubisco really a reserve protein, along with its task in the photosynthetic CO_2 fixation?

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The Head of the Centre of Excellence is academician Endel Lippmaa, Professor in chemical physics and in physical chemistry, DSc in physics and mathematics, Head of the Division of Physics and Astronomy of the Estonian Academy of Sciences, Chairman of the Board of NICPB and Head of the Laboratory of chemical physics.

The first decade of this century is dominated by new forms of cooperative dynamics and coherence. Entanglement has been established as a general property of all elementary particles and can span and bind at the quantum level significant distances in space and time. New forms of spin co-operativity have led to explosively rapid growth of spintronics and to new forms of matter such as the Bose-Einstein condensates. Dynamics-enhanced nonlocal quantum tunneling phenomena have been established in enzyme catalysis and in regulatory and “action at a distance” phenomena in DNA. Coherent lattice modes have been introduced as the thermal driving force in heterogeneous catalysis. All this, combined with the latest analytical techniques, forms the solid basis for rapid growth of both basic and applied research and development in physics, chemistry, materials science, and new biology. All this also forms the mainstay of scientific activities of the Centre of Excellence of Analytical Spectrometry (CEAS) at the National Institute of Chemical Physics and Biophysics (NICPB). CEAS was formed on the basis of six research groups of the Laboratory of chemical physics (LCP) of NICPB and one biology-related research group by the Dec. 13, 2001 decree no. 855 of the Ministry of Education and it is included into the list of 10 Estonian National Centres of Excellence for five years by the Nov. 05, 2002 decree no. 1202. The strategic plan of R&D activities confirmed

for the 5 years 2002-2006 in the founding documents draws upon the latest trends of development in physics but since some applications are in materials science, environmental research, proteomics and functional genomics, it is decidedly interdisciplinary. Since NICPB is a fully independent public body, all activities of the Centre of Excellence are also aimed at fundamental research with no commercial or service functions, but it would participate in work with PhD students and postdoctoral fellows.

The fundamental strategy of CEAS and the main aims of current R&D activities were already clearly set out in the June 11, 2001 application for establishing the Centre. For shaping the current research at NICPB, the Institute has an International Advisory Board, headed by the Nobel Prize winner Prof. K. Wüthrich, that also serves as a Steering Committee for CEAS.

The members of the Committee are:

- Prof Kurt Wüthrich, TSRI, La Jolla, USA/ETH and NCCR, Zurich, Switzerland, nuclear magnetic resonance spectrometry
- Prof David C. Baulcombe, Norwich, UK, functional genomics
- Prof Carlos F. Ibáñez, Stockholm, Sweden, molecular neurobiology
- Prof Leevi Kääriäinen, Helsinki, Finland, molecular biology
- Prof Michael Mehring, Stuttgart, Germany, nuclear magnetic resonance spectrometry
- Prof Lauri Niinistö, Helsinki, Finland, analytical chemistry
- Prof Risto Orava, CERN, Switzerland, high energy physics
- Prof Eiliv Steinnes, Trondheim, Norway, environmental research

The research groups of CEAS are:

- High energy and quantum physics group. In collaboration with CERN, both theoretical and experimental studies of Higgs field and boson(s), vacuum structure, energy and metrics of the Universe; quantum logic; coherence phenomena in quantum chemistry, spintronics, materials science, chemical kinetics and catalysis.
- Liquid phase nuclear magnetic resonance (NMR) spectrometry group. Structural studies of enanthiomers, diastereisomers and organic stereoisomeric compounds with numerous chiral centers, peptides and other polymers.
- Solid state nuclear magnetic resonance (NMR) spectrometry group. Development of uni- and biaxial MAS/DOR-NMR multidimensional high resolution nuclear magnetic resonance techniques with applications in contemporary bio- and solid state physics and in strong magnetic fields.
- Low temperature physics group. Low temperature far infrared terahertz Fourier transform spectrometry of low-dimensional quantum magnets, superconductors and other solid state spin systems in strong magnetic fields.
- Mass-spectrometry and catalysis group. High resolution quadrupole, time-of-flight (TOF) and ion cyclotron resonance (ICR) mass-spectrometry, development and application of new ionization methods for ion dynamics and catalysis studies of solids.
- Environmental chemistry group. Studies of air, water and soil pollution-limiting technologies.
- Proteomics and functional genomics group. Studies of the role of protein-protein interactions in the regulation of free energy conversion and mitochondrial activity in muscle cells; linking of embryo- and tumorigenesis in PTCH-signaling networks.

The Centre has a research staff of 60, including 28 senior research scientists (DSc and PhD) and 24 research scientists (MSc and Mag), and PhD students. Three members of the Estonian Academy of Sciences work at CEAS.

The past performance and future plans of the seven research groups participating in CEAS were evaluated by an international panel Nov. 15, 2001 with the highest summary rating "Outstanding" and the best points count (119) among the 13 final contestants. The earlier six international evaluations of various groups and laboratories of NICPB in 2000/2001 yielded ratings between excellent to good in chemical physics and good in the AST biology group.

The targeted financing of CEAS from the state budget was 666 700 EEK in 2001, 666 000 EEK in 2002, 1 350 000 EEK in 2003 and 2 844 000 EEK in 2004. Estonian Crown is firmly pegged to Euro at 1 EUR = 15.65 EEK.

As it was mentioned before, all research at CEAS is basic science-oriented, open and non-confidential, as befits a public body. All research is covered by financing from the state budget, which contains in addition to the targeted financing of scientific excellence, also the recurrent basic financing, the maintenance costs of infrastructure, and individual research grants from the Estonian Science Foundation. Of course, several groups also have grants and

sponsorships from outside Estonia. CEAS is reasonably well equipped with all the necessary laboratory facilities, research equipment, computers and professional software, including that for parallel computing at clusters and supercomputers, mechanical and electronics workshops, a liquid helium (^{4}He and ^{3}He) and liquid nitrogen facility, a well-equipped scientific library with more than 150 leading professional journals in physics, chemistry, materials science, electronics, scientific instrumentation, computing, modern biology, medicine, energy and environmental research; also internet with free electronic access to many journals and fully electronic publications, and a supercomputing GRID facility.

During the past two years of CEAS activity 115 high level peer-reviewed scientific papers have been published, or more than 50 publications at the *Current Contents* (ISI) level per year and CEAS has had numerous research grants from the Estonian Science Foundation (ESF), in 2002 21 ESF grants for 2 211 000 EEK, in 2003 19 grants for 2 285 000 EEK, in 2004 20 grants fro 2 605 900 EEK.

CEAS has active cooperation with the two leading universities, the University of Tartu and the Tallinn Technical University, in preparing Ph.D. students and has good contacts to more than 30 scientific partners in Europe, USA and Japan.

HIGH ENERGY AND QUANTUM PHYSICS

The research group includes as senior research scientists M. Raidal, E. Lippmaa, R. Stern, G. Blumberg and in part J. Subbi and M. Lippmaa, and as research scientists A. Rummel, A. Trummal, A. Hektor (PhD students), A. Sirk.

MAJOR RESULTS

The high energy physics group (M. Raidal) is studying both theoretical and experimental particle physics in the CERN Large Hadron Collider (LHC) Compact Muon Solenoid (CMS) collaboration. The main theoretical research topics of the group include explaining the observed baryon asymmetry of the Universe *via* leptogenesis [1-4], relating it to the neutrino masses and mixings as well as to the inflation of the Universe [3], and predicting the rates of lepton flavor violating charged lepton decays observable at the experiments under construction [4]. This research requires making precise predictions for the leptogenesis in heavy neutrino decays aiming at taking into account all the processes influencing leptogenesis in the early Universe. Since the precision of new astrophysical observations (WMAP) of the properties of the Universe has reached a few percent, detailed theoretical investigation is required to analyze and to explain the present observations. We used the results of the WMAP satellite to unify the inflation and leptogenesis in supersymmetric theories [3] in which the inflaton is heavy sneutrino (supersymmetric partner of the heavy neutrino). In this case the inflation and reheating of the Universe are described with the known neutrino parameters, and the unknown cosmological quantities are replaced with the neutrino couplings and masses. Such a theory predicts observation of lepton flavor violation at the planned experiments [4]. The present experimental physics program includes searching for lepton number violating decays of the tau-lepton at CMS [4]. Our group also studies new physics in CP violation in the Standard Model quark sector, for example in the processes $B\to\phi K$ and $B\to\psi K$ [5] which are currently under experimental investigation in the b-quark factories in USA and Japan.

The research program and activities in experimental high energy physics are currently expanding. We actively prepare scientists for experimental particle physics research (which has never been done in Estonia before) and, at the same time, prepare technical devices necessary for collaboration with the CMS experiment at CERN [7]. We have established close contacts with the CMS groups of the Nordic countries with whom we organize common workshops in order to obtain experience in experimental high energy physics (A. Hektor, M. Kadastik). We also have built a Xeon-Linux computer cluster (A. Rummel, A. Trummal) which will be used through the GRID supercomputing system for CMS data analyses.

The very basis of contemporary theoretical physics, quantum mechanics, has turned out to be a fertile field of fundamental studies in conjunction with the rapid development of quantum logic and quantum information processsing. Hundreds of papers have been written about the inner meaning of wavefunction entanglements, about the possibility or impossibility of their reductionist classical description,

and about the feasibility or fallaciousness of universal error correction codes at the quantum level, but no consensus has been found. Our theoretical analysis (E. Lippmaa) has shown the impossibility of any classical description of all the implications of quantum entanglements and the deceptive nature of all universal error correction codes at the quantum level. All this makes the cellular Type II QC [15], quite similar in architecture to the common storage classical supercomputers, the only realistic choice for large scale quantum computing (QC). The experimental proof of this concept belongs to the year 2004 workplan of CEAS and shall be carried out using NMR techniques. The nuclear spin is by far the best manipulated two-level system in all physics that easily forms addressable entangled states of very high order. It serves as a good model for the superconducting squid matrixes or related spintronic devices. In this connection various forms of spin coherence in solids are also studied, including high temperature superconductivity (G. Blumberg [16-22]). It was shown that antiferromagnetic fluctuations-based superconductivity is of the same origin in both electron- and hole-conductivity cuprates [18,19].

One of the most interesting, challenging and productive classes of materials of the present decade has been the class of transition metal oxides. Because of the extreme variability in local environments and dimensionality, those materials offer an unprecedented rich area of physical systems and lie due to the involved preparation techniques at the frontier of materials research. Especially novel and important are the (quantum) magnetic materials with ordered spin structures (R. Stern) and catalysts and solid electrolytes with mixed conductivity (J. Subbi).

In quantum magnets we have concentrated our efforts on new phenomena occurring in high magnetic fields, such as Bose-Einstein condensation (BEC) and the corresponding plateaus in magnetization. Until recently, BEC was only recognized in superfluid helium and as Cooper pairs in superconductivity. Yet magnetic tripleton-based BEC is also possible in spin-ordered quantum magnets, where the singlet ground state of a lattice of Cu^{2+} ion pairs (dimers) is separated by an energy cap of only a few meV from the first spin triplet excitations. At low temperatures and in a very strong magnetic field the spin triplet states (tripletons) become part of the new ground state and, depending on the lattice-dependent degree of frustration, can either crystallize [26,27] or condense [23,28] in a phase-coherent state, thus forming a new form of matter with new properties. The crystallization of tripletons manifests itself as plateaus in the magnetization *versus* field. Compared to the ultra cold quantum gases, the “kagome” or bamboo basket-weave type and some other highly ordered lattices can be studied at relatively high (helium) temperatures under easy-to-achieve experimental conditions (20 T to 40 T magnetic fields at NHMFL). We have just started kagome lattice collaborative NMR studies.

The studies of catalytically active oxide materials have been centered around the H^+ ion mobility in the strongly acidic Brønsted reaction centers of zeolite catalysts (E. Lippmaa) and research on solid oxide fuel sell (SOFC) components (catalytic electrodes and ionic conductors), mainly with electric impedance spectrometry (J. Subbi). Numerous oxides, such as perovskites, can serve both as high temperature superconductors and as efficient SOFC catalysts. Both phenomena are based upon the presence of oxygen defect chemistry, creating highly mobile vacancies and ionic conductivity in structures that can be meso- or macroporous, amorphous or even plastic [30,31].

In quantum chemistry the main emphasis has been upon the influence of lattice dynamics upon the activity and (super)acidic properties of the reaction centers of petrochemical zeolite catalysts, keeping in mind using the same approach later in enzymology. A good measure of the zeolite high temperature solid state acidity is the H^+ ion mobility, or proton hopping between the Al-coordinated oxygen atoms in the Brønsted acidic center. It has been studied both experimentally by NMR and impedance spectrometry, and by quantum chemical calculations. Activation barriers, tunneling and stabilization energies have been calculated for various static cluster-, potential- and hybrid models of the active center. Our studies have been carried out in the context of lattice dynamics. H-FER and H-ZSM5 zeolites were simulated by the intrinsic reaction coordinate (IRC) method for the evolution of the reacting system (H^+ + lattice) from the active complex towards the stationary state with the proton localized at various oxygens, coordinated with the same Al-defect.

The dynamic reaction coordinate (DRC) method was used for process simulation in case of selective excitation of some degrees of freedom of the system. Evolution of the lattice modes thus determines the reaction dynamics. Char-

ting the evolution of the system modal structure along the reaction path for a periodic system with a large number of degrees of freedom is a very large computational task. For H-ZSM5 (Pnma symmetry, 289 atoms) and H-FER (Immm symmetry, 109 atoms, but 216 in a double unit cell) it is realistic only at the semiempirical potential energy hypersurfaces (Mopac PM5). Modal analysis along the reaction path after mapping the reaction coordinate in relevant points allowed to find relations between the normal modes and the reaction coordinate, energy exchanges between the degrees of freedom, and the crucial process-enhancing and inhibiting lattice modes. These results form the basis for establishing relations between the characteristic zeolite rigid unit modes (RUM) of lattice tetrahedra and the lattice dynamics driving the acidic proton and thus the catalytic activity of any particular zeolite. The computational results were satisfactorily consistent with the results of high temperature MAS-NMR measurements of proton mobility in zeolites [32].

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LIQUID PHASE NUCLEAR MAGNETIC RESONANCE SPECTROMETRY

The research group includes as senior research scientists T. Pehk, L. Vares, J. Jarvet and as research scientists S. Vija, E. Kiirend.

MAJOR RESULTS

The importance of nuclear magnetic resonance (NMR) spectrometry for the liquid state studies cannot be overestimated. It is the most important single method for structure determination of organic compounds. With modern instrumentation and proper experimental setup, most useful information can be obtained about the structure and dynamics of molecules and their intra- and intermolecular interactions. The targets for the liquid state NMR research in CEAS are such products of organic synthesis, natural products, materials and bioactive molecules, for which other instrumental methods cannot give adequate information. First of all isomeric compounds should be noted, and among them the most important are stereoisomeric chiral molecules. Absolute configurations of chiral centers can be studied only in the diastereoisomeric compounds or complexes. For this some kind of diastereoisomerism must be present or introduced into the molecules. Our use of differential shieldings of the corresponding atoms from the fully assigned ^{1}H and ^{13}C chemical shifts of diastereoisomeric compounds *via* the 2D Fourier transform ^{1}H -^{1}H and ^{1}H -^{13}C chemical shift correlation diagrams provides a solid basis for the application of conformational models in order to determine the absolute configurations of chiral centers of the compounds under investigation. This method is applied in the configurational analysis of various chiral compounds, among them for the products from asymmetric syntheses. In the configurational analysis of aliphatic and alicyclic vicinal chiral diols and polyols crowding effects connected with the bulky aromatic rings must be taken into account. Effects of new derivatizing agents are studied and semiempirical methods (AM1, PM3) of quantum chemistry are used in the interpretation of the small differential chemical shifts.

In the studies of compounds with several asymmetric centers, the change of absolute configuration of an individual site results in a new diastereoisomer, which gives in principle different from the starting compound NMR spectrum. However, the observed differences depend on the structural details of the compound and distances between the chiral centers. Prostaglandin molecules are good examples of such multichiral compounds. Absolute configurations of synthetic and natural prostaglandins have been studied. Stereoselectivity and kinetics of enzymatic acylation of prostaglandins with up to 3 different OH groups can be followed by NMR spectroscopy to obtain valuable information about the active site of the enzyme.

A systematic NMR-MS study of successive generations of poly(amidoamino)-dendrimers grown upon an ethylenediamine 2-carbon core was carried out [1]. The study allowed to establish new approaches for the interpretation of these crowded spectra and for describing the long-distance NMR effects present. Enanthiomeric 2,2'-biaziridinyl derivatives and the parent compound itself were synthesized for further use as new chiral ligands [2]. A three-part NMR-guided systematic study of asymmetric oxidation of 3-alkyl-1,2-cyclopentanediones was successfully concluded [3,6,18]. New efficient methods for the synthesis of enanthiomeric alkyllactonic acids, hydroxylactonic acids and spirodilactones were developed. Decidedly interesting is the use of 1D- and 2D-^{1}H,^{13}C and ^{31}P-NMR spectrometry for establishing the specificity of ATP-converting activity of a new enzyme from the marine sponge *Axinella polypoides*. The enzyme turned out to be an ATP N-glycosidase [4].

In addition to the chiral stereoisomeric configurations, the conformers and conformational dynamics are gaining importance as important structural parameters, critical in determining the chemical, catalytic, aggregational (plaque-competence) and other physiological properties. Thus in degenerative amyloidosis diseases (Alzheimer's disease, Creutzfeldt-Jakob disease, kuru and other prion diseases) that can be found in all organs of human body, the infectious pathological molecular agent is structurally identical to the normal native form (same configuration), but the conformation is different.

In the case of Alzheimer's disease the 39-43 amino acid residues long toxic Aβ peptide has a very high propensity for the formation of aggregates. Eventually regular fibrillar structures, rich in the β-sheet motif, are formed. Fibril formation is preceded by extended, and well soluble left-handed 3_1 helix conformation that interconverts with a flexible random coil conformation, increases sample stability in solution and lowers transition to the insoluble β-structure (J. Jarvet)

The new Oxford Instruments superconducting magnet of the 600 MHz 2D-FT-NMR spectrometer.

[8]. All this is a significant improvement over the earlier results of K. Wüthrich et al., who did not use far ultraviolet circular dichroism (CD) optics and could conclude that even high field 750 MHz homonuclear 2D-TOCSY (total correlation spectroscopy) and both homo- and $^{15}N\{^{1}H\}$ heteronuclear 2D-NOESY (nuclear Overhauser effect spectroscopy) fail to identify significant conformational differences between the two Alzheimer peptides with widely different plaque-competence [9]. Combination of < 200 nm CD with easily accessible ^{1}H NMR at 600 MHz turned out to be more efficient and allowed to establish as a general conclusion that a putative random coil peptide is not always random [8].

The high resolution NMR spectrometry group has numerous contemporary 2D-FT-NMR multi-resonance high resolution spectrometers, equipped with superconducting Oxford Instruments magnets and the ^{1}H working frequencies equal to 200 MHz, 360 MHz, 500 MHz and 600 MHz. The laboratory also has the necessary facilities for organic synthesis and sample preparation, including GC-MS and HPLC-MS chromatographic instruments.

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SOLID STATE NUCLEAR MAGNETIC RESONANCE SPECTROMETRY

The research group includes as senior research scientists: A. Samoson, I. Heinmaa, P. Sarv, E. Kundla, J. Past and as research scientists T. Anupõld, A. Reinhold and T. Tuherm.

MAJOR RESULTS

Studies of relations between the structure and functionality forms a very important part of CEAS activities. Solid state high resolution nuclear magnetic resonance (NMR) is equally informative and useful in finding either structural or lattice dynamics and kinetic parameters of the sample. All solid state high resolution studies are based upon averaging the line-broadening tensor interactions with rapid mechanical rotation of the sample around axis tilted from the direction of the polarizing magnetic field. The tilt angle dependencies of the averaged NMR spectral line forms are well described by spherical harmonics defined through Legendre polynomials, just like the elementary atomic wavefunctions are. The solid state linewidths can

thus be narrowed by up to two orders of magnitude at the "magic" sample spinning angles that correspond to the zero values of the 2. and 4. order angle dependent Legendre polynomials. The actual forms of the angle dependence correspond to the shapes of the well-known d- (l = 2) and g- (l = 4) atomic orbitals. If the interactions being averaged out correspond to spherical harmonics of different ranks, then rapid switching of the tilt angles in dynamic-angle spinning (DAS) or simultaneous double rotation (DOR) around two tilt angles is necessary. The actual engineering of MAS and DOR is described in two seminal patents, both of which have found wide application through licenses sold to Bruker, Chemagnetics and Doty Scientific:

1. United States Patent No. 4,254,373
   Mar. 31, 1981
   Sensor for Generating Nuclear Magnetic Resonance Signals
   Inventors: E.T. Lippmaa, M.A. Alla, A.A. Salumyae, T.A. Tukherm
   Assignee: Institut Kibernetiki
2. United States Patent No. 4,899,111 Feb. 6, 1990
   Probe for High Resolution NMR with Sample Reorientation
   Inventors: A. Pines, A. Samoson
   Assignee: The Regents of the University of California

The faster the "magic angle(s)" rotation, the better the averaging, and the more informative is the measured MAS-NMR or DOR-NMR spectrum. In 2003 up to 70 kHz MAS [1] and 10 kHz DOR have been achieved with rather small precisely machined rotors, self-balanced in gas lubricated bearings a few tens of micrometers thick. It must be stressed that at such high rotation rates the rotor materials work very close to the absolute limits of stress for high-strength materials [2] and stable rotation requires machining to 1 micrometer tolerances even for rather large items. Of considerable practical importance is also the inverse proportionality between homogeneous line broadening and the product of magnetic field strength and spinning speed. Single pulse experiments at 1.066 GHz ^{1}H frequency showed that the combination of very high field strength with very fast sample spinning yields ^{1}H MAS-NMR linewidths approaching the intrinsic limit determined by anisotropy of magnetic susceptibility [3].

The applicable temperature range for MAS sample spinning at present stretches from 25 K to 700 K [1], which is quite sufficient for optimum temperature studies of many important solid state phenomena from superconductivity to petrochemical zeolite catalysis. Ramped-speed MAS-NMR is a useful technique for achieving optimum efficiency in heteronuclear cross polarization and in selective homonuclear polarization exchange [4]. Reversible spinning acceleration up to 1 MHz/s has been achieved. Four superconducting magnet-equipped high resolution 2D-FT-NMR spectrometers (600, 500, 360 and 200 MHz ^{1}H frequency) are in daily use and up to 45 Tesla fields are accessible through collaborations. It must also be mentioned that direct digital synthesis (DDS) is now in use for frequency synthesis, allowing rapid and frequency-continuous pulse switching, crucially important in quantum logic, solid state physics and materials science. Recently, rotation sweep NMR has been used for homonuclear 2D-NMR spectroscopy of fully ^{13}C-labeled compounds, such as LVFFA peptide sequencing [4] and studies of the Crh phosphocarrier protein. A fairly novel high rotation rate effect is low-power XiX decoupling, which is efficient in MAS-NMR experiments if the sample spinning frequency exceeds the interaction strengths between hydrogen nuclei [5]. Lower decoupling field strengths used in XiX decoupling are especially beneficial in case of temperature-sensitive biological samples. The technique can be applied for ^{13}C/^{15}N-labeled peptide sequencing. The recommended high 40 kHz rotation rate spinning was successfully used in ^{1}H, ^{31}P CP/MAS-NMR studies of trabecular and cortical human bones [7]. Only the expected carbonatoapatite B was found with no evidence for the disputed presence of brushite.

Solid state ^{17}O DOR-NMR 3-Quantum MAS-NMR and Gaussian 98 calculations were used to interpret the ^{17}O resonances in the identical spectra of solid D- and L-glutamic acid hydrochlorides. As expected, the ^{17}O spectrum of L-monosodium glutamate hydrochloride with 5 resolved oxygen shifts from the 8 structurally distinct sites turned out to be rather different [8]. ^{17}O NMR turned out to be much more informative than ^{1}H and ^{13}C resonance in this case. In order to further enhance the potentialities of the quadrupole nuclei in structural analysis, such experiments were also carried out in ultra strong magnetic fields [9].

Traditionally, ^{29}Si NMR occupies central position in NMR studies of inorganic solids. In this connection, direct oxidation of silicon [10] and possibilities of preparing novel mesoporous aluminosilicates with larger 37-38 Å cavities

available for catalytic reactions, were studied [11]. The novel approach of changing the Si/Al ratio of mesoporous materials through postpreparative doping with silicon or aluminium certainly has merit. This allows separate regulation of cavity size and the choice of (Brønsted and Lewis) catalytic acid centers [12].

In the realm of applied science, ^{13}C CP/MAS-NMR methods were used for a rerun of Estonian oil shale organic matter – kerogen structure determination. The NMR-determined distribution of structural motifs and C/O-based functional groups [13,14] turned out to be rather close to the results of purely chemical analysis [15]. Extensive presence of phenolic aromatic structures with ether bonds in the native kerogen was confirmed.

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LOW TEMPERATURE PHYSICS GROUP

The research group includes as senior research scientists T. Rõõm, U. Nagel, G. Liidja, E. Joon and as research scientist D. Hüvonen (PhD student).

MAJOR RESULTS

Low-dimensional quantum spin systems with a finite spin gap have become the subject of intensive advanced research. One of the reasons is the progress of solid-state chemistry enabling tailoring of various low-dimensional spin systems for the experimental verification of concepts brought about by theoretical studies. For example geometrical spin frustration in antiferromagnetic systems has been an interesting and challenging issue in the condensed matter physics. Recently another interesting aspect of quantum magnets appeared, the Bose-Einstein condensation (BEC) of magnons.

Phase transitions are usually examined as a function of temperature. For quantum spin systems magnetic field can be used as the experimental parameter as the magnitude of the spin gap and quantum spin fluctuations can be tuned by the magnetic field. Therefore studies of magnetic excitations in quantum spin systems in high magnetic fields are attracting more and more interest.

The main objects of study are low-dimensional solids with gapped spin excitations and a singlet ground state. These systems merit serious attention because of Bose-Einstein condensation of triplet excitations (magnons) in $TlCuCl_3$ and $KCuCl_3$ spin dimer systems, quantization of magnetization in $SrCu_2(BO_3)_2$ that exhibits magnetization plateaus due to the interplay of spin frustration and quantum fluctuations, and syperconductivity in $Sr_{14-x}Ca_xCu_{24}O_{41}$. The main research instrument is far infrared spectrometry that allows to measure both lattice and spin excitations, and their mutual interactions as well as movement of change carriers.

$SrCu_2(BO_3)_2$ and α'-NaV_2O_5 measurements carried out in Tallinn and in Tallahassee (NHMFL), taken together with theoretical calculations, show that optical transition from singlet to triplet takes place through virtual excitation to a lattice vibrational mode and is thus an electric dipole transition. This proves the important role of lattice vibrations in spin state mixing which takes place through the dynamic Dzyaloshinskii-Moriya (DM) antisymmetric interaction and allows forbidden optical transitions between the antisymmetric singlet ground state and the symmetric triplet excited state [1]. In α'-NaV_2O_5 the DM interaction is created by optically active phonon modes that lower the crystal symmetry. One such phonon is polarized along the ladder rungs of the lattice and the other at right angles to the ladder planes. Far infrared measurements of $SrCu_2(BO_3)_2$ showed that in this case, just as in α'-NaV_2O_5 , the singlet-triplet optical transition has the symmetry of an electric dipole transition [3] that is partially allowed through the DM interactions. A spin cluster simulation of the Shas-try-Sutherland model was used to identify the absorption lines. Exact diagonalization of the spin Hamiltonian, including the nearest and next-nearest exchange couplings and DM-interactions, was carried out for clusters of up to 10 (24) spins using the Lanczos algorithm [4].

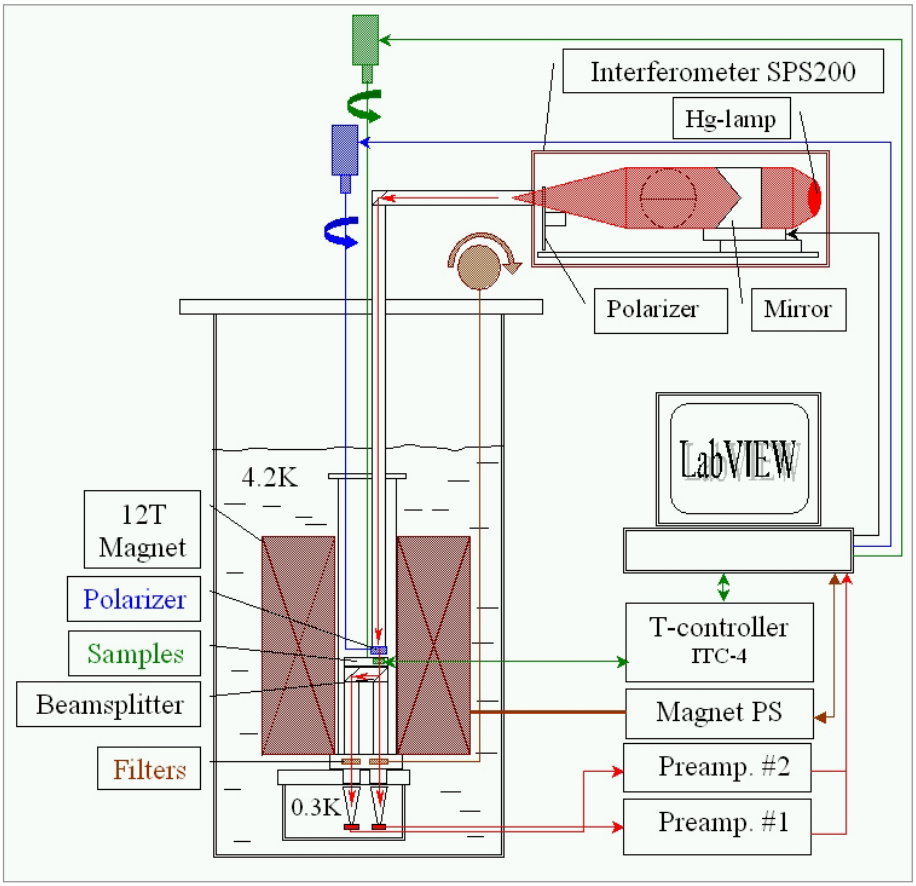

Fig. 1.
Layout of the far-infrared Tesla FIR^2 spectrometer.

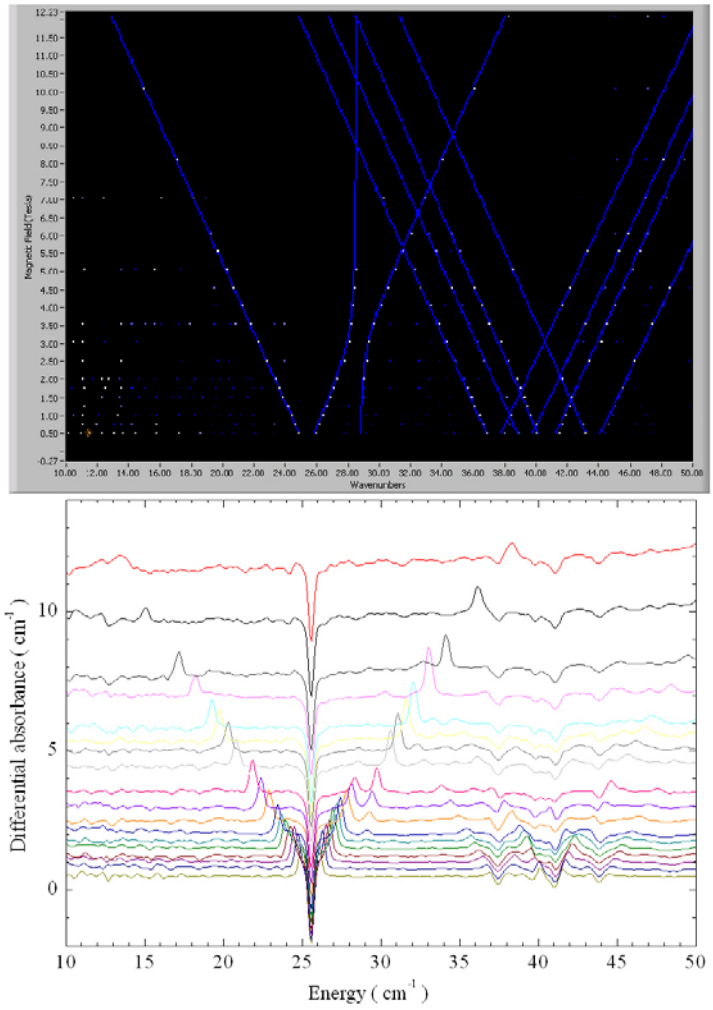

Fig. 2.
Magnet field dependence of the infrared spectra of $SrCu_2(BO_3)_2$ at 4.4 K. Lower panel – differential absorption spectra relative to zero field, from T. Rõõm, U. Nagel, E. Lippmaa, H. Kageyama, K. Onizuka, Y. Ueda, Far-infrared study of the two-dimensional dimer spin system $SrCu_2(BO_3)_2$, Phys. Rev. B61, 14342-14345 (2000). Upper panel – absorption peak positions shown by dots and the theoretical fits.

The $Sr_{14-x}Ca_xCu_{24}O_{41}$ is rather special among cuprate superconductors because it lacks the usual square lattice. It has a rather involved magnetic structure of spin chains and spin ladders. Calcium doping introduces holes into the ladders and it is presumed that the hole pairs form bosons which lead to superconductivity. Indeed, if $x \geq 11.5$ the compound turns metallic and under pressure also superconductive. If $x < 10$, a phase transition into charge density wave state takes place. The gap of this state diminishes with the growth of x and charge density wave competes with the superconductive state. Thus transition into superconductive state starts from two-dimensional charge dynamic state and not from a one-dimensional charge density wave state [5,9].

All far-infrared measurements are carried out in the 0.1 to 6 terahertz frequency range (3 to 200 cm^{-1}). The very good low frequency performance of the Tesla FIR^2 spectrometer is achieved through the use of very sensitive silicon bolometers working at 0.3 K and a Sciencetech (Canada) SPS200 polarizing Martin-Puplett type interferometer, equipped with an up to 12 Tesla variable field Oxford Instruments superconducting magnet with two inserts, a 2 K insert and a 7 mK ^{3}He/^{4}He dilution refrigerator cooled insert (also Oxford Instruments). Stronger magnetic fields, up to 45 Tesla are available in collaboration with the National High Magnetic Field Laboratory (NHMFL) in Tallahassee, Florida.

In conclusion – far infrared terahertz spectroscopy is a new powerful and very universal new tool that allows comprehensive studies of both lattice and spin excitations as well as the combined DM-phenomena in a new field of solid state physics centered around quantum magnetism, spin frustration, Bose-Einstein condensation and superconductivity in a whole class of novel antiferromangetic and spintronic materials.

In addition to spectroscopy, there has been ongoing activity in detectors design for particle

physics (U. Nagel) [7,8] and in high field electron spin resonance (ESR) at both the X-band (10 GHz) and Ka(Q)-band (35 GHz) frequencies. The higher frequency is necessary for studies of triplet states and magnetic systems. The formation under the influence of ionizing radiation of carbonate radicals in tooth enamel bioapatite was studied by Q-band ESR at 35 GHz (G. Liidja). Various forms of CO_2^- radicals were found in the enamel hydroxyapatite of both fossil (*Elephas primigenius, Rhinoceros antiquitas*) and contemporary (*Loxodont*) material. The ESR signals can be used of paleonthological dating purposes.

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MASS SPECTROMETRY AND CATALYSIS PHYSICS

The research group includes as senior research scientists J. Subbi, R. Pikver and R. Tanner and as research scientists H. Kooskora, R. Aguraiuja, J. Pahapill and in part A. Hektor (PhD student).

MAJOR RESULTS

The research in mass spectrometry was at first oriented to high energy physics at CERN and in particular, to the physics and operation of new

gas-filled particle detectors [1]. Ion cyclotron resonance as a mass-spectrometric tool was first developed for ultraprecise measurement of the ^{3}T and ^{3}He mass difference with an error below 1/20 000 000 for the measurement of the rest mass of electron antineutrino [2]. The result pointed to a small positive rest mass, which later proved to be right. At present the main aims of the mass spectrometry group are catalysis and gas phase physics together with some applications in biochemistry.

Two matrix assisted laser desorption ionization (MALDI) time of flight (TOF) mass spectrometers, one linear and one reflectron, and one high field Fourier transform (FT) ion cyclotron resonance (ICR) mass spectrometer have been built by the Group and are in daily use. In addition to MALDI, electrospray (ES) ionization is also in use. There are also two commercial quadrupole instruments, one attached to a gas chromatograph (GC) and the other to a high pressure liquid chromatograph (HPLC). As a recent development in MALDI-TOF mass spectrometry, a special delayed extraction ion source has been designed and built under the project for investigation of the MALDI plume dynamics. The whole mass spectrometer was modelled with the SIMION 3D version 6.0 program and built in the mechanical workshops of NICPB. This allowed to compare the experimental ion flight times with theoretical models. The results showed that the optimal delay grows with desorption laser intensity and is correlated to the analyte signal strength. At the same time the actual optimal delay is always longer than the simple models of simultaneous ion departure at various speeds predict. These investigations indicate that there are indeed nonadiabatic prompt fragmentation pathways and fast energy and charge transfer processes involved, as proposed by some more sophisticated models of MALDI ionization processes (J. Subbi).

In high field MALDI-FTICR mass spectrometry, using a Bruker 4.7 Tesla vertical superconducting magnet, a new acceleration-deceleration (AD) method for reducing and focusing the ion kinetic energies has been developed [3]. The aim of the method is first to equalize and then significantly reduce the kinetic energies of the MALDI-produced ions, initially distributed over a broad energy range, by means of delayed acceleration and deceleration. By applying high asymmetric voltages to the ICR ion trap endcaps, a deep potential well can be created in the region where the ions are cooled to near immobility at very low kinetic energies [4]. MALDI-generated ions can thus be kept trapped for hours. For example, using 6-aza-2-thiothymine (ATT) as the matrix, one can scan the mass spectrum of adenosine triphosphate ATP in the negative ion mode with 180 000 resolution and a signal to noise ratio (S/N) of 13:1 after 2 hours trapping time. This is the longest registered trapping time for a MALDI-created ion. Since the new technique traps all ions including those with very high initial kinetic energy, it has high inherent sensitivity and respectable mass resolution close to 70 000 for substance P (R. Pikver).

MALDI-TOF allows mass resolution of about 12 000 and is much easier to use. It has found wide use in collaborations with Estonian universities. These cooperative projects have provided the technical means to establish the synthetic specificity of marine sponge oligoadenylate synthetase [5], to identify the closely related forms of snake venom enzymes [6-9], to develop methods for determining enzymatic specificity of model synthetic peptides and to identify the products of bioactive compounds synthesis [10], and develop methods for the analysis of synthesis and modification of PAMAM dendrimers [11].

The combined HPLC-ES-MS apparatus is actively used for studies of the lifecycles of blue-green algae in Estonian lakes (R. Tanner). These bacterial algae can produce dangerous poisons and also carcinogenic compounds, such as microcystins. Concentrations of the liver poisons (the microcystin group of compounds) in

J. Subbi with his MALDI-TOF mass spectrometers.

the lakes correlates fairly well with the abundance of *Microcystis*, and microcystins LR, dmLR, RR and dmRR are dominant. Unfortunately, the Narva reservoir of drinking water is also contaminated with *Microcystis* and the dangerous *Anabena* that can produce the nervous system poison anatoxin that can cause death through respiration blockade.

The original importance of gas-phase chemical physics in the development of TOF-MS is also returning because the Large Hadron Collider (LHC) in nearing completion at CERN and the new detectors use many gas-filled particle detector elements. A new, but closely related field of research is fuel cell chemical physics, in particular direct oxidation of hydrocarbons and related compounds at the anodes of medium temperature solid oxide (and hybrid) fuel cells (SOFC). These dynamic studies require direct online analysis of the gas vented at the anode. Very good results have already been achieved with the use of $La_{0.75}Sr_{0.25}Cr_{0.5}Mn_{0..5}O_3$ type perovskites as medium temperature SOFC anodes on cerium/gadolinium oxide ion-conducting solid electrolyte membranes [14]. These studies at present aim at increasing the catalytic activity of the anode with chosen additives such as titanium (Ti) that can facilitate direct hydrocarbon oxidation. The stability and improved conductivity of the electrolyte membrane are also important issues, especially in a reducing atmosphere.

RECENT RELEVANT PUBLICATIONS

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ENVIRONMENTAL CHEMISTRY

The research group includes as senior research scientists U. Kirso, N. Irha, E. Maremäe, A.-T. Pihlak and J. Reinik.

MAJOR RESULTS

The main emphasis of the current studies has been on Estonian shale-burning power stations and their renovation with the introduction of the novel circulating fluidized bed (CFB) technology.

In the current study the aerosol and dust samples were taken and analyzed. The sampling was carried out in Tallinn and in the Ida-Virumaa County. The main attention was paid to the fine fractions of aerosol particles, which contribute most to the health effects, e.g., PM2.5 (respirable fraction, which reaches alveoli) and PM10 (thoracic fraction). The results of the analyzes proved that the chemical composition of various size fractions of suspended particles varied. Thus, the environmental impact and health effects of aerosol depend on the chemical composition and the physical properties of the particles. The concentrations and speciation of the priority pollutants in air samples were determined. Quantitative measurements of the most important carcinogenic pollutants, attached to the fine fly ash and diesel exhaust particles, were carried out using contemporary analytical instrumentation and methods, such as GC-REMPI-MS with mass-selective detector, and HPLC analysis. Phenanthrene, fluoranthene, pyrene, benz(a)anthracene, chrysene, benzo(b)fluoroanthene, benzo(k)fluoranthene, benzo(a)pyrene and other important polycyclic aromatic compounds (PAC) were determined in dust samples collected from the ambient air. Most of these PAC are cancerogenic, mutagenic or both. The distribution of these compounds in dust fractions is very uneven, but the most dangerous compounds tended to collect into the finest particles which reach the alveoli. This is a dangerous tendency which needs further study.

All these results can and shall be used in monitoring the current boiler renovation where the existing technology is being replaced with CFB technology with quite different environmental impact.

Finally, the ash samples collected in different stages of the combustion process were characterized by the MAS-NMR method (I. Heinmaa). A typical ^{27}Al MAS-NMR spectrum indicated only tetrahedral Al sites. The ratio of Al to Si remained almost the same throughout the technological process, while the content of both Si and Al increased from boiler to stack, with decreasing particle size. The X-ray (Tallinn University of Technology) and BET analysis were performed with the ash samples. Essential quantitative differences were observed between the oil shale ash samples originating from different stages of the combustion process. Another objective of the study was to investigate the mobility of the compounds of environmental

significance in oil shale processing solid wastes such as ash and semi-coke. Even very hydrophobic (low solubility) compounds as PAC were found in the water phase. It means that they started to be bioavailabe.

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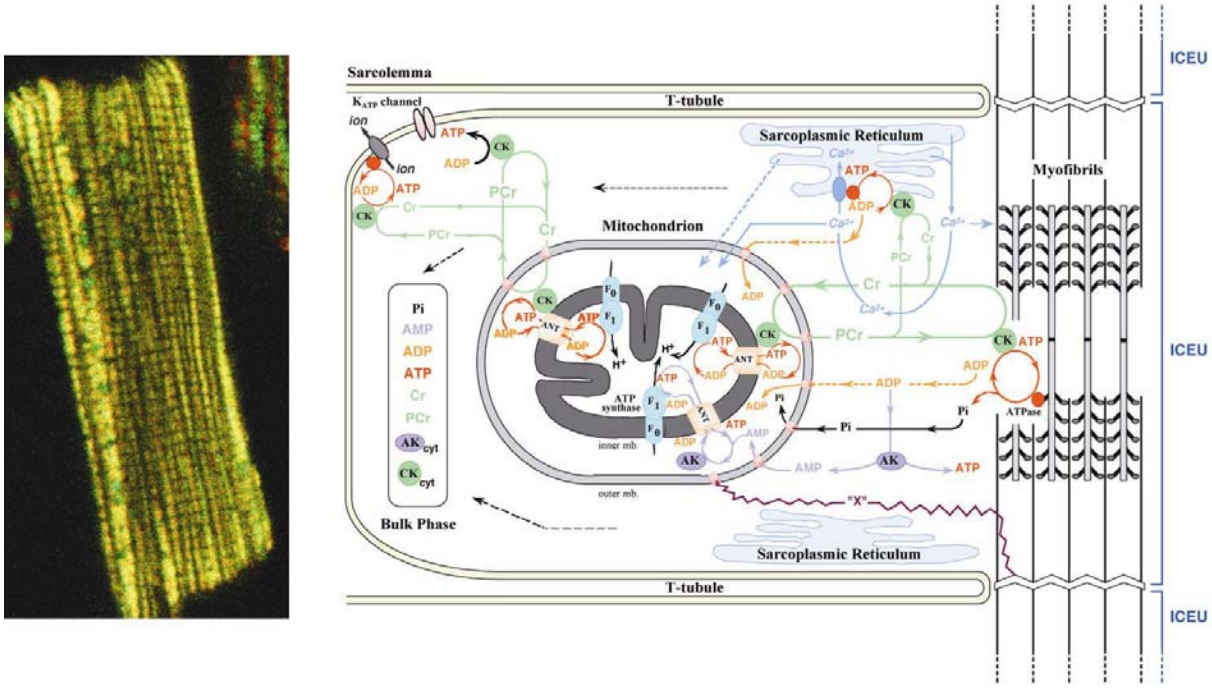
PROTEOMICS AND FUNCTIONAL GENOMICS

The research group includes as senior research scientists V. Saks, P. Sikk, P. Kogerman, A. Valkna, M. Drews and as research scientists T. Käämbre, T. Tiivel, H. Vija, I. Tammiste (PhD student).

MAJOR RESULTS

The main goal of the group led by V. Saks is to study the role of protein-protein interactions between the cytoskeletal and cytoplasmic proteins in the regulation of free energy conversion and mitochondrial activity in the heart muscle cell bioenergetics *in vivo* in normal and pathogenic conditions. The functional genomics (P. Kogerman) aims at elucidating the molecular genetic mechanisms underlying the formation of some forms of (skin) cancers and the regulation of these processes through protein-protein interactions. The current research program on cancer focuses on the signaling networks emanating from the transmembrane receptors.

The organization of the signaling networks with many inputs and outputs is both sophisticated and flexible, and the compartmentalized metabolic pathways are just as highly organized and optimized for maximum efficiency. Regulation itself depends in both cases upon highly selective protein-protein interactions [1-4]. The concept of the intracellular energetic unit (ICEU) is a good example of both compartmentalization and complexity, see Fig. 7. The ICEUs are functional complexes between myofibrils and sarcoplasmic reticulum which have synchronized metabolism and mechanical stress behavior in heart muscle cells. Structural and functional changes of the ICEU in pathological conditions of cardiac muscle cells can provide the basis for an analysis of whole cell and muscle behavior. These studies are carried out by using skinned fibers, ghost fibers without myosin and permeabilized cardiomyocytes. Morphology of muscle fibers is studied by confocal microscopy. Kinetic studies on the cellular respiration are performed by oxygraphic registration of the respiratory rate or by spectrofluorometry. Structural and functional changes in the ICEUs under pathological conditions (high Ca^{2+} concentration or lack of substrates) are studied by reperfusion of pig heart. 2D-PAGE maps (polyacrylamide gel electrophoresis in a nonlinear pH-gradient) of proteins from cardiac and *m. soleus* skinned fibers and ghost fibers are used. The spots from 2D-PAGE are analyzed by MALDI mass spectrometry. Vesicles of the outer mitochondrial membrane are prepared by hypo-osmotic rupture of isolated mitochondria. Surface plasmon resonance (SPR) method is used for studies on the complex formation interaction of the mitochondrial outer membrane with identified proteins. All information thus obtained is used for the development of mathematical *in silico* models of compartmentalized energy transfer in heart metabolism. The heart muscle research is carried out in collaboration with Estonian universities and with the Joseph Fourier' University (Grenoble).



The ICEU structure.

The studies in functional genomics are centered around linking embryo- and tumorigenesis through PTCH signaling networks (Howard Hughes Medical Institute grant), where the regulatory mechanisms of the triple Hedgehog signaling activity provide good model for these regulatory mechanisms. The Sonic hedgehog SHH signaling pathway has unique functions during the external genitalia (male and female) development starting with the embryonic GT development and carried out through extensive apoptosis. The role of SHH is in this respect quite similar to that of glucosylated AFP during the whole embryonic development, which likewise proceeds through extensive apoptosis. SHH acts through the PTCH1, PTCH2 and SMO transmembrane receptors and the SUFU- and DYRK1-regulated transcription activators GLI1, GLI2 and GLI3 directly on the genetic transcription, whereas the following protein synthesis may be preceded by organ- or cancer-specific splicing. Since SHH signaling network also directs cell proliferation and angiogenesis, it can be of crucial importance in the development of various forms of cancer or malformations in the skin or other organs [20-24]. Of course, some skin cancers may be regulated by other pathways as well, involving, for example, CYLD [22]. The workplans of CEAS include the PTCH-type and SMO-receptor proteins for SHH, the regulatory SUFU and DYRK1 and the regulated GLI-type activator proteins. Every inherited change or mutation, or retention of some embryonic motif in adult organism, or overproduction of GLI can cause basal cell carcinomas (BCC), cylindromas and other cancers.

The Centre of excellence is equipped with all the necessary equipment and facilities for working with cell biology and molecular biology techniques. The laboratory is equipped with all the necessary apparatus for DNA analysis, cell and tissue culture apparatus, preparative fermentation facilities, and access to work with laboratory animals and plants. The equipment includes cold rooms, radioactivity lab, plant growth rooms and chambers, scintillation counter, spectrophotometers, ultracentrifuges, horizontal and vertical electrophoresis systems, gel documentation system, HPLC-s, FPLC, cytofluorimeter, ABI 310 Genetic Analyzer, PCR thermocyclers, ELISA readers, TRFIA readers, hybridization oven, UV crosslinker, phosphoimager, incubators, laminar flows, research microscopes (fluorescence, Nomarski, phase contrast), inverted microscopes (fluorescence, phase contrast), stereo microscopes, video imaging fluorimeter, amino acid analyzer, fermenters, etc. The new animal facility is being finished. The reference databases are CD-vault based and internet-connected.

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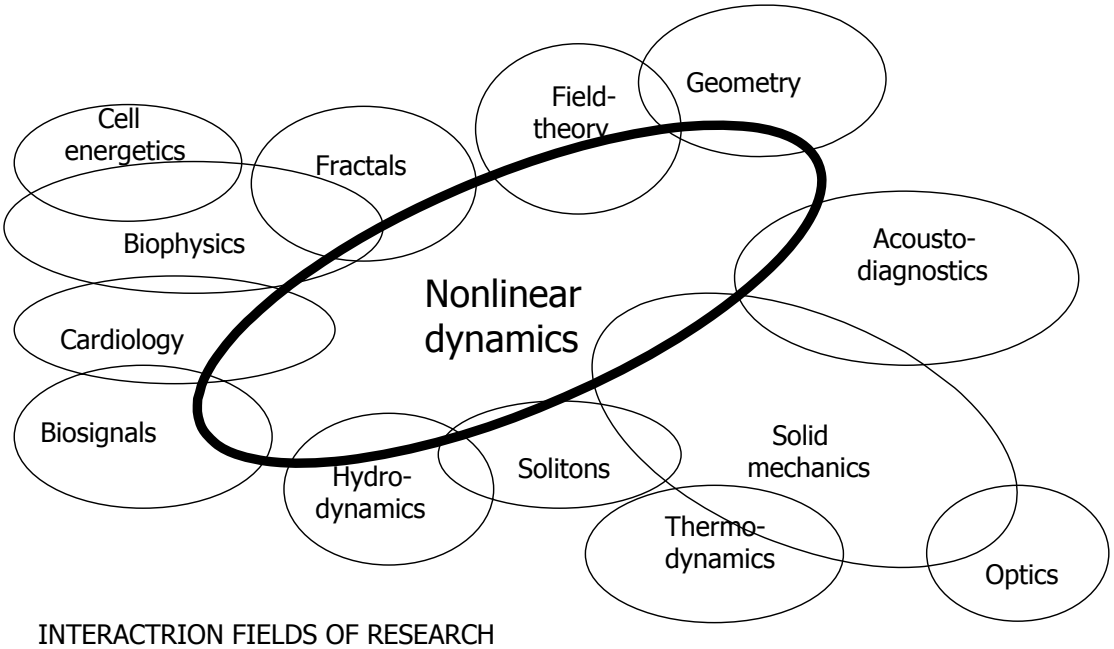
The CENS was founded already in 1999 in order to bring under one umbrella the scientific potential in Estonia engaged in interdisciplinary studies of complex nonlinear processes ("nonlinear science"). Many problems on the frontier of science that stem from solid mechanics, fluid dynamics, fractality of nature, biophysics, optics together with the theory of differential equations are interwoven into the general framework of complexity and nonlinear dynamics.

This framework includes both coherent (eg soliton dynamics) and chaotic phenomena. Nonlinearity is a fundamental property of nature and the additivity is lost in nonlinear systems that gives rise to new phenomena and is extremely important as for understanding nature as well for high technology.

The present research of CENS involves:

- Nonlinear waves: complexity of wave motion in solids, coherent wave fields, solitonics and surface waves, phase-transformation fronts, acoustodiagnostics of material properties, micro-structured materials, impact;
- Fractality and biophysics: complexity in biophysics, in silico modelling of cardiac mechanics and cell energetics, heart rate variability, turbulent diffusion, statistical topography and flooding, econophysics;
- Nonlinear integrated photoelasticity: stress field tomography (tensor tomography), complexity of interference fringes;
- Water waves: marine physics, multimodal waves, wind wave forecast, anomalies of wave fields, extreme waves;
- Geometric approach: Lie-Cartan methods, flows of vector fields on tensor fields;
- Nonlinear signal processing: analysis of physiological signals (EKG, EEG), and applications in cardiology and brain reasearch (hypoxic states of the brain).

The main aim of CENS is to be at the frontier of science in all these fields and also react to national interests.



INTERACTRION FIELDS OF RESEARCH

The International Advisory Board:

Prof Josef Ballmann, RWTH Aachen;
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Dr Andras Szekeres, Budapest Technical University;
Prof Dick van Campen, Eindhoven University of Technology;
Prof Embrecht van Groesen, Twente University

has approved this aim and the main results of recent years:

- the concepts and analyses of of hidden solitons, soliton patterns and solitary ensembles;
- thermodynamical modelling of phase transition front propagation and FGMs;
- methods of acoustodiagnostics for NDT;
- mathematical models of hysteretic piano hammers;
- novel models for describing cardiac mechanoenergetics and cell energetics;
- explanation of cardiac arrhythmias on the basis of a quiescent nerve pulse equation;
- solving an inverse problem of a 2D soliton pattern with interaction solitons,
- kinetic theory for multimodal water waves;
- explaining complexity of geophysical turbulence;
- theory of interference blots in photoelasticity;
- optical tensor field tomography;
- algebra of supersymmetry and Lie derivatives;
- nonlinear EEG signal processing.

More detailed results are described below by teams

CENS is funded by the Ministry of Education and Research and by Estonian SF grants, altogether in 2003 in sum about of 4 MEEK There have been several international grants (BMBF, NATO etc) and presently an ESF programme (NATEMIS), the Parrot programme and the EU contract PAPA. A project of the 6th FP is to be starting. Several international contracts are related to photoelasticity.

There are many international co-operation agreements and working contacts (Paris 6, Twente, Eindhoven, Helsinki, Uppsala, Lyngby, Turin, Aachen, Grenoble, Wroclav, Hong Kong; Budapest, Loughborouh). The fellows have been recognised by the Humboldt Fondation, Marie Curie Fond (two recent post-doc positions), Fulbright Fond, etc. In Estonia, the collaboration is with the NICPB, TU, MSI at TUT, IG at TUT, Estonian Diagnostic Centre. Contracts from Marine Department and Tallinn Port are related to measurements of wave fields.

During the last 5 years 5 PhDs have been promoted, presently there are 8 PhD students. The International Schools are organized (in 2003 the Third Glass Stress Summer School and the Advanced Study School in "Nonlinear Processes in Marine Sciences".

CENS has a cluster of Athlons (altogether 32) functioning as a system of parallel networks. The Laboratory of Photoelasticity is well equipped including automatic polariscopes and a polariscope for magnetophotoelasticity.

NONLINEAR WAVES

The main idea of research is to understand and explain complex nonlinear phenomena in wave motion and use new information for applications either in materials science or hydrodynamics.

SOLITON DYNAMICS

Resulting from the balance between nonlinear and dispersive effects, solitons can emerge and exist in dispersive media like alloys or granular materials with certain microstructure.

The cycle of studies on soliton dynamics in such materials using the KdV-type models has revealed: (i) the existence of hidden solitons and soliton ensembles; (ii) the mechanisms of soliton amplification in a force field (Fig. 1); (iii) the coherent patterns of soliton trajectories in long run.

In shallow water the dispersion is caused by the finite depth. The interaction process of solitons is characterized by the existence of interaction solitons (Fig. 2). It has been shown how the interaction patterns can be constructed and used for solving the inverse problems – determining velocities and wave amplitudes from aerophotos.

Collaboration with Paris 6, Twente, MSI at TTU.

THERMOMECHANICAL MODELLING

The propagation of waves and phase-transition fronts in thermoelastic solids are studied. Based on continuum mechanics, an effective numerical solver is derived allowing to take the discretness (singularities) into account. The accuracy of the solver is quaranteed by introducing special thermodynamical contact quantities satisfying thermodynamic consistency conditions. The problem of stress-driven propagation of phase-transition fronts is described (Fig. 3) and stress fields in FGM are determined. Results are applicable in technological designs.

Collaboration with Paris 6, Berlin TU.

ACOUSTODIAGNOSTICS

The novel idea of using nonlinear ultrasonic waves for determining material properties in NDE is developed. The methods based on continuum mechanics permit: (i) to determine the prestress field parameters (Fig.4); (ii) to. determine the physical properties of inhomogeneous nonlinear elastic materials. A novel approach includes using the information from the interaction of two probing waves. A reso-

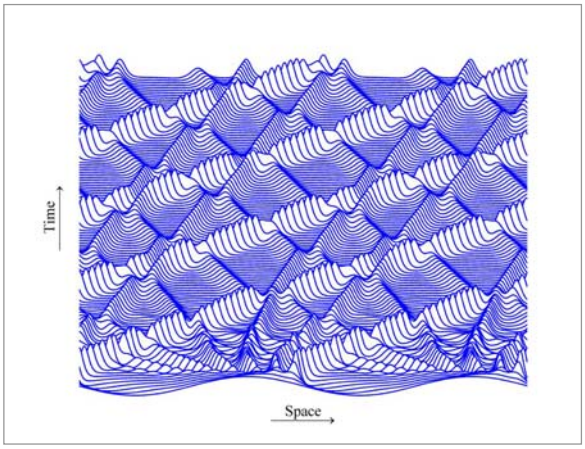


Fig. 1.
Formation of solitons from an harmonic excitation in force field. After a certain transfer period the emerging coherent pattern is seen with amplified solitons

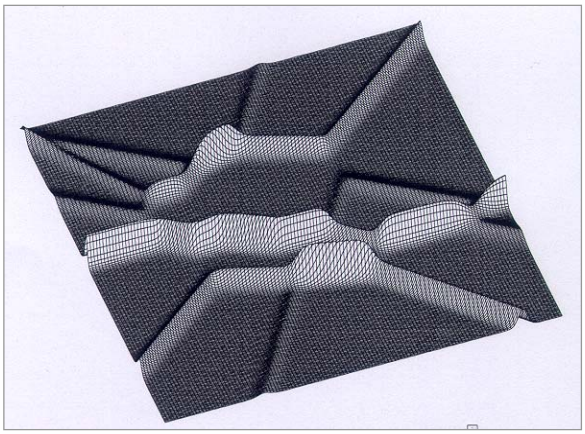


Fig. 2.
Interaction of five solitons on the water surface. Clearly seen are interaction solitons with higher amplitudes and the complex pattern of interaction.

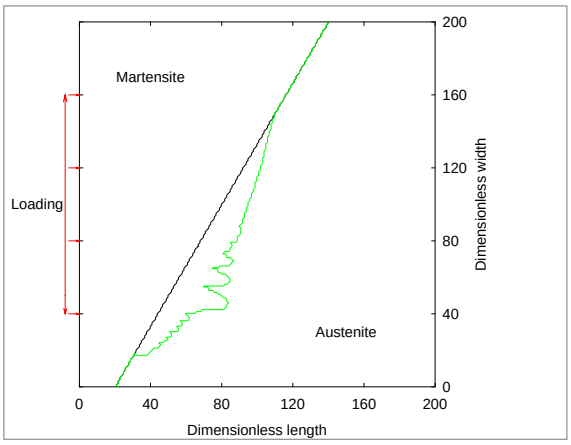


Fig. 3.
Shift of a phase boundary (green line) between martensite and austenite under localized pulse-type stress load at the left boundary. The influence of shear causes a rugged interface.

nance method is proposed based on measuring the frequency shifts in inhomogeneous materials. The studies form a part of the ESF programme NATEMIS, collaboration with Fraunhofer IZFP in Saarbrücken.

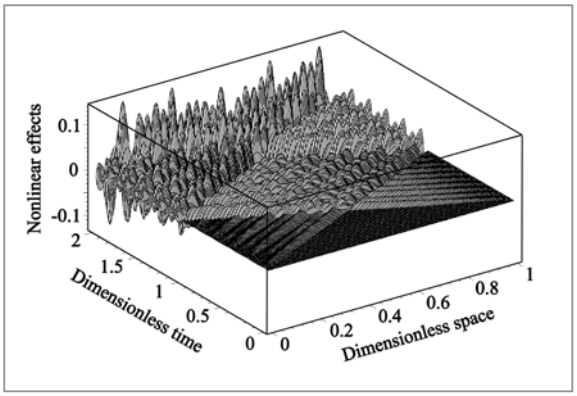
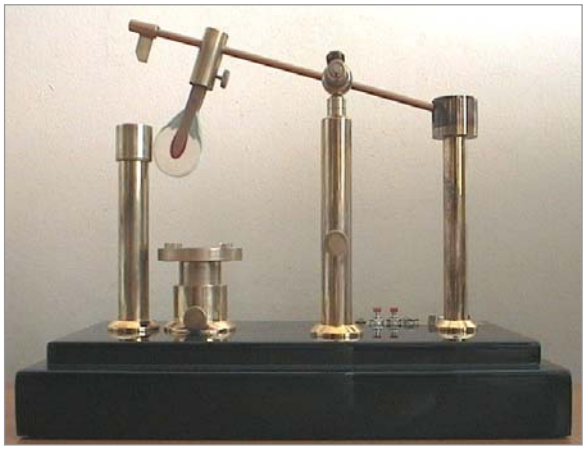


Fig. 4.
Nonlinear effects in a prestressed solid: generation and interaction of the 2nd harmonic at harmonic excitation from both boundaries. Amplification of the amplitude is clearly seen in the wave interaction interval



Testing device for piano hammers. The hysteretic parameters of felt are determined from the measured nonlinear force - compression curves

IMPACT – PIANO HAMMERS

The novel piano hammer mathematical models are derived and experimentally verified. For that purpose a special testing device is constructed (photo). The crucial point in felt modeling is to account for hysteretic effects. The studies are in close cooperation with Tallinn Piano Factory for enhancing the quality of grand pianos.

GENERAL

Ongoing studies are directed to hot problems of dynamics of microstructured materials and dispersive waves. Functionally graded materials are studied, new NDE methods are derived based on consistent modelling of continua, the mechanisms of emerging soliton complexies are investigated, explanation is given to anomalous and extreme wavefields in water basins.

Challenges include explaining the spatio-temporal chaos and Farey-tree formalism for emerging solitons and also hierarchical dispersion mechanisms in microstructured materials. Complexity of nonlinear waves includes many new phenomena for which the general theoretical background together with numerical simulation is developed.

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FRACTALITY AND BIOPHYSICS

The main aim is to understand the complexity of natural processes and learn to describe those processes, which have been beyond the reach of the classical monodisciplinary physics.

CARDIAC METABOLISM AND CONTRACTION IN HEALTH AND DISEASE

ATP, a major energy carrier in cells, is synthesized in the mitochondrial matrix and its major use in muscle is for myofibrillar contraction and ion pumps. There is much debate on the mechanism of the regulation of the ATP synthesis in the mitochondria to balance ATP consumption during changing workloads. The model of transfer of energy-rich phosporyl groups has also been disputed for decades It turns out that the cell cannot be explained from knowledge of the behaviour of its constituent macromolecules in the test tube, i.e., the whole is greater than the sum of its molecular parts.

Therefore, computer models are now considered necessary to understand the complex interplay of macromolecules in the cell. We have built a mathematical model consisting of three parts: production (OxPhos), transport, and consumption of the high energy phosphates in myocytes (see Fig. 5). The model of biochemical reactions has been furnished with a spatial organization of the major intracellular structures resulting in a complex reaction-diffusion model of a working cardiac cell. Simulations with this model, validated against numerous experiments, have shed new light to compartmentation of the high energy phosphates in both physiological and pathological conditions. An integration of the reaction-diffusion model of the cardiac cell metabolism into a 3D mechanical contraction model of a whole heartis in progress. Such a model will be suitable for studying the contraction of the ischemic or post-infarcted heart.

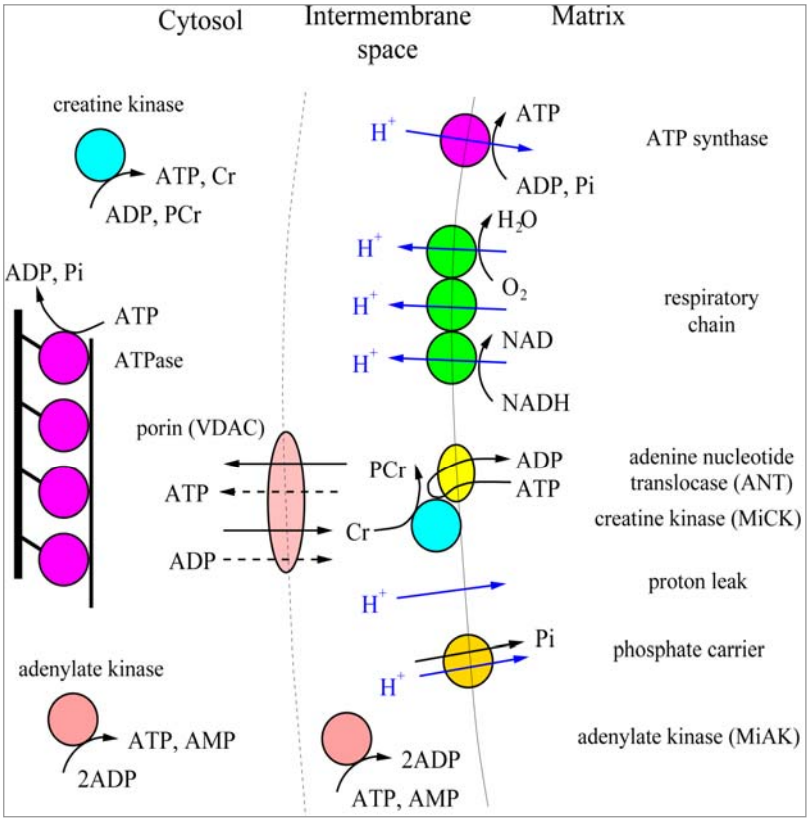

Fig. 5.
Schematic representation of the biochemical processses in the reaction-diffusion model of the heart cell.

CARDIAC ELECTRICAL ACTIVATION: ARRHYTHMIAS AND BISTABILITY

The sick heart can be bistable exhibiting coexisting modes such as normal behavior and reentry tachycardia. In terms of nonlinear dynamics, these two modes can be viewed as coexisting attractors, because without any change in external factors such as vagal or symphatetic activity, or drug level, the heart can function in either mode. The switch between the modes can occur by the temporary disturbances such as ectopic beat or the impulse from an artificial pacemaker or defibrillator. The reentry mechanism, either anatomical or functional, is possible only in the tissue with certain size and geometry together with a proper velocity of the activation front and a repolarization time. We have adapted a van der Pol-type model of the nerve pulse propagation to simulate the electrical activation of the distal part of the cardiac conduction pathway – the Purkinje tissue. With this model, we were first to propose that complex bifurcation scenarios (see Fig. 6), including global bifurcations leading to bistability, may happen in tiny regions of the distal parts of cardiac conducting system without involving the reentry mechanism.

STATISTICAL TOPOGRAPHY OF THE SYSTEMS AT SELF-ORGANIZED CRITICALITY (SOC)

For many systems at SOC, several important features of the system can be expressed in terms of random self-affine (or multi-affine) surfaces and self-similar (or multifractal) contour lines. Examples of such surfaces and lines include interfaces in various growth models, fracture surfaces, streamlines of turbulent flows, surfaces of geological landscapes, gradient-limited surfaces, isodensity lines of passively convected scalar, cloud perimeters, ripple wave turbulence etc. The statistical analysis of the geometrical properties of surfaces and contour lines is referred to as statistical topography.

Our main research results during recent years can be listed as follows. First, we have suggested a new simple model for describing the multifractal properties of chaotically mixed passive scalar (see Fig. 7). This is applicable to the distribution of pollutants, temperature etc. in turbulent flows. The model allows risk estimation arising from the leakage of environmentally harmful substances. Further, we have constructed an efficient model for numerical analysis of random self-affine surfaces, the four-vertex (4V) model. We have also suggested a new model for the evolution of geological

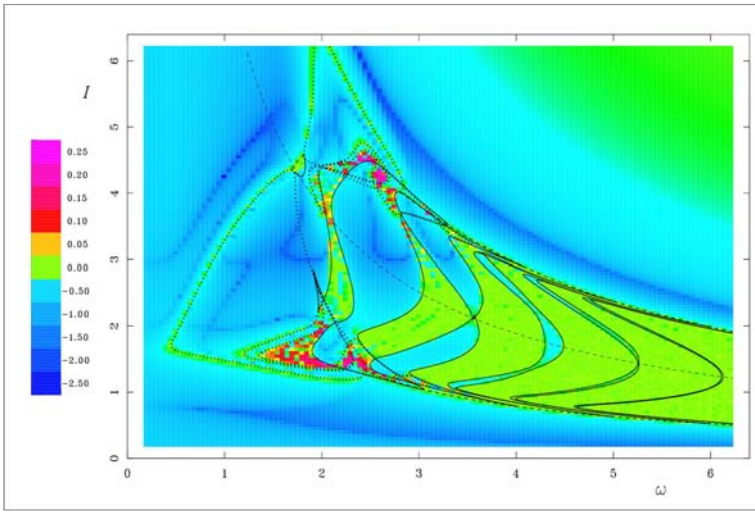

Fig. 6.
Lyapunov exponent map on the parameter plane for the periodical driven nerve pulse equation modelling cardiac conduction.

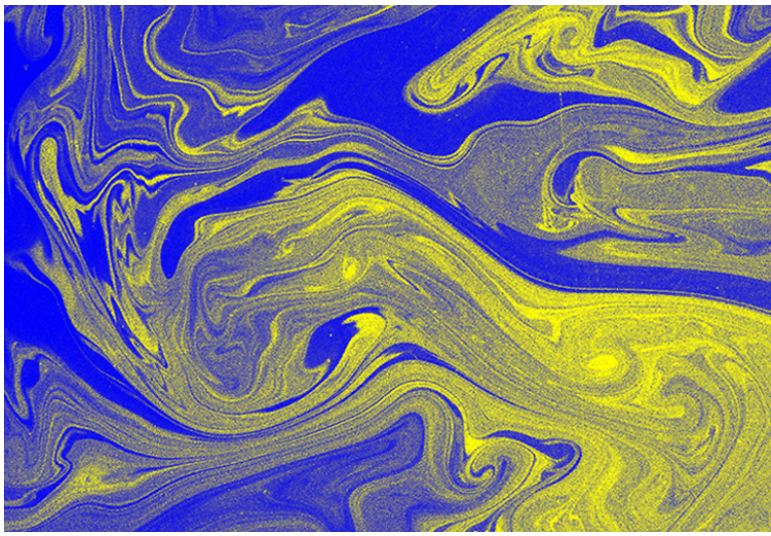

Fig. 7.
A chaotic mixing of an initially smooth field of dye by a smooth chaotic velocity field leads to complex multifractal patterns.

landscapes, the model of gradient-limited surfaces. This model captures the most universal features of real landscapes (e.g. scale-dependence of differential roughness exponent). Finally, we have introduced a new object of analysis, the "oceanic coastline"; we have shown that for negative roughness exponents, these coastlines are mapped to the percolation clusters of the correlated percolation problem.

Our current studies in the field of statistical topography include numerical analysis of the contour line statistics of the surfaces with negative roughness exponent, application of the 4V model for the calculation of turbulent transport

in quasistationary turbulent stream, analytical and numerical studies of the diffusion in fully developed turbulence, applica-tions in geophysics.

ANALYSIS OF NON-LINEAR TIME-SERIES

Non-stationary time-series are characteristic to a wide variety of processes, such as heart rate, electrical activity of brain (ECG), rainfall, geotectonic activity, financial time-series etc. Standard linear measures are far from being adequate tools for the analysis of these intermittent data. The methods based on non-linear deterministic models (e.g. correlation dimension) are neither appropriate. It is widely recognized that an appropriate approach to the analysis of non-stationary data is based on multifractal analysis.

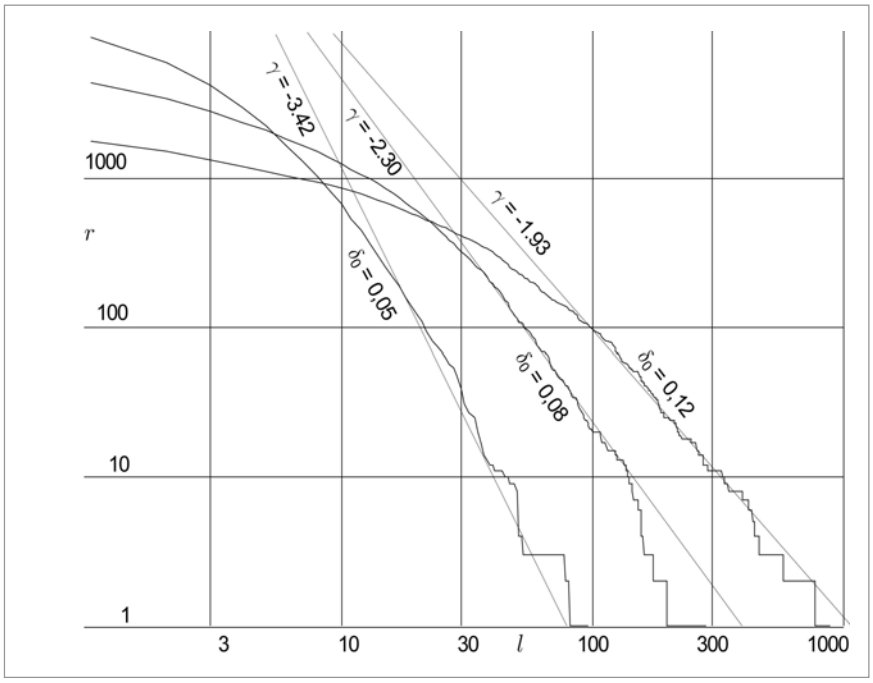

Fig. 8.
The length-distribution of low variablity periods of human heart rhythm is described by the multiscaling Zipf's law: The scaling exponent γ depends on the parameter δ_0 .

We have shown that even multifractal analysis is not sufficient for revealing all the features of such time series, the most important omission being the failure to describe long-term clustering of low-variability periods. To address this aspect, we have introduced the method based on multiscaling Zipf's law describing the distribution of low-variability periods (see Fig. 8). For heart rate variability, the measures based on this distribution law have a good diagnostic performance. We have also shown the relevance of this method to financial data. Further, we have studied the possible sources of false detection of deterministic chaos in he- art rate signal. We have shown that the mode-locking between the heart rate and respiration plays an important role in the formation of apparent structures in the reconstructed phase space. Our current studies involve comparative analysis of known nonlinear techniques of intermittent time-series analysis, and investigating the role of Lévi flights in the heart rate dynamics.

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NONLINEAR INTEGRATED PHOTOELASTICITY

The goal of this research project is to widen the possibilities of integrated photoelasticity by non-destructive measurement of three-dimensional stress fields. The main application area of the results is residual stress measurement in various glass articles. Nonlinearity of the problem follows from the fact that the relationships between the parameters of the stress field and experimental data are nonlinear. Additional nonlinear effect is caused by the bending of the light rays when polarized light is passed through an inhomogeneous birefringent medium.

The first step consists of the investigation of the limits of application of the linearized solution of the equations of integrated photoelasticity. It has been shown that by measuring residual stress in axisymmetric glass articles (bottles, drinking glasses, neck tubes of CRT bulbs, etc.) the linear approximation gives reliable results. The algorithm, which is based on the nonlinear solution of the equations, is being developed

mography deals with the measurement of scalar fields, in photoelastic tomography we have to determine a tensor field. This complicated problem of tensor field tomography has been decomposed to several problems of scalar field tomography for separate components of the stress tensor. The method has been implemented at the Laboratory of Photoelasticity of the Institute of Cybernetics using the automatic polariscope AP-05 SM, which is supplied with a rotary stage for rotating the specimen.

A tomographic photoelastic method for the measurement of arbitrary three-dimensional stress fields, based on linear approximation, has been developed. The section under investigation is illuminated in many directions making photoelastic measurements on many light rays for every direction. While the classical to-

As an example, Fig. 9 shows geometry of a high-pressure lamp, the stress field in section A-B is shown in Fig. 10.

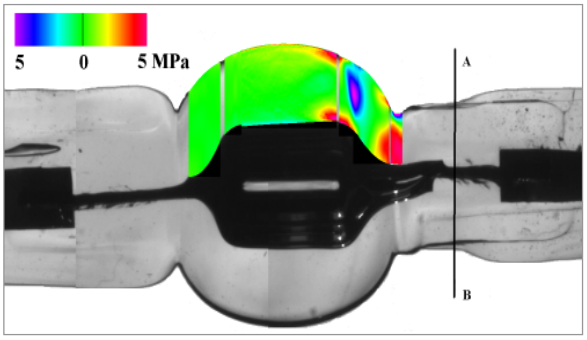

Fig. 9.
Geometry of the high-pressure lamp and axial stress field in the axisymmetric part.

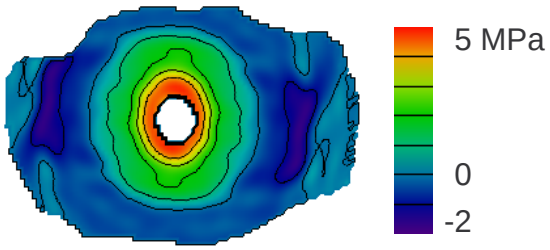

Fig. 10.
Normal stress field in section AB of the high-pressure lamp; 180 projections.

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WATER WAVES

The interests of the working group include (bu are not limited to) various nonlinear phenc mena occurring in different wave systems i marine environment. A large part of research i concentrated on wave-wave interactions in th framework of the kinetic equation (that des cribes slow evolution of weakly nonlinea waves). Rossby waves (large-scale oscillation in the oceans and the atmosphere) serve as rich model system where many attractiv results can be derived analytically. Considerabl efforts have been directed to analysis c existing surface wave models, in particula towards including specific effects of the Balti Sea environment into these models. During th last years, specific properties of fast ship wave in the vicinity of the Tallinn-Helsinki ship lan have been studied.

HIGHLIGHTS 2001-2003

Shown was that the structure of the set c solutions to kinetic equations mostly depend on the number of interacting waves. Th energy exhange between specific modes c Rossby waves in a three-layer ocean model fail if and only if an eigenvector of the potentia vorticity equations has a zero entry. Thi happens in the case of several simple vertica structures of the ocean.

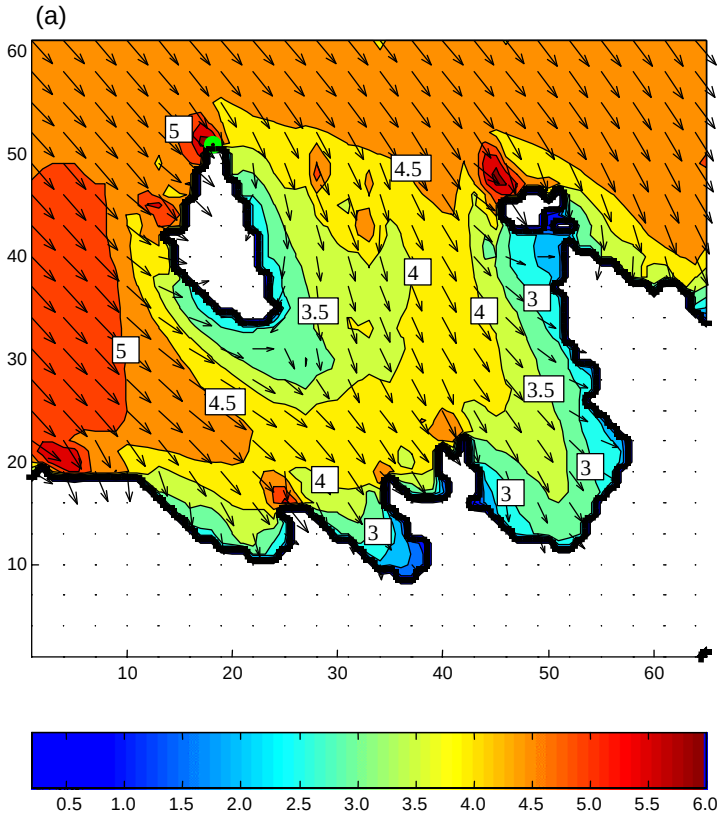

Fig. 11.
Significant wave height and wave propagation direction in Tallinn Bay during an extreme strom 15.11.2002

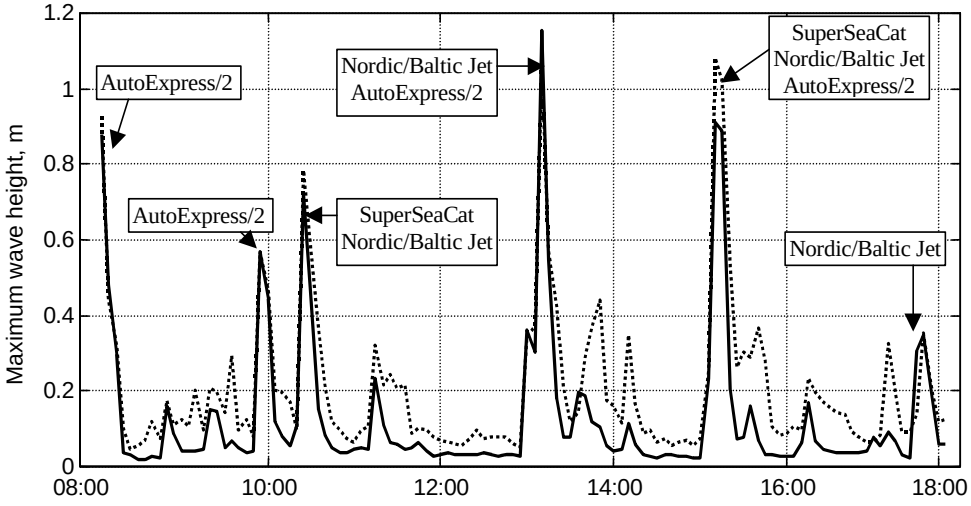

Fig. 12.
The maximum height of the long wave components (periods >5s, bold line) and of the whole wake of fast ferries (dotted line) near the Aegna jetty on 14.04.2002.

It was demonstrated that in many areas of the Baltic Sea the wind anisotropy much more affects wave properties than the fetch length. As a practical application, it has been demonstrated that the wake of fast ferries is a new forcing component of vital impact of the local ecosystem of semi-open bays that may cause considerable intensification of beach processes and have significant influence on the aquatic wildlife.

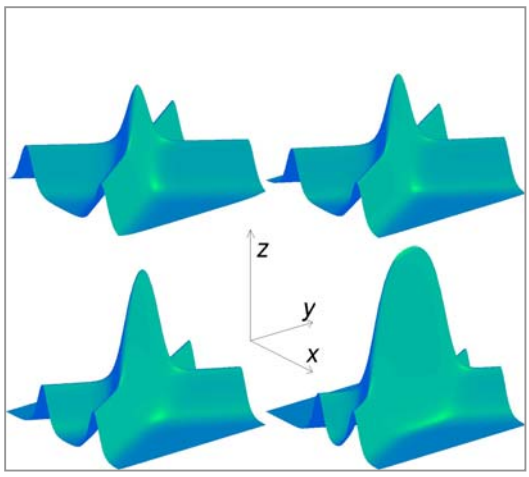

Fig. 13.
Surface elevation in the vicinity of the interaction area, corresponding to incoming solitons with equal amplitudes but different angles between their crests.

SELECTED EXAMPLES OF STUDIES

Many wave systems (e.g. Rossby waves, internal waves) can be described as a superposition of a number of vertical modes in which energy exhange rate depends on both interaction and coupling coefficients. As an example of multi-modal kinetic equations for wave systems with comparable frequencies, the kinetic description of baroclinic Rossby waves in a multi-layer model ocean is analysed. Explicit expressions for the coupling coefficients are obtained for the three-layer model. Several types of interactions vanish in the case of simple vertical structures of the ocean. The largest number of void interactions occur when the top and the bottom layer are equal in depth and the medium layer is twice as thick as the top layer. Such a situation normally does not occur in the open ocean but frequently appears in the Baltic Sea conditions.

The structure of the set of thermodynamically equilibrated solutions to kinetic equations depends on the particular wave class. It was shown that this structure basically depends only on the parity of the number of resonantly interacting waves whereas wave action is conserved only in the framework of interactions of an even number of waves. Formally, solutions that correspond to negative energies in certain area of wave vectors may arise. The existence of such solutions, their stability, physical meaning and realizability conditions in realistic wave systems has been examined in detail.

Laboratory experiments with closely packed clusters of vortices of one sign (Grenoble, 13-m rotating platform "Coriolis") demonstrated several anomalous features of quasi-2D geostrophic vortices. First, relatively long-living structures consisting of two concentrated cyclones were detected. Second, concentrated anticyclones showed a tendency to penetrate into large cyclones and to form axisymmetric mostly cyclonic structures with oppositely rotating 'eye'.

The wind field in both Baltic proper and in the largest subbasins of the Baltic Sea has an extremely complex and spatially nonhomogeneous nature. The wind anisotropy has considerably influence on the properties of wind wave fields. Wind wave statistics and wave height anomalies in the Baltic Sea are studied using the third generation wave model WAM. In certain regions wave height may increase in extreme cases about 2 m as compared to wave heights in the open sea. In many areas of the Baltic Sea the wind anisotropy much more affects wave properties than the fetch length.

High speed craft (HSC) ships of various size cross Tallinn Bay up to 70 times per day during the navigation period.The ships frequently sail with speeds close to the critical velocity and produce extremely long-crested waves.

The annual mean energy of ship waves is about 10% from the bulk wave energy and wave power (energy flux) as high as 40% from the bulk wave power in the coastal zone of the bay. The highest components of ship wakes with the heights about 1 m have frequently periods 10-15 s. Such surface waves do not exist in natural conditions in the area in question. They cause unusually high near-bottom velocities at the depths of 5-20 m. Such waves form a new forcing component of vital impact on the local ecosystem that may cause considerable intensification of beach processes as well as enhanced vertical mixing in the water body, and have significant influence on the aquatic wildlife.

Interaction of two long-crested shallow water waves (such waves are frequently generated by high speed ships) is analysed in the framework of two-soliton solution of the Kadomtsev-Petviashvili equation in cooperation of the group of nonlinear waves (P. Peterson, J. Engelbrecht). The wave system is decomposed into the incoming and the interaction soliton that represents the particularly high wave hump analogous to Mach stem in the crossing area of the waves. Shown is that extreme surface elevations up to four times exceeding the amplitude of the incoming waves typically cover a very small

area but in the near-resonance case they may have considerable extension.

AWARDS:Estonian State Science Award 2002 in technical sciences: T. Soomere, together with J. Elken (group leader), T. Kõuts, J. Kask and U. Liiv for a cycle of studies "Hydrodynamical and geological investigations of possible deep harbour sites in north-western Saaremaa Island".

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GEOMETRY AND DYNAMICS

The main idea of research is to study the universal properties of the structure of infinite jet space

Proved theorem about universality of jet space allows to study on the manifold M different differential operators (Laplacian, Hessian, curvature tensor of connection) and their symmetries. The knowledge of symmetries is impor-tant in many aspects e.g. to calculate the integ-rating factors, multiply the solution and first integrals of differential equations, prolong the group operators or study of map singularities. As a result we have a new vision about the nature of differential equations and dynamical systems, connections in fiber spaces, represen-tations of Lie groups and classification of geo-metrical objects by algebraic and differential invariants. The ties between classical theories (highest order differential geometry, envelopes and catastrophes, stability of singularities, mechanics of continuous media) appear.

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NONLINEAR SIGNAL PROCESSING

The aim of this study is to obtain information about physiological systems, first of all brain and heart, using analyses of the bioelectrical signals created by the physiological sources. New knowledge and understanding of the principles of their operation can be applied in developing medical technology. Physiological processes are nonlinear by nature. Complex feedback and regulation mechanisms are involved. This implies that applying nonlinear analysis methods has an important role in describing and understanding these processes.

EFFECT OF MICROWAVE AND PHOTIC STIMULATION ON THE EEG SIGNAL, ATTENTION, AND MEMORY

Mechanisms of stimulation by electromagnetic fields (EMF) are not clear up to now. Clarification of the EMF biological effects is important for understanding of the principles of nervous activity and applications in medical practice – development of treatment methods for psychological disorders, rehabilitation etc.

Research group focused its efforts to the effects of low-level modulated microwave radia-

tion during several years. Two types of experiments were carried out aimed to direct EMF effect on human EEG rhythms and indirect effect on mental performances. Field power density of the applied 450 MHz microwave radiation was about an order of magnitude lower than the existing health protection requirements.

Our experimental results demonstrated that effect caused by microwaves as a nonspecific stressor was noticeable but less than that of photic stimulation. Most effective was 7 Hz modulation frequency. In the majority of cases, photic stimulation caused changes in the EEG energy level in the occipital and microwave stimulation in the frontal region. Changes varied strongly from subject to subject. The variability of the EEG parameters increased under microwave exposure

We applied Higuchi fractal dimension analysis to the EEG signals. The results showed that photic stimulation consistently caused increase in the fractal dimension of the EEG signal while the results for the microwave stimulation were more difficult to interpret. However, in some subjects clear correlation between the microwave stimulation and the fractal dimension was seen (see Fig. 14).

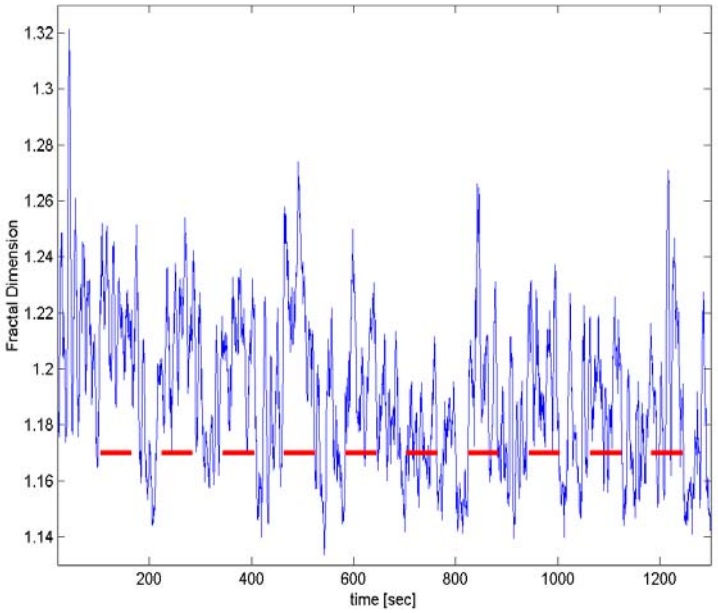

Fig. 14.
Correlation between the fractal dimension of the EEG and microwave stimulation (stimulation periods are marked with red lines).

The results of psychological tests showed that in the case of the most complicated task the number of errors increased when microwave radiation was switched on. In the case of a simpler test a significant decrease in errors in the exposed group was seen. This experiment provides additional evidence that acute low-level exposure to microwaves modulated at 7Hz can affect cognitive processes, such as attention and short-term memory.

ASSESSMENT OF DEPTH OF ANESTHESIA AND THE PHENOMENA CAUSED BY ANESTHETIC AGENTS IN THE EEG

Traditionally the depth of anesthesia has been assessed using such indirect measures as the reaction of the patient to verbal stimuli, motor reflexes etc. This kind of assessment, however, has proved to be not sufficient in many cases.

Recently several methods have been presented for the assessment of the depth of anesthesia using the EEG signal. Probably the best known such measure is the bispectral index incorporated to several commercial anesthesia monitors. The assessment of the depth of anesthesia is based on understandig the changes in the function of the nervous system caused by anesthetic agents. In cooperation with finnish scientists we have studied the phenomena caused in human brain by propofol, a modern popular intravenous anesthetic agent. By calculating the coherence between the EEG measured from subthalamic nucleus and from scalp we found that while depth of anesthesia increases a jump in the frequency of synchronous EEG rhythm from 10 Hz to 20 Hz occurrs. This is followed by gradual decrease of the frequency until burst-suppression pattern appears (see Fig. 15). The independence of the different components of the burst-suppression pattern were also studied using the Independent Component Analysis (ICA) method. Although the physiological meaning of these findings is still unclear, the discovered phenomenon is an imporatnt step towards understanding the mechanisms behind propofol anesthesia.

DETECTION AND CLASSIFICATION OF CARDIAC ARRHYTHMIAS

Investigation of cardiac arrhythmias together with French and Polish scientists resulted in remarkable achievements in control algorithms for cardiac pacemakers. Further investigation was focused on the ECG signal analyses to evaluate the possible correlation between the level of myocardial electrical instability assessed

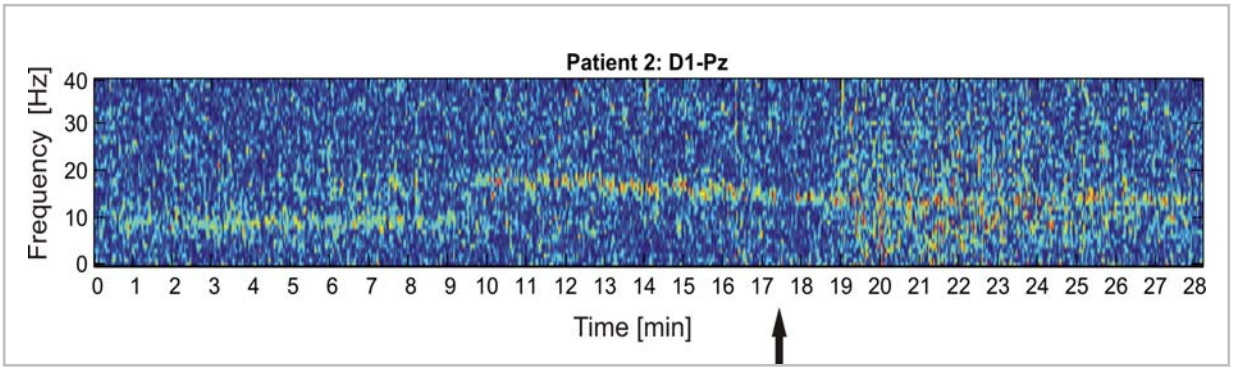

Fig. 15.
Coherence between depth and scalp electrodes during the course of anesthesia. The onset of burst-suppression is marked by an arrow.

during Holter monitoring and certain ventricular repolarization parameters. The majority of the parameters containing prognostic significance for increased myocardial electrical instability seem to be related to the first part of the RT interval. RTs interval, i.e. the fragment from R-wave peak to the onset of the T-wave, was proved to be one of the most sensitive parameters of myocardial electrical instability. RTs interval duration did not correlate with RR interval. It has very weak correlation with RT interval and therefore it seems to be an independent diagnostic parameter.

The approximate entropy parameter was used to assess the value of the above described parameters in detecting the risk of cardiac death. It was found that entropy increases and the dynamics of the entropy value decreases in correlation with the increase in ventricular instability. The study was carried out in co-operation with Estonian Institute of Cardiology and Tallinn Diagnostic Centre.

Further investigations are focused on application of the nonlinear signal processing methods to analyses of the EEG signals in existing databases and experimental studies aimed to clarification of the interaction mechanisms of different physical and chemical factors with brain.

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Recent decades have witnessed the accelerating development of two broad disciplines – behavioural sciences and health sciences – which both have great impact on society and are characterised by their multidisciplinary approach.

Both of these scientific fields make use of a wide array of methodologies, often in combination; the methods applied by these two fields are, however, largely similar, as sometimes are the research questions addressed. Estonian Centre of Behavioural and Health Sciences has the aim to ensure appropriate conditions for research to the already available competence in these disciplines in Estonia, to guarantee further development and world class standards through a co-ordinated research network and efficient and integrated graduate study programs, and to bring together theoretical and applied research with a special emphasis on the multidisciplinary approach.

The main directions of research at the ECBHS are the processes of perception and cognition, the structure of personality and its biological and cultural underpinnings, child development and assessment and promotion of children's health, assessment of persistence of individual differences and their neurobiological modelling, the physiological, psychological and social determinants of health, the convergent influence of personality and environment on behaviour and health, and longitudinal and multilevel assessment of health impacts. The Centre's International Steering Committee includes Neil Armstrong (University of Exeter, U.K.), Steven Blair (The Cooper Institute, Dallas, U.S.A.), Risto Näätänen (University of Helsinki, Finland), Endel Tulving (University of Toronto, Canada), and Björn Wittrock (University of Uppsala, Swedish College for Advanced Studies in Social Sciences).

Prof Endel Tulving, member of the international steering committee of the ECBHS, lecturing to the Centre's doctoral students.

The ECBHS promotes both in-depth studies in specific areas of research and interdisciplinary contacts. In joint efforts to conduct doctoral training the intention is the provide future scientists and specialists with the experience of aiming at the highest standards in specific methodological competences and of using this expertise for tasks which cross boundaries between research fields. The Centre provides incentives for aiming at higher achievements to the PhD students. Regular interdisciplinary seminars and annual conference have already led to novel collaborative projects. Currently members of the ECBHS hold six target financed projects of the Estonian Ministry of Education and Science, one post-doctoral target financed project, 27 grants of the Estonian Science Foundation, and several international grants, and are involved in a number of international networks. Two major advances, an EC 6th Framework Integrated Project NEWMOOD, and the Estonian project of the European Science Foundation's European Social Survey, are about to begin. The Centre has modern equipment for neurobiological, behavioural and movement studies which to a large extent has been obtained in the few recent years, and adequate hard- and software for data analysis.

Researchers of the ECBHS have achieved broad international recognition with studies such as the localization of phoneme analysis in the brain, published together with colleagues at the University of Helsinki in Nature and Nature Neuroscience, identification of the hierarchical nature of collectivism, theoretical modelling of depression and development of novel experimental models of affective disorders, a psychophysiological model of visual masking, demonstration of the critical role of alcohol use in male suicide, and epidemiological analyses of risk factors of some diseases.

PERCEPTION AND PERSONALITY

Research team: Prof Jüri Allik (PhD), Anu Realo (PhD), Olev Must (PhD), Kairi Kreegipuu (PhD), Talvi Kallasmaa (PhD), Aave Hannus (MSc), Kenn Konstabel (MSc), Kaia Laidra (MSc), Kätlin Nummert (MSc), Helle Pullmann (MSc), Monika Schmidt (MSc), Raivo Valk (MSc), Toivo Aavik (MSc), Aire Mill (MSc), Maris Kaskmann (MSc).

The main research areas of the Perception and Personality Research Group are visual perception (programming of eye movements; movement perception), personality, mental abilities, and cross-cultural psychology. In the year 2003, the research group has published 15 papers in journals covered in ISI Web of Science. In the following, we mention the group's most important research results of the past few years.

Among the most important results in the field of perception is a novel mathematical model explaining how the parameters (e.g., direction and amplitude) of a planned movement are programmed. The data fit almost perfectly to the model, showing that, contrary to the commonly accepted view, the amplitude and direction of saccadic movements are programmed separately rather than as a single vector. The novel temporal disassociation method for studying programming of movements, and the model of growth processes, are applicable to other information processing problems, where binding and coordination of separate features are necessary. Another series of studies is about perception of spatial and temporal properties of moving objects. The localisation errors of moving objects are commonly explained by delays caused by slow processing. The result that spatial and temporal decisions are inconsistent with each other shows the erroneousness of this practice.

In the field of personality psychology, we have adapted the world's most widely used and theoretically soundest instrument for measuring personality traits, the revised NEO Personality Inventory, which has enabled us to investigate the sources cross-cultural variations in personality trait structure. In collaboration with one of the world's leading personality psychologists, Dr. Robert R. McCrae (among the first 10 most frequently cited social scientists), an edited book on cross-cultural applicability of personality taxonomy has been published at Kluwer/Plenum. Five-factor, an attempt to organise the scientific knowledeg about personality into a coherent scheme, was proposed in 1996 by R. McCrae and P. Costa. The most comprehensive and up-to-date overview of this theory has been written by Allik and McCrae. In elaborating the five-factor theory, Allik and McCrae discovered strict regularities in the global geographic distribution of personality traits.

In studying people's beliefs about their own ability of person perception, it was surprisingly found that there is no correlation with actual ability to understand other people's mental states, to recognize emotions and personality traits. Differently from actual performance, the subjective beliefs had no correlation with psychometric intelligence, but were related to personality traits.

Studies in the field of mental abilities have explored the sources of the Flynn effect (gains in intelligence test scores with every next generation or cohort); the results show that the gains are primarily in the sub-tests which are less related to general intelligence.

In the framework of an international collaboration programme (Social Representations of HIV/AIDS in Central and Eastern Europe), the relationship of attitudes and values with sexual behavior was studied. People who value openness to change, hedonism and self-enhancement, tend to engage in risky sexual behaviours, whereas people with higher score on collectivism are more conservative and restricted in their sexual behaviour. The possible role of social attitudes and representations in the spread of HIV/AIDS epidemic was demonstrated.

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PSYCHOPHYSIOLOGY

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Main research directions of the group are experimental and theoretical modelling of depression, neurochemistry of noradrenergic-dopaminnergic interactions and related neuropeptides, psychopharmacology of individual differences, and biological psychology of impulsivity. Thus focus has been placed on the neurobiological regulation of affect, and its meaning for behaviour.

Research group which initially consisted of the group leader and one MSc student includes now besides its leader two researchers, one technician, three PhD students and five MSc students. Since 1999 the group has a target financed project of the Estonian Ministry of Education and Science. Currently the group hold two grants from tha Estonian Science Foundation and has a research contract with the Estonian Road Administration. In 1998-2003, 42 articles in international journals or chapters in books by major publishers have been produced. The work of the group leader has according to SCI been cited over 1400 times.

Psychophysiology Research Group has developed the most comprehensive pathogenetic theory of depression, and a couple of new experimental models of depression to facilitate discoveries of antidepressants with principally novel mechanisms of action. We have demonstrated the existence of previously undescribed aspects of control mechanisms over dopaminergic neurotransmission by other neurotransmitter systems, and localised in the brain specific neurochemical processes which govern affects. While most of this research is carried out in animals, some constructs are being studied in humans by means of search for biomarkers of personality and behaviour. Recently we demonstrated in collaboration with other groups that the activitity of platelet monoamine oxidase (MAO) which is a marker of serotonergic capacity in the brain is significantly lower in men caught driving while intoxicated by alcohol. These subjects also have higher dysfunctional impulsivity, and thus probably a general deficiency in control of behavioural urges. In another study with a longitudinal design it was found that platelet MAO activity can predict regular smoking in adolescents. Most interestingly, this association is clearly nonlinear, regular smoking being predicted by the size of deviation from the average.

The strategy of the group has been a creative combination of different techniques. Multidisciplinary methodological competence is achieved by means of active collaboration with several leading experts in the field. Current priority projects include joint studies on noradrenergic-dopaminergic interactions using dual-probe

In the psychophysiology laboratory.

microdialysis with Ben Westerink, Department of Biomonitoring, University of Groningen, ELISA and EMSA studies on transcription factors together with Lars Oreland, Department of Neuroscience, University of Uppsala, and immunochemical studies on neuropeptides and neuropeptide antibodies together with Tomas Hökfelt, Department of Neuroscience, Karolinska Institutet. Psychophysiology Group has an extensive network of collaborations in the University of Tartu, including its activities as the Psychopharmacological Drug Development Group in the Centre of Medical Technology in Biomedicum. Active collaboration is also ongoing with the Tallinn Pedagogical University and the National Institute for Health Development. The group was instrumental in developing the concept of the Centre of Behavioural and Health Sciences in 2001, and in conducting of its activities thereafter.

The group has sufficient equipment for studies in behavioural pharmacology and of biomarkers of personality, and very modern equipment for intracerebral neurochemical studies in freely moving animals. Further developments will be based on the activities of the EC 6th Framework integrated project NEWMOOD consortium which consists of 13 partners. This is built to foster multidisciplinary research on depression – from molecular genetics and genomics to human brain imaging and drug development. This project expands the technological scope of the group by means of adding new equipment, and know-how from new colloborators from nine countries.

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DEVELOPMENTAL AND EDUCATIONAL PSYCHOLOGY

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Developmental and Educational Psychology Research Group aims to study the influence of culture – more specifically, that of home socialization and school education – on the development of children. The studies are grounded by the theoretical approach of Peeter Tulviste. While the emphases of the research of the Developmental Psychology Group is on home socialization, the School Psychology Group deals with the problems of the development of thinking but also with the problems of the development of children with special needs and the ways of helping them.

Studies in developmental psychology address the characteristics of language socialization – i.e., the socialization of how to use language and the socialization through language – in mother-child interactions and peer interaction. In addition to the real-life video recordings of family mealtime interactions and peer interactions at the day-care centrums, the mothers' attitudes towards social issues such as value preferences, and child-rearing goals provide comparative background information.

Comparative research on mothers' interaction with adolescents at meals demonstrated that the directive conversational style preferred by Estonian middle-class mothers contrasted strongly not only with American mothers of adolescents, but also with mothers residing in the neighbouring countries Finland and Sweden, including the Estonian-speaking mothers living in Sweden. Furthermore, the studies revealed that the Swedish sample was as talkative as the American, differing in this respect from all Finno-Ugric samples, and that different social norms and values were emphasized in Estonian, Finnish, and Swedish mono- and bicultural families. The Estonian monocultural mothers place less emphasis on self-direction (creativity and independence) than the Swedish mothers. The items rated most important as the parents' developmental goals were "I wish that my child would believe in his/her abilities" by the majority of Swedish and Finnish mothers of preschool age children, while the Estonian mothers emphasized "I wish that my child would grow up to be a diligent and capable person" and "I wish to raise my child into a conscientious and reliable person" more frequently.

In conclusion, the Estonian mothers appear to value and exercise somewhat less democratic and more traditional socialization styles than their Finnish and Swedish counterparts.

The studies in school psychology have contributed to the discussions if children's concepts are coherent and integrated into theoreties or fragmented, the relations between thinking and ability level and knowledge, the development of knowledge in the course of learning. We have studied the concepts of astronomy and chemistry. We have shown the fragmentality of concepts but also how synthetic concepts and verbalisms evolve during learning. Due to the teacher-centered teaching methods and emphases on teaching factual knowledge, Estonian state school children develop verbalisms, however, in contrast, the development of synthetic concepts has been shown to occur while using experimental teaching methods.

Also, we have analysed the activities of school psychologists, the attitudes of clients towards these services; the comparisons between various cultures have been made. Estonian school psychologists work mainly with individual children, and this work is very time-consuming. Although both psychologists and clients like the model, it is economically inefficient and there-

fore less and less used in other countries. Additionally, we also develop and adapt tests. This part of the research is of great practical value in Estonian context, providing better opportunities for helping children with special needs.

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PERCEPTION AND CONSCIOUSNESS

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Recent research in Perception and Consciousness Research Group has been focused on the microgenesis of visual images, spatial attention, masking, and flash-lag effect. In collaboration with German colleagues, a collection of articles has been published on cognitive processes in the perception of spatiotemporal events, including an overview of Bachmann's theory of perceptual retouching. In addition to a novel explanation to visual masking phenomena, the theory provides a coherent account of seemingly disparate microgenetic phenomena. Bachmann has published a monograph presenting a systematic overview of microgenesis in the context of consciousness research; Francis Crick and Christof Koch convey their agreement with most of the ideas expressed in that book.

Flash-lag is a perceptual effect which occurs when a constantly changing (e.g., moving, or altering colour) object is compared to an unchanging object flashing in its proximity: the flashing object seems lagged behind the changing object in the attribute space, although it was presented as equal to it. Bachmann and Põder showed that the flash-lag effect occurs even when the stream of objects is not changing in the feature space. Bachmann, Luiga, Põder, and Kalev showed that the entire complex of flash lag phenomena can be explained by the theory of perceptual retouching, and introduced the universal perceptional principle of

Prof Talis Bachmann (on the left); spatially quantized face.

accelerated processing of the earliest objects in a stream.

An important problem in research on perception of visual objects (e.g., faces) is the relative importance of spatial frequencies of contrast, local features, and overall configuration, in the process of visual recognition. Using spatially quantised images (see illustration) is one of the most useful methods to explore this issue. Among the most frequently cited papers in this field is Bachmann's study which first demonstrated, by systematically varying the degree of quantisation, a paradoxical relationship between the degree of quantisation and exposition time; this paradox is critical for object recognition. In a more recent study, quantised images were used for forward masking the test images of faces. Random noise, unrelated faces, and the critical test faces were used, in quantised form, as masks. The differences in identification level resulting from different types of masks and different degrees of quantisation were found to indicate a higher importance of holistic configuration as compared to the spatial frequency spectra and local features. It was found that a coarsely quantised non-test face, presented as a mask, did not disturb the initial phase of the microgenesis of the test face; moreover, in the initial phase of perceptual process, such mask may serve as a surrogate for the test face. An experiment in collaboration with English colleagues showed that McGurk effect (illusory auditory perception resulting from the visually presented image being in conflict with the phonemes in the auditory stream) is present even when a coarsely quantised image of the speaker's face is presented.

In the field of visual attention, we have studied the perceptual features enabling an effective search for target objects. Research by Põder has shown that the target defined by relative position of an element can be easily found from among distracting objects when the difference in the position of the critical element defines the target as an object having a feature that is different from those of distractors, and that the target object can be selectively attended to in a rapidly presented stream of spatially overlapping objects. The result that certain spatial frequency bands are more important than others in character recognition has been explained as a property of the symbols' spatial spectrum, not as a characteristic of human processing system as had been thought before. Bachmann and colleagues have demonstrated that higher processing demands to the precue have no effect on the efficiency of spatial focusing of attention. Bachmann has published a theoretical comment on a discussion on substitution masking.

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FAMILY AND WELFARE

Research team: Prof Dagmar Kutsar (PhD), Mare Ainsaar (MSc), Avo Trumm (MA), Anu Laas (MA), Katre Pall (MA), Kadri Koreinik (MA), Marju Selg (MA).

The following research topics are studied at the Family and Welfare Studies Research Unit:

- Psychological and economic coping of households and individuals in a transitional society: poverty and social stress. Main results: method for calculation national poverty line; guidelines for poverty alleviation strategies in Estonia; model of social stress and coping.
- Socio-political issues of a transitional country: social welfare, democratisation, social exclusion and re-integration. Main results: method for measuring living conditions in the Baltic States; model of social exclusion analysis; conceptual framework of social inclusion.
- Family and comparative family policy. Main results: analyses on family formation, quality and stability of family relations, interpersonal perception of spouses; family policy conception for Estonia; methodological framework of comparative family policy.
- Childhood and childhood policies. Main results: application scheme for the perspective of sociology of childhood; evaluation of impacts of household economic situation on perceived relative deprivation of childhood and parenting.

The research unit is participating in a comparative research project 'Improving Policy Responses and Outcomes to Socio-Economic Challenges: changing family structures, policy and practice' financed by the 5th Framework Programme. The results of the latter project show that, in comparison to its EU neighbours, Estonia stands out as a country with the steepest decline in marriage rates since the 1960s, while at the same time reporting one of the youngest ages at marriage and one of the highest teenage pregnancy rates. Estonia is also distinguished from the EU average and the other two candidate countries that it had gone furthest in de-institutionalizing family forms, while nonetheless retaining more conventional timing of family formation. Estonian governments have responded to these trends by giving greater recognition to non-traditional living arrangements than in the other two candidate countries and the southern European countries.

Currently the research group is involved in EU COST A19 project 'Children's Welfare' (2001-2005), that brings together outstanding European sociologists, economists and political scientists in the field of childhood studies to focus on children's economic performance, access to time and space and childhood discourses from generational perspective. A broad-scale edited overview about the status of children in these countries is under preparation and will be published in two volumes early in 2004.

On the initiative of the Family and Welfare Studies Research group, Estonia is being involved in the European Social Survey financed by the European Science Foundation.

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SUICIDOLOGY

Research team: Prof Airi Värnik (MD PhD), Kairi Kõlves (MA), Merike Sisask (MSc), Karmel Saveljev (MSc).

Suicidology Research Group (Estonian-Swedish Institute of Suicidology, ESIS) studies the causes of suicides and possibilities for their prevention, both at the individual and societal level, and in the combination of both levels.

SOCIETAL LEVEL. ESIS has gained international recognition with extensive epidemiological studies of suicides in the republics of former Soviet Union, which explored the prevalence and trends of suicide in different socio-political, economic, and cultural conditions. The Wasserman-Värnik research group opened the path for studies that interpreted changes in the prevalence of suicides and other externally caused deaths in transitional societies, calling attention to a social pathology. The first studies on that topic are published in six articles in a volume of Acta Psychiatrica Scandinavica Supplementum, and in Airi Värnik's doctoral dissertation. The studies are continuing in collaboration with the Swedish colleagues.

The collaborative research project “Country-based Guidelines for Suicide Prevention Programs for Europe” (WHO/Euro and Mental Health Europe) is in the stage of setting up the research design. In this project, the strategies of measuring the efficacy of suicide prevention programmes will be worked out; Prof. Airi Värnik is involved as a member of Steering Group, and as a head of the publication group.

INDIVIDUAL LEVEL. The laborious method of psychological autopsy was used to reconstruct the details of life and death of the persons having committed suicide in 1989 and 1999 (504 cases). Data from a representative control group have been collected for the group of 1999 suicidents. These data are being analysed together with analogous data collected by the psychiatry research group at Goethe-Institut Frankfurt; joint publications are following in 2004.

Beginning with 1995, ESIS is participating in the WHO/EURO Multicentre Study on Parasuicide (monitoring study of suicide attempts in 28 centres in Europe), and in 2001-2004, in the WHO SUPRE-MISS study of suicide attempts, representing Europe among 8 internationally selected centres. In the latter study, data on more than 4000 suicidents and control persons will be collected, together with testing the efficiency of specific rehabilitation programmes.

SOCIETAL AND INDIVIDUAL LEVELS IN COMBINATION. The complicated integration problems of ethnic minorities in contemporary Estonia as a transitional society have raised the need to study the differences in suicidal death in Estonians and non-Estonians, to analyse alcohol as a risk factor in preventable deaths and in the prevention of suicidal behaviour, and to monitor the specific trends of auto- and hetero-aggression in the Baltic countries.

The close connetedness of the Suicidology Research Group with the Faculty of Social Sciences of the University of Taru is adding the necessary component of multidisciplinarity of our studies. ESIS has developed into an organisation where young researchers are being prepared for defending dissertations in different universities and institutes (Kairi Kõlves, Karmel Saveljev and Helen Biin at the University of Tartu, Merike Sisask at Karolinska Institute, Stockholm, Piret Laur at Nordic School of Public Health, Gothenburg). The aforementioned part of work has gained momentum with the creation of the ECBHS.

PUBLIKATIONS

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BIOSTATISTICS AND HEALTH CARE

Research team: Prof Raul-Allan Kiivet (MD, PhD), Krista Fischer (PhD), Anneli Uusküla (MD, PhD), Liis Rooväli (MD), Taavi Lai (MD), Jarno Habicht (MD), Ly Rootslane (MSc), Oleg Novikov (MSc).

The main directions of research are the needs assessment for health care services, access and quality of medical care, epidemiology of HIV and sexually transmitted diseases in Estonia, methodology for analysis of medical data, public health aspects of pharmacoepidemiology and pharmacoeconomics.

Studies of hospital utilization showed that hospital use decreased significantly with increasing travel time from place of residency to the nearest hospital. The decline was major by discretionary hospitalizations and was not significant by mandatory hospitalizations. The accessibility of hospital care is most problematic for elderly. Studies on asthma treatment revealed the correspondence to the evidence based standards. The prescription and other treatment practices of psychiatrists varied considerably and the variability among psychiatrists in one hospital was larger than between different countries.

To differentiate the individual health care needs, the validated questionnaires SF-36 and EuroQol were used. Postal survey among patients being hospitalized in Tartu University Clinics due different chronic conditions (gastroenterological, rheumatic, pulmonological, cardiac) was carried out. The results were compared with general population data. Patients with rheumatoid arthritis had the lowest perceived health due their physical condition and social problems connected with it.

Analysis between relations of health care services use and socio-economic (SES) status revealed that population groups with lower SES utilize less health care services, e.g. people with lower education utilize less specialist and dental care than people with higher education. Education is one of the most important socio-economic factor influencing health in Estonia. Lower education has relations with lower income and social status, but the influence on health appears earlier. Also regional differences were found: rural people use less specialist and dental care but more primary health care than urban inhabitants do. There is almost 25% differentce in hospital utilization between counties in Estonia.

HIV and sexually transmitted diseases are a rapidly growing problem in Estonia, but its epidemiology has been addressed poorly. HIV epidemic is concentrated among injecting drug users in Estonia, but there is no reliable data on either the prevalence of HIV or injecting drug use in the population. Physicians have a vital role in interrupting the spread of sexually transmitted diseases (STD) through early diagnosis and appropriate treatment. In 11% of cases the drug prescribed to treat STD was inconsistent with guideline recommendation; in addition to that, in 9 % of cases the drug was chosen accurately but the treatment dose was too low, therefore at least 20% of cases treatment could be considered inappropriate.

Changes and trends in morbidity and in utilization of health care services, which are essential knowledge for proper planning and provision of services, are analysed. A book giving an overview of health in Estonia and describing most pertinent demographic variables, data on morbidity, trends in health determinants during the 90's, recent developments in the health care sector, socio-economic impacts on health and more important trends in the past decade was published.

Extending existing methods and developing new methodology for the analysis of medical data, when the data does not contain complete information on quantities of interest is under process. There are at least two general cases that one can consider as the problem of incomplete information. Missing information can lead to bias and cause problems for causal inference. The methodology of structural mean models leads to unbiased estimates in the presence of selectivity and is developed for placebo-controlled trials. The plan is to extend that methodology for more general cases: trials comparing two active treatments, trials with repeated measurements and observational epidemiological studies. Besides estimation methodology, it is necessary to develop tools for model diagnostics in all contexts mentioned above.

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HEALTH-RELATED BEHAVIOUR

Research team: Maarike Harro (MD, PhD), Kersti Pärna (MD, PhD), Diva Eensoo (MA), Argo Soon (MD, MA), Liis Merenäkk (MSc), Inga Villa (MSc).

In close collaboration with the Department of Psychology, University of Tartu, our main research theme has been assessing the relationships between personality characteristics and risky behaviour. In collaboration with the Department of Neuroscience, Uppsala University, we have studied the platelet monoamine oxidase B (MAO-B) activity in relationship with risky behaviour. In recent years, we have also begun to study the efficiency of intervention programmes, due to a practical need to increase their efficiency.

The research group has since 1999 participated in the target financed theme of Institute of Public Health; currently we have 2 grants from the Estonian Science Foundation and a project financed by the Health Insurance Fund. From 1998 to 2003, we have published 29 papers, including 16 full articles, 2 chapters in books published by international scientific publishers, 7 chapers or monographs in Estonian, and 4 articles in the Estonian medical journal Eesti Arst.

In collaboration with the perception and personality research group, we have demonstrated a relationship between risky behaviour and personality traits; the personality trait most indicative of risky behaviour is low conscientiousness. In collaboration with the psychophysiology group we have shown that a correlation with certain behavioural characteristics and MAO-B activity is reduced to zero when smoking is controlled for. In collaboration with the psychophysiology and biostatistics research groups we have shown that both high and low MAO-B activity increase the probability of being a regular smoker.

The PI has recently moved to the position of director of National Institute of Health Development NIHD); due to that, the collaboration with the general and molecular epidemiology research group is gaining momentum.

The NIHD is coordinating four national programmes, and since 2003, the programme for HIV prevention financed by the Global Fund. In relation to these programmes, the research focus of the group is shifting to the assessment of intervention programmes.

PUBLICATIONS

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Viru, A., Harro, M. Biological aspects of physical activity and health. In: Riddoch, C., McKenna, J. (Eds.) Perspectives on Health and Exercise, Palgrave MacMillan Limited Publishers, 229-262 (2002).

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GENERAL AND MOLECULAR EPIDEMIOLOGY

Research team: Prof Mati Rahu (PhD), Prof Toomas Veidebaum (PhD), Tiiu Aareleid (MD PhD), Mall Leinsalu (PhD), Mare Tekkel (MD PhD), Alex Baburin (MSc), Kaire Innos (MD PhD), Kaja Rahu, Sigrid Vorobjov (MSc), Tatjana Veidemann (MD PhD), Piret Veerus (MD).

The General and Molecular Epidemiology Research Group consists of 13 persons. The nucleus of the group is the Department of Epidemiology and Biostatistics of the National Institute for Health Development (the former Institute of Experimental and Clinical Medicine). Five of the researchers hold a PhD degree and two have a Master's degree; there are two data analysts working in the team. Since the year 2000, two doctoral dissertations have been defended and the same number of dissertations is currently being written. In addition to the aforementioned members, the department, but not the group, includes the Estonian Medical Birth Registry, the Estonian Abortion Registry (with the total of four employees) and the Estonian Drug Monitoring Center (three employees).

The main research activities include studies of the occurrence and risk factors of cancer, tuberculosis and other diseases, occupational and radiation epidemiology, reproductive health, registration of diseases and other health-related events, and data quality in registries. A number of the scientific projects are essentially register-based studies – data contained in medical registries and other databases are linked together. Record linkage has become indispensable around the world in epidemiological studies and other studies related to public health.

The most important studies in recent years include: Epidemiological resources in Estonia: registries, databases and their quality (K. Innos); Survival of cancer patients in Estonia and other European countries, an EU co-project (T. Aareleid); Occurrence of cervical cancer and human papillomavirus in Finland and Estonia: implications for vaccination programs M. Kibur-Nygård); Visual disability due to macular degeneration in elderly European populations: a multi-center study of prevalence and risk factors, a co-study of seven European countries (M. Rahu); Postmenopausal hormone replacement therapy – benefits and risks, a randomized population-based trial carried out in co-operation with Finnish scientists to find out the long-term effect of hormone replacement therapy on health, its social effect on ageing and its effect on health services utilization (P.Veerus); Reconstruction of doses for Chernobyl clean-up workers, a co-study of five countries (M. Tekkel); Radiation-induced molecular genetic changes among children and adults in Estonia, a joint Estonian-Finnish project (M. Tekkel, T. Veidebaum); Socioeconomic inequalities in physical and mental health and some possible explanatory mechanisms (M. Leinsalu); Validation of biomarkers of exposure and susceptibility to aromatic carcinogens in workers of oil shale petrochemistry (T. Veidebaum).

Important achievements of the research group in the recent years include:

- registration, description and evaluation of epidemiological data resources in Estonia,
- creation of mortality database in cooperation with the Statistical Office of Estonia,
- characterization of population health in Estonia and creation of database within the framework of the Estonian Health Interview Survey,
- continuous research on the occurrence of diseases, particularly cancer, in Estonia, and in comparison between Estonia and other countries,
- publishing the Cancer Atlas of Northern Europe including data from Estonia,
- participation of Estonia in a global cancer monitoring system.

PUBLICATIONS

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Innos, K., Horn-Ross, P. L. Recent trends and racial/ethnic differences in the incidence and treatment of ductal carcinoma in situ of the breast in California women. Cancer 97, 1099-1106 (2003).

Innos, K., Rahu, K., Rahu, M., Baburin, A. Suicides among cancer patients in Estonia: a population-based study. Eur. J. Cancer 39, 2223-2228 (2003).

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KINANTHROPOMETRY

Research team: Prof Toivo Jürimäe (PhD), Vello Hein (PhD), Jaan Loko (PhD), Ants Nurmekivi (PhD), Jaak Jürimäe (PhD), Terje Sööt (MSc), Leila Oja (PhD), Andre Koka (MSc), Aire Leppik (MSc), Jarek Mäestu (MSc).

There are 6 senior researchers, 2 researchers, 4 PhD students and 4 MSc students in the group (see the photo). Last five years we have been studied intensively the relationships between physical activity, motor abilities, anthropometrical parameters, motor skills and biological age in children. Most of the results are presented in the monograph.

Members of the research group at the annual congress of the European College of Sport Science in Salzburg (2003).

The body composition measurement methods in children have been studied intensively. Surprisingly we found that in measuring body fat percentage, body girths are more important than skinfold thicknesses. However, body composition measured by DXA method (trunk, arms, legs) correlated significantly with skinfold thickness. Body fat percentage measured by bioelectrical impedance method depended on the different anthropometrical parameters and especially on skinfold thickness. Some of the results are published in the monograph. Several aspects of body composition measurements and blood lipids are studied in cooperation with professors from Graz University (Austria). The results were published in international elite journals.

Among elite athletes a lot of experiments were done in rowers. A new test battery has been presented for testing motor abilities in rowers. Overtraining and overexcertion problems were studied using different biochemical parameters. The changes of the leptin concentration are probably sensitive parameter of the overexcertion. Very useful are the complex investigations where blood biochemical markers are studied together with psychological tests. A new scale for measuring readiness to start a new lap during interval running has been presented for middle- and long-distance runners. As an interesting conclusion we can say that the perceived readiness index correlates significantly with heart rate but not with blood lactate concentration.

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NUTRITION AND EXERCISE PHYSIOLOGY

Research team: Prof Vahur Ööpik (PhD), Prof Mati Pääsuke (PhD), Lennart Raudsepp (PhD), Tamara Janson (MD, PhD), Eve Pihl (MD, PhD), Kalle Karelson (PhD), Luule Medijainen (MSc), Jaan Ereline (MSc), Merike Kull (MSc), Saima Timpmann (MSc), Helena Gapeyeva (MD, PhD), Ivi Saaremets (MSc), Karin Tammik (MSc), Saima Kuu (MSc), Ege Johanson (MSc), Eric Roots (MSc), Roomet Viira (MSc).

The research group of nutrition and exercise has in recent years worked on the explaining of the effect of several food supplements on the metabolism and physical performance of highly

trained athletes. Creatine monohydrate is at present the most widely consumed food supplement by athletes. Our research has provided a systematic approach to the efficiency of using creatine in combat athletes on the background of body weight manipulation. Research on the effect of medium-chain triglyceride ingestion in middle- and long-distance runners has shown that although regular consumption of the mentioned compounds induces explicit metabolic changes in the organism, however, their endurance-enhancing effect emphasized by producers and distributors is debatable. The ingestion of sodium citrate shortly before physical effort can produce a definite effect on energetic processes in skeletal muscle during work and the fluid balance of the organism and result in endurance-enhancing effect. High loads applied in elite sport are related to considerable metabolic and hormonal changes in the organism. Our research has shown that adequate physical load and good cardiovascular performance relate to lower oxidative stress and level of inflammatory indices in the serum. In the mentioned area is conducted co-operation with several Estonian elite athletes for the purpose of improving routine testing methods and avoiding overtraining.

Neuromuscular adaptation during athletic training was measured using electrophysiological methods. The results indicated that power training induced a significant increase in force-generating capacity, speed of contraction and relaxation of plantarflexor muscles, while endurance training did not cause significant changes in contractile properties of the skeletal muscles. However, endurance training induced a marked increase in reflex excitability of motoneurones and in fatigue-resistance of neuromuscular system. Age-related changes in twitch contractile properties of skeletal muscles has been measured. A marked age-related reduction in voluntary force-generating capacity of the plantarflexor muscles, and speed of contraction of the electrically evoked twitch takes place after 40 years of age, while reduction in force-generating capacity and speed of relaxation of the twitch occurs after 50 years of age. Lower limb performance in older sedentary female patients with mild-to-moderate Parkinson's disease was examined. The data suggest that subjects with Parkinson's disease are more deficient in the regulation of force-time parameters, rather than simply in force production of the knee extensor muscles. Biomechanical studies of human movements using modern movement analysis system BTS ELITE 2002 have been launched.

Measurement of aerobic performance.

Biomechanical studies of human movements using BTS ELITE 2002.

The results of the studies of health behaviour indicated that moderate to vigorous physical activity of adolescents was longitudinally predicted by exercise behaviour of significant others (friends, siblings, parents), body satisfaction and physical self-perception, and enjoyment of physical activity. However, the relative impact of psychosocial correlates of adolescents physical activity behaviour changed over time.

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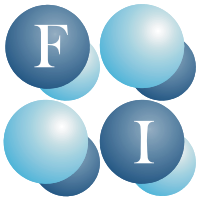

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The Centre embraces the Institute of Physics of the University of Tartu as a whole, all its labs. The research groups correspond in general to the research teams of the target financed themes (projects). The Institute is one of the eldest and most significant research establishments in Estonia. It was established in 1947, then as the Institute of Physics, Mathematics and Mechanics of the Academy of Sciences of the Estonian SSR. Approx. 80 fellows of the Institute/Centre possess the doctoral degree (PhD, DSc).

The main lines of the scientific activities and the groups behind:

- materials' science (the materials for lasers, luminescent lamps and -displays, radiation dosimeters and gas sensors are under consideration) – the groups SPECTROSCOPY OF LIGHT-SENSITIVE MATERIALS, NANOTECHNOLOGY, and RADIATION PHYSICS; theoretical support from the THEORETICAL PHYSICS group;
- theory of the fundamental structure of matter (elementary particles and fields, molecules and solids serving as objects) – THEORETICAL PHYSICS group,
- laser physicas and laser optical technologies (development of the excimer lasers, superconfined laser beams) – OPTICS group;
- environmental physics (radioactivity in Estonia) – ENVIRONMENTAL RADIOACTIVITY group;
- biophysics (elementary processes of the photosynthesis) – BIOPHYSICS group.

Institute endeavours to assist to the formation and development of the high-tech industry in Estonia. At the moment Estonian enterprises have special interest in the development of the excimer lasers (small companies Estla in Tartu and Neweks in Tallinn), as well as in the development of the new types of the gas sensors, necessary in medicine and industry. The Swedish enterprise NQUIP in Lund manufactures a student/foolproof variant of the scanning point microscope, suitable for training and industrial

Fig. 1.
Main investigation objects at the Institute of Physics of the University of Tartu: luminescent crystals, grown at the Institute.

purposes. The device is elaborated in collaboration with the Institute.

The elaboration of technology has been started to design field effect transistors based on C_{60} single crystals. Efficient is the collaboration with the Dermatological clinic of the University of Tartu in the field of laser therapy of skin diseases, and with Estonian environment conservation offices on the topic of radioactivity in Estonia and its spread, including consultations on the treatment of radioactive wastes.

Especially lively is the joint research with the universities and science centres in Sweden, Germany, USA, Finland and Italy, but also with the scientists of Latvia, Lithuania, the Netherlands, Denmark, Iceland, Canada etc. The reseachers' exchange has considerably animated starting from the year 2001, under the auspices of the European Commission: in the year 2000 the Institute was selected to be a Centre of Excellence of the European Commission.

During the years 2001-2003 5 PhD and 10 MA theses have been defended, containing the results, obtained at the Institute; underway are 8 PhD and 9 MA theses.

From the most conspicuous finacial supports should be mentioned:

- NATO "Science for Peace" grant SfP-973510 for elaboration of new scintillators (S.Zazubovich, 2000-2003);
- Grant from the organization NORFA for the synchrotron radiation based electron spectroscopic investigations (A.Kikas, 2003-2006);
- Contract between the Institute and OSRAM SYLVANIA Development Inc. (Beverly, USA) aimed at development of spectral transformers and gas discharge devices (A.Lushchik, 2000-2001);
- An INCO-Copernicus grant, Contract ERBIC15CT for development of short-wavelength laser optics (V.Denks, 1997-2000);
- A contract with the Canadian Space Agency No 9FO28-6-6045/001/XCD aimed at improvement of radiation resistant laser materials and frequency multiplication crystals (V.Denks, 1996-97).

THE BASIC EQUIPMENT

SPECTROSCOPY OF LIGHT-SENSITIVE MATERIALS:
Super-resolution (1 MHz) laser spectrometer (on the basis of a Coherent-supplied scanned single ferquency dye laser) for single molecule spectroscopy and spectral hole burning;

Laser spectrometer for registration of two-dimensional emission/excitation spectra;

Time resolved (down to 10 ns) high sensitivity spectrometric complex to test small samples (nanofilms, quantum dots) – temperatures down to 2 K, DC magnet fields up to 4 T;

High pressure system (15 kbar) for low temperature (2-300 K) spectroscopy of compressed samples;

Spectrometer for the Optically Detected Microwave Resonance (ODMR).

NANOTECHNOLOGY:
Two devices for Atomic Layer Deposition (ALD);

Laser ablation device;

Scanning Point Microscope AutoProbe CP;

Near field microscope NSOM-100;

Electron diffractometer;

Auger electron spectrometer.

BIOPHYSICS:
Fluorescence spectrometer with picosecond time resolution (based on a Coherent laser);

Ti:sapphire solid laser (Spectra Physics) with an registration system;

Several different high pressure systems, incl. a cell with diamond anvils (Diacell), for optical measurements in the 0-30 kbar pressure range and at temperatures between 4 to 300 K.

Microspectroscopic device, composed of a Zeiss microscope, Andor CCD-camera, and EGG avalanche photodiode;

Device for single photon correlated registration (Ortec) to measure subnanosecond decay times of luminescence.

ENVIRONMENTAL RADIOACTIVITY:

High-resolution low-background ORTEC (USA) HPGe γ-spectrometer with a p-type coaxial detector GEM-35200;

Low energy low-background HPGe γ-spectrometer with planar BDRG-32 detector (BSI, Latvia)

Area monitoring system AAM-90

Radon Monitor RM-3B

OPTICS:

Cu laser system (1.5 W, green emission, fiber light duct) for clinical applications;

Setup for investigation optical properties and electronic conductivity of solids down to 0.3 K based on a single-shot ^{3}He magnetooptical cryostat with fields up to 2.5 T, and sensitive DC resistance measurement apparatus (Keithley);

System for magnetoresistance measurements in fields up to 8 T;

Time-of-flight mass-spectrometer for studying laser-induced erosion and damage of optical materials and coatings; laser-assisted elementary analysis of solids;

VUV-UV-VIS spectrometers for light emission studies; equipped with computer-controlled gated ICCD cameras (Andor Tec. Inc.) and a digital delay pulse generator (Stanford Research Systems);

Interferometric/holographic-grade optical tabletop setup for ultrashort light field and signal processing studies (based on a picosecond dye laser system (Spectra Physics); an synchroscan streak camera (Hamamatsu) and computer-controlled CCD cameras (Electrim Corp).

RADIATION PHYSICS:

Setup for detection of weak cathode luminescence in the spectral region 1.8-11 eV (incl. double VUV monochromator;1-10 keV electron beam; T = 9-400 K);

Setup for the registration of fast emission pulses ($h\nu$ = 1.7-8.0 eV) at a crystal excitation by single powerful electron pulses (300 keV, 10^1-10^3 A·cm^{-2}, 3-15 ns) at 80-700 K;

Setup for polarisation spectroscopy ($h\nu$ = 1-6 eV, T = 1.7-500 K, double monochromators);

ESR spectrometer ERS 231 (X-band) with a continuous flow nitrogen cryostat STT3 (90 - 550 K) and an Oxford Instruments continuous flow helium cryostat ESR 900A (3.9-300 K);

Electron spectrometer Gammadata-Scienta SES100;

TLD Reader System 310 accommodated for thermoactivation spectroscopy of irradiated (VUV, X-ray, α-particles) samples in the temperature regions 2-500 K and 300-750 K;

Setup for the investigation of photoluminescence spectra (1-6 eV) and the spectra of luminescence excitation by 4-13 eV-photons (VUV monochromator, discharge lamps) at 5-300 K;

Device for optical absorption measurements in the spectral region of 1.4-6.7 eV based on a spectrophotometer JASCO 550;

Unconventional setup for thermoactivation spectroscopy in the range of 5-600 K that allows to investigate the annealing of optical absorption or of the flash of photostimulated luminescence of crystals previously irradiated by monochromatic VUV radiation of 6-13 eV or by X-rays (~ 50 keV);

Setup for measuring the absolute quantum yield of photoluminescence in phosphors under the excitation by 4.5-13.0 eV photons (intensity of 10^8 to 10^{11} photon/cm^2);

X-ray spectrometer (photon energies of 50-1000 eV)

Crystallization devices for growing high-melting (up to 3000°C) oxides, ultra-highly pure and doped alkali halide single crystals.

SPECTROSCOPY OF LIGHT-SENSITIVE MATERIALS

The processes of interaction of light and matter (light absorption, emission and propagation in the matter), explored by the optical spectroscopy, are significant both by their applications (lasers, optical communication, information storage) and importance for the physical world view. Advent of lasers raised the spectroscopic research to a principally new level.

At the Institute it lead to a top achievement in the physics in Estonia – the phenomenon of spectral hole burning was discovered in 1974. The phenomenon allowed to develop new ultra-high resolution spectroscopic methods. Spectroscopy of single molecules emerged as a natural step towards continuously growing sensitivity of the spectral methods.

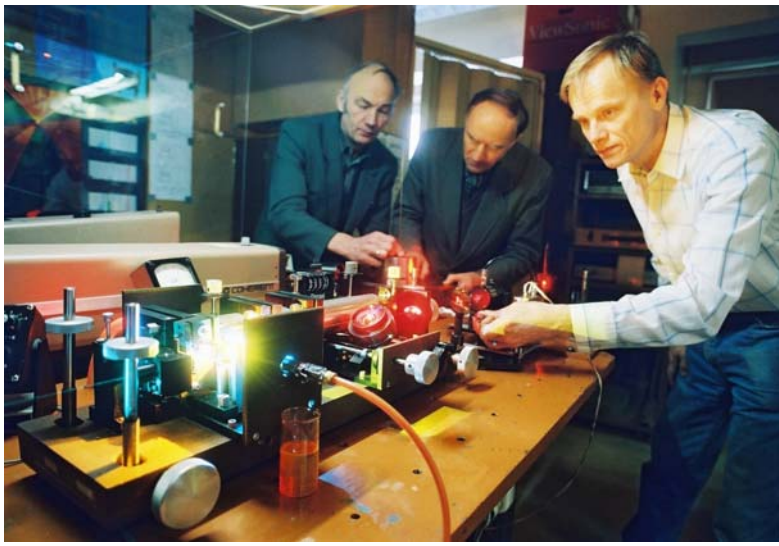
Under certain conditions, the spectral hole burning and single molecule spectroscopy allow to address the molecules quite selectively, a single molecule with a certain transition frequency being the limit. Similarily as a human being in a crowd responses to his name, an impurity molecule in the solid responses only to the light quantum, having the frequency, characteristic to the molecule. This property proceeds from the existence of ultra narrow spectral lines, called zero phonon lines, in the spectra of the impurity molecules. The zero phonon lines turn the impurity molecules into highly sensitive probes, transmitting information about their environment and its transformations. At the same time, they offer possibilities of very delicate manipulation with the matter at nano- and sub-nanolevel. Enjoying a quite unique combination of the experimental conditions (available only in 1-2 labs over the world): low temperatures + high pressure + supermonochromatic laser radiation, we have demonstrated that under such circumstances the properties of the polymeric glasses change drastically, e.g. the relaxation processes are suppressed in them, diminishes the extent of "inner freedom", distinguishing glasses from crystals. Based on such observations are further developed the models, used to describe the amorphous systems.

If former spectroscopic investigations mainly dealt with such "classical" solids as crystals (incl. molecular crystals), then, during last years, we have expanded research to several "nonclassical" solids, such as so-called noncommensurate systems ("almost crystals", but lacking translation symmetry).

With the aid of impurities as probes we have revealed in these systems processes, usually characteristic for amorphous (highly disordered) systems. In addition to high spectroscopic resolution, the to-dimensional excitation-emission spectra were here of great aid (i.e. the dependences of luminescence intensity on the both excitation and registration wavelengths). In such 2D spectra the spectral information is presented in a "un-wrapped" form – as in a topographic map with the contour lines. As a map presents more information as compared with the landscape view from a single point, so the 2D spectroscopy is more rich in comparison with the ordinary spectroscopy.

Besides the objects which can be prepared by relatively simple methods, we have turned more and more attention to the structures, which can be fabricated only by high-tech techniques, but being quite actual for practical applications. Such are thin oxide layers (different phases of titanium oxide, zirconium and hafnium oxides), grown by atomic layer deposition (i. e. growth by single atomic layers).

Carrying out single molecule spectroscopy.



In the laboratory of laser spectroscopy.

Light propagation in such films presents interest for applications, but the spectral properties of the films also offer information about the structure of the films. This information assists in development of the atomic layer deposition method itself.

PUBLICATIONS

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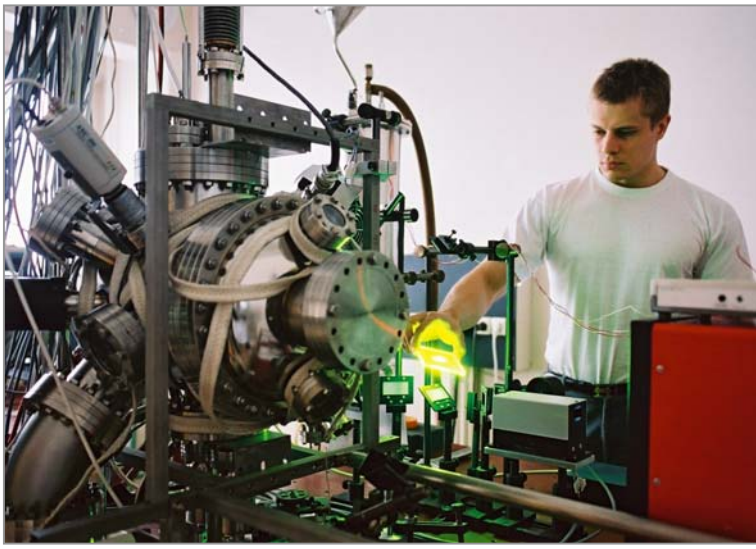
NANOTECHNOLOGY

The properties of a solid depend significantly on the arrangement (packing) of the atoms in the crystal lattice. One of the purposes of nanoscience is to reveal the relations between packing peculiarities in the nanometer range (nanometer = 10^{-9} m) and the characteristics of a solid. Nowadays intensive experimental and theoretical investigations are focussed onto these relations. Such high resolution microscopy techniques as transmission electron microscopy, tunnel microscopy and atomic force microscopy (the last ones are known as scanning point microscopy) are here of tremendous value. The nanotechnology of solids deals with synthesis of nanostructured and nanodimensional materials.

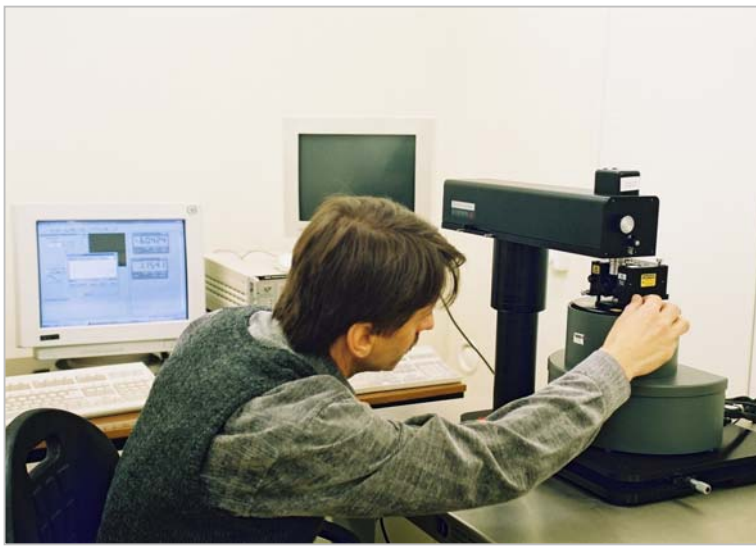
Activities of the group are concentrated on the atomic layer deposition (ALD) of metal oxide films, characterization of the deposited films, development of the depostion techniques and diversification of the applications of the nanofilms.

ALD is a special pulsewise synthesis method of solid films. It is based on the selfsaturating surface reactions and offers a possibility to perform the synthesis by single atomic layers. It enables a better deposition control and gives good prerequisites to fabricate perfect films. In the last years, the method attracts more and more attention. Electronics industry is intending to introduce into the next generation of the integrated circuits super thin isolating films with high dielectric constant. But a lot of problems remains and efforts are made in a number of labs over the world.

Recently the group obtained good results in ALD of isolating material HfO_2 from new combinations of precursor substances. It was established how the film structure of this and other oxides (TiO_2, ZrO_2, SnO_2) varies in dependence of the deposition parameters. The films with improved electrical, optical and luminescence properties have been grown.



Laser ablation procedure running.



In the lab of scanning point microscopy.

Fig. 2 demonst-rates as packing defect free and abruptly segregated is a SnO_2 epitaxial layer. It was established that if the high quality SnO_2 films are ultrathin (~10 nm), they can be applied as functional elements of a new type of semicon-ductor gas sensors.

The group deposits the films also by laser ablation. This is also a pulse method. The deposition proceeds from a plume, created by laser evaporation of the target. The method has significant advantages for deposition of the layers with a complex composition. The technique enables also a controlled etching of the layers. Nanostructured $Cr_xTi_{1-x}O_2$ films have been prepared by the group for gas sensors.

Further, some words about the works, belonging to the field of scanning point microscopy (SPM), a major imaging method in nanoscience.

The group succeeded in hybridisation of the methods of SPM and transmission electron microscopy. The aim of this integration is getting information about the nanocontact between the scanning point and the object. It assists to elucidate the nature of the contact, incl. such parameters as the tearing-off force at the contact and its electrical conductivity. The core of the constructed hybride system (Fig. 3) is a tiny scanning point microscope.

By the sol-gel technique, we succeeded to prepare a point with both good electric conductivity and transparency (Fig. 4). This point is perspective for linking optical near field microscopy with tunnelling microscopy. The new point is far cheaper as compared to the diamond points, used for this purpose up to now.

A novel combined method is dubbed nanotomography, a compound of SPM and successsive removal of the atomic layers from the object. The etching (removal) is carried out by laser ablation. The method allows to establish the packing structure of the near-surface layer.

The light reflection from the nanometers-thick films has been examined theoretically. The obtained analytical relations are applicable for determination of the parameters of ultrathin layered structures by optical measurements.

Fig. 2.
An .-Al_2O_3 (top) – SnO_2 (beneath) junction, as displayed with atomic resolution with the aid of a tunnel microscope.

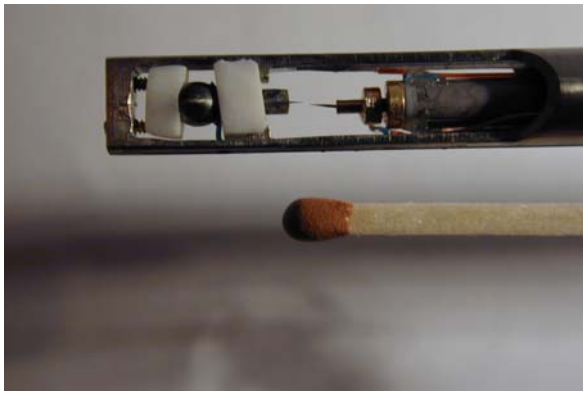


Fig. 3.
A scanning point microscope, which can be fitted into the transmission electron microscope.

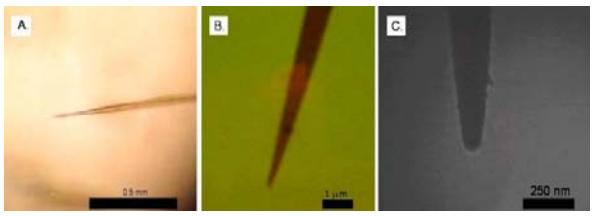


Fig. 4.
A new tip (in different magnifications) for the near field optical microscopy in combination with the tunnelling microscopy.

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BIOPHYSICS

The biosphere exists thanks to the energy, irradiated from Sun. The process of getting this energy is called photosynthesis. Thus, one can argue that the biology starts from the light absorption in special protein complexes – in the light harvesting antennae. This is a critical stage from the standpoint of the biological energy transformation. To get the best result, light must be absorbed in a maximally wide spectral range (energy span). Absorbed energy must reach, with minimal losses, into a special site in the photosynthetic membrane. This site is called photochemical reaction centre. In this centre it is transferred into potential energy of the chemical bonds. To compete with the possible energy losses, unavoidable from the standpoint of the laws of thermodynamics, the energy transmission and successive electron transitions must proceed at an extremely high speed (see Fig. 5). These parameters (a wide spectral range and superfast energy transfer) establish strict limits to the structure and properties of the photosynthetic chromoproteins.

As a result of joint efforts of several laboratories, including this lab, it was revealed already some decades ago that the spectra of antennae complexes are nonhomogenously broadened. This means that the spectra of single antennae are not too wide, but their spectral position is somewhat different. Thus, taken together, as in a photosynthetic antennae, they cover a rather wide spectral band.

From one side the existence of such a wide spectrum is rather beneficial for efficient absorption, but, on the other hand, a question arises, how energy transport is possible at all. Indeed, the speed of energy transfer and its efficiency depends on the energetic resonance (equality of the distances of the levels of the energy supplier and energy receiver molecules. To a considerable difference in the energies corresponds a slow transport or even its interruption, in the worse case. Scientists speak in this case about energy localization. Nature has been smart enough to use several ways to avoid the disadvantageous stopping of energy in the antenna before it reaches its target, i.e. the reaction centre. A main one, exciton self-localization we revealed recently. What that means? – Electron excitations, arising at light absorption, embrace quite a number of antenna molecules simultaneously: the primary excitation is delocalized. This delocalized excitation is called the exciton. Exciton transport can be per-

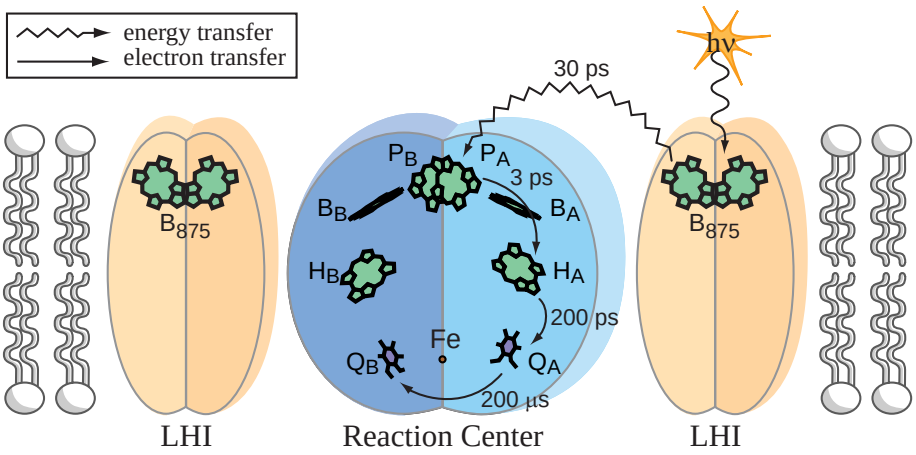

Fig. 5.
An artist's vision of the co-existence of the antennae complex and the reaction centre in the photosynthetic membran. The typical energy and electron transfer times are indicated.

turbed by the thermal vibrations of the atomic lattice of the chromoprotein. Usually, this possibility was assumed to be negligible. However, we succeeded to prove the opposite. The excitons localize dynamically already during a quite short time interval, merely ~150 fs. Differently from the above mentioned static or inhomogenous localization, such a dynamic or autolocalization (self-trapping) induces a broadening of the emission spectrum and its red shift relatively to the absorption spectrum. As a result, the efficiency of the energy transfer is enhanced. First, the broadened emission spectrum more widely overlaps with the absorption spectrum of the probable candidate of the energy acceptor. Second, the red shift of the spectra gives a certain direction to the energy transfer: energetically downhill, and energy can move via shortest route to the reaction centre.

In the investigations, having lead to these conclusions the methods of ultrafast spectroscopy (temporal resolution ~ 100 fs) were used in parallel with the means of high resolution spectroscopy (spectral resolution ~ 0.1 cm^{-1}). The tested specimens were squeezed by high pressures (up to 10 kbar). The results were analysed by computer modelling.

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ENVIRONMENTAL RADIOACTIVITY

In the field of environmental physics in the Institute (Laboratory of the nuclear spectroscopy) the focus is on the abundance of radioactive substances, their spread and migration in Estonia. The radiations of the radionuclides are one of the most cunning ones among various environmental hazards. So as we do not sense them in any way, we do not get any warning from our senses about these hazards , until the morbid changes take place in our body. In soviet times the local radiation hazards were almost not investigated and the population remained uninformed about the risks. The research work had to be started from zero.

At the northern coast of Estonia there are minerals and soils with enhanced radioactivity. The war preparations of the Soviet Union left here a lot of sources of radiation risks (uranium production/enrichment wastes at Sillamäe, extensive nuclear equipment at the training centre of nuclear submariners at Paldiski etc). In the North-East Estonia are running power plants on oil-shale fuel. Their smoke and fly ash disperse the radionuclides from the subspoil plots. These power plants are sometimes considered to belong to the greatest pollution sources in Europe. Now we know all this in detail thanks to the efforts of the environment researchers at the Centre/ Institute.

For the research they have managed to develop contemporary laboratory. It enables to elucidate, besides the radiation measurements, which kind of radionuclides emit the radiation. At the international inter-comparisons the skills of local researchers, their equipment and results, have got the highest marks.

At the lab of nuclear spectroscopy are running the devices, which immediately would alarm about emerging radiation hazard of any origin, e.g. in the case of an accident at a nearby nuclear plant.

By the analysis of soil samples the researchers have got a detailed picture of the spread of radioactivity in the Estonian soils and into depth. The obtained data have been introduced into international data banks.

Investigations are underway of the radioactivity of common building materials, as well as of the most widely used fuels – wood and peat and their ashes. Computer modelling is conducted on the pathways of radioactive contamination and the predicted radiation doses received by the population of different regions in Estonia.

The environment physicists of the Institute have contributed to the assessment of the depositories of the radioactive wastes, the contemporary as well as these planned in the future. The wastes stem, e.g. from the hospitals (the radiation therapy units, having surpassed their usability term), from industry (sensors, counters etc, containing a radiation source, gamma-defectoscopes etc) as well as from research institutions and universities.

The researchers have elucidated

- that in Estonia there are sites unique for all Europe by their high radium content in soil;
- the environmental hazards of the nuclear equipment, remained at Paldiski;
- long term environmental effects of the depository of radioactive wastes at Tammiku;
- that the fly ashes of the thermal power plants contaminate soil, water, and air in the environs with a number of radioactive substances, incl. radioactive lead. It is remarkable that the thermal power plants emit far more radioactive pollution as compared with nuclear power plants, of course, if the accidents can be avoided in the last ones.

Anyhow, it is comforting to confirm, supported by the research results of the Tartu physicists, that the level of radioactivity is nowhere in Estonia exceeding the tolerable limits and turned alarming. We were relatively lucky also during and after the Chernobyl catastrophe, as compared with our northern and western neighbours: the dominating winds were blowing then, and the rains falling, so that they did not carry to us too much of the radiopollution, released from the blown up nuclear plant.

The group collaborates tightly with the Estonian Radiation Centre, participates in many international programmes, has assisted in drafting the Estonian radiation legislature, and participates in the training of students in the radioecology and radiation protection.

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THEORETICAL PHYSICS

Theoretical physics is a traditional research area at the Institute, being closely connected to local experimental research and also to research in the Department of Physics of UT and in Tallinn University of Technology. The research in this frame belongs to areas of solid state theory, theory of elementary particles and relativistic theory of gravitation. A number of earlier results of our theoreticians (the nuclear fusion catalyse mechanism of μ^+-mesomolecule, the theories of zero-phonon line and of secondary emission, the discovery of hot luminescence, the microscopic separation of electronic phases in high-temperature superconductors, the vibronic theory of phase transitions, the transform method in Raman scattering etc.) have been internationally recognised. The members of the research group actively participate in relaying achievements of contemporary science to students, young scientists and the community.

In the following some details on the main research areas.

SOLID STATE THEORY

In the solid state theory, the optical and magnetic properties of new solids and molecular systems necessary for contemporary technology, also the migration of particles in these systems are investigated and predicted. Special attention is paid to new high-temperature superconductors discovered in recent years, the mechanisms and properties of their superconductivity are investigated.

The main recent results in this area are a new theory describing unusual magnetic properties of high-temperature superconductors, a theory explaining properties of a novel superconductor MgB_2, and a two-component model of cuprate superconductors describing their state transitions. Conductivity and superconductivity of insulator films, organic films and fullerenes are studied.

The theory of vibrations of crystal lattice (nonlinear dynamics[1]) is being actively developed. Special vibrational states of crystals – lattice solitons are studied. A theory allowing one to compute these excitations for real crystals with account of quantum effects has been developed. A theory of multiquantum processes was created; this theory for the first time predicts a critical behavior of quantum phenomena when the strength of interaction of particles changes. Also the properties of disordered and defect-rich structures at atomic level are studied. A theory explaining anomalous behavior of glasses under pressure at low temperatures has been developed.

An important field of study is the behavior of laser radiation in substances. Here the main attention is paid to new nonlinear quantum phenomena. In collaboration with experimentalists, there are predicted several of them, mentioning for example a new mechanism of the directed emission of matter. The subject of laser radiation exceeds the usual limits of the solid state theory, being directly connected both to actual problems of quantum field theory as well as to some aspects of quantum astrophysics. A topical field of study in laser optics is singular optics. In this area, interaction with matter of new type laser beams having orbital angular momentum is studied and new phenomena at refraction and reflection of such beams have been predicted.

Optical spectra of crystals with defects and these of micro-objects used in nanotechnology (atomic clusters, nanostructures) are computed. There was found a new mechanism increasing the width of the zero-phonon line[2], caused by effects of connected movement of defects upon electronic transitions in the lattice. The reasons of temperature dependence of spectra were clarified. A theory describing the scattering of short pulses of intense laser light in solid matter was elaborated. A theory of nonlinear optical time-dependent transitions in doped crystals was developed, including the theory of spectral hole burning based on zero-phonon transitions.

All this information is necessary for creating new and more effective lasers, luminescence bulbs, monitors, radiation detectors etc.

THEORY OF ELEMENTARY PARTICLES AND RELATIVISTIC THEORY OF GRAVITATION

In the theory of elementary particles, the particle interaction models looking further from the generally accepted Standard Model are considered: the evidence of possibility of non-

[1] In nonlinear theory the relations are not limited to the simple linear ones, but also the contribution of higher powers of the variables included in theory to the values of functions is taken into account.

[2] A zero-phonon line is a narrow spectral line, emission and absorption of which is not accompanied by the generation of vibrations of the crystal lattice.

standard interactions in processes of creation and decay of vector bosons at accelerators with colliding beams, the theories of interactions of particles with higher spins ($s > 1/2\hbar$) are developed.

In the theory of gravitation and string theory, under attention are new type cosmological models regarding our Universe as existing in a higher-dimensional space which surrounds it.

Also more general problems of quantum theory are considered, including questions related to the operator of time and the modification of the quantum mechanics in curved spacetime.

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OPTICS

The group consists of several subgroups, dealing with a number of different topics. In the following laconic summaries of the goals and main recent results of each team are presented. Finally, the applications and development activities are summarized.

NONLINEAR DYNAMICS OF SELF-TRAPPED EXCITONS IN RARE GAS CRYSTALS

Goal – to develop physical understanding, theoretical description and methods of experimental study of peculiar mechanisms of vibrational relaxation in some cryocrystals; main results – in Xe and Kr an abrupt increase of the relaxation rate near a critical vibration level has been detected and it has been shown, by making use of analytic method elaborated and software for fast and accurate solution of the quantum-mechanical energy eigenvalue problem composed, that the effect confirms the predictions of the new nonperturbative relaxation theory worked out within the Institute's other project "Theory of the fundamental structure of the matter".

DYNAMICS OF EXCITON INTERACTION WITH CHARGE CARRIERS IN SEMICONDUCTOR CRYSTALS

Goal – to study the interaction with laser-induced free carriers in GaAs and clarify some contradictions in literature data; main results –a decreased exciton generation rate at a higher temperature of charge-carriers, and a strong exciton scattering on hot free carriers that heats the excitons and effectively quenches luminescence have been revealed by a novel picosecond-domain-time-resolved dual channel modulated luminescence correlation technique.

ELECTRON TRANSPORT PROPERTIES OF LOW-DIMENSIONAL SYSTEMS

Goal – to study thin two-dimensional tungsten films used as sensors in cryogenic particle detectors, Ta_4Te_4Si quasi-one-dimensional nano- and micro-scale fibers at cryogenic temperatures; main results – at temperatures down to 0.35 K and in magnetic fields up to 11 T electron-electron and electron-phonon scattering lengths have been determined, which are important for further development of the detectors.

LOCALIZED ELECTROMAGNETIC WAVES

Goal – to develop physical understanding, theoretical description and methods of experimental generation of ultrawideband nonspreading pulses, which were recently discovered in mathematical physics as exotic solutions to wave equations and intensively studied in ultrasonics; main results – experimental tests of the feasibility of these waves as electromagnetic waves were successfully carried out on the sample of the so-called optical Bessel-X wave and applications of specially designed femtosecond-duration Bessel-X pulses in optics and ultrafast spectroscopy have been proposed.

MULTIPHOTON PROCESSES IN INTENSE LASER FIELDS

Goal – to develop non-linear spectroscopy of gases by implementation of nontraditional light beams (e.g., Bessel beam and other localized beams, which are of great interest owing to their prospective applications in generation of coherent UV-VUV radiation, laser treatment of materials, etc.); main results – three-photon resonances of rare gases have been studied with methods developed and a simple and reliable way to control the nonlinear response was found.

HIGH-RESOLUTION LASER SPECTROSCOPY OF JET-COOLED ORGANIC MOLECULES

Goal – to obtain molecular constants, which allow to predict their chemical and biological properties; main results – molecular constants for a number of biologically-important organic molecules have been determined via the analysis of rotationally and vibrationally resolved electronic spectra.

SPECTROSCOPY OF PLASMO-CHEMICAL PROCESSES IN THE ACTIVE MEDIA OF DISCHARGE PUMPED UV-VUV GAS LASERS

Goal – to reveal key reactions and engineering of new generation of "sealed-off" discharge-pumped excimer laser tubes with long operation lifetime and improved efficiency; main results – different modifications of compact excimer lasers have been developed in cooperation with several Estonian high-tech companies.

LASER PHYSICS OUTSIDE PHYSICS

Goal – to develop public-oriented applications of laser optics; main results – a compact, easy-to-handle and portable (16 kg) copper vapour laser system for medical applications has been designed, clinically tested and sold to clinics in Estonia and Finland.

APPLICATIONS

Using Cu-laser, an effective laser biostimulation method for the therapy of chronic and severe skin diseases (acne, allergodermatoses, leg ulcers, psoriases) has been developed in collaboration with the Dermatological Clinic of the University of Tartu. The same laser enables to

Copper-vapour laser treatment of a patient at the dermatological clinic of the Tartu University.

remove various skin defects in cosmetic surgery (teleangiestatic lesions). No side-effects of the laser treatment have been noticed, while it is well tolerated by the patients and does not have interaction with systematic or topical medicines. Laser treatment has been introduced in Dermatological Clinic as a standard method of treatment (over 200 patients in month). The results indicate that this new method significantly complements clinic's potential in the cure of serious skin diseases as a treatment without medications.

Development of compact "sealed-off" UV-VUV excimer lasers has been accomplished in tight collaboration with "Neweks" – Estonian high-tech small company. New serial model of compact excimer laser PSX-501 with enhanced resource, ouput energy (12 mJ KrF-248 nm; 10 mJ ArF-193 nm; 2 mJ F_2-157 nm) and pulse repetition rate (up to 300Hz) was developed. Nowadays this laser is the most compact commercially available excimer laser on the world market (weight 14 kg, size: mid-tower computer case). Results achieved are a real step toward designing of a new generation of sealed-off discharge-pumped excimer lasers with high repetition rate and long operation lifetime. True modular design with recycling laser enclosure can offer reduced production and maintenance costs, improved safety and reliability of these lasers. This would help to accelerate development of new areas of technological application of excimer lasers in Europe.

Development of compact easy handled and portable (16 kg) copper vapour laser (CVL) system for medical purposes has been accomplished in collaboration with "Estla" – Estonian high-tech small company. CVL is mounted into a single standard PC Mini Tower box, operates with air cooling and requires only single phase line voltage (1.5 kW). CVL is an effective high frequency (16 kHz) source of visible (511 and 578 nm) coherent radiation pulses at an average power of 1.5 W. The device is supplied with a fiber manipulator or with a PC controlled automatic scanner. The original laser has been tested in the Medical Research Centre (Helsinki) and in the Dermatological Clinic of the University of Tartu. Medical Cu laser system has been introduced into production in the laser company Estla Ltd.

Recently Estonian company Laser Diagnostic Instruments Ltd. was recognized with several prizes in the 51th World Exhibition of Innovation, Research and New Technology "Eureka" (Brussels, 2002), in particular, LDI's laser based medical system "Maria" won the gold medal. Another spin-off company from the Estonian Academy of Sciences, NEWEKS has developed and sold more than 600 miniature excimer lasers worldwide, among others to the customers like NASA, US Navy, Los Alamos National Laboratory, etc.

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IRRADIATION PHYSICS

Irradiation is influencing upon an object with radiation. Here we consider radiation, first of all, as ionizing ("hard") radiations: X rays, emissions of radioactive substances, short wavelength ultraviolet, beams of particles from accelerators. In difference with the visible light, these radiations are invisible, their fluxes can be revealed only by artificial sensors. The group of irradiation physics investigates radiation effects upon solids, mainly ionic crystals (such as common salt, NaCl) and metal oxides (such as unslaked lime, CaO), but also upon much more complicated compounds, e.g. $MgAl_2O_4$, $Y_3Al_5O_{12}$, $BaMgAl_{10}O_{17}$. In crystals the atoms are packed into a regular crystal lattice, where the structure elements are repeated many times, as bricks in a wall.

Under the influence of radiation several solids shine light or emit luminescence, their absorption spectrum and electrical conductivity change, and, what is especially significant, the hard radiations "shake up" their crystal lattice. The defects of atomic dimensions, or microdefects are created, e.g. some of the lattice sites remain unfilled (a vacancy is produced), but the atom or ion, ejected from the site takes irregular position, "out of the row" (an interstitial is generated). This, in order, leads to the modification of the absorption spectrum, in its optical part as well as in the region of radio frequencies. (In the last case the spectra of electron spin resonance, briefly ESR are detected.) The emission spectrum becomes also changed.

From one side, the research of irradiation physics belongs to fundamental physics: it gives new information abot the atomic structure of solids and its conversions under radiataion, and about the excitation states, migrating about in the crystal lattice – uncharged excitons, conduction electrons and -holes etc.

On the other hand, the irradiation physics has high applied value, elucidating radiation sensitive as well as radiation resistant materials. The first ones are needed to fabricate radiation sensors and dosimeters. The second ones are needed in nuclear energetics, luminescent lamps, laser irradiatiors, details of laser optics etc.

The main caharacteristic features of the investigations of the group are:

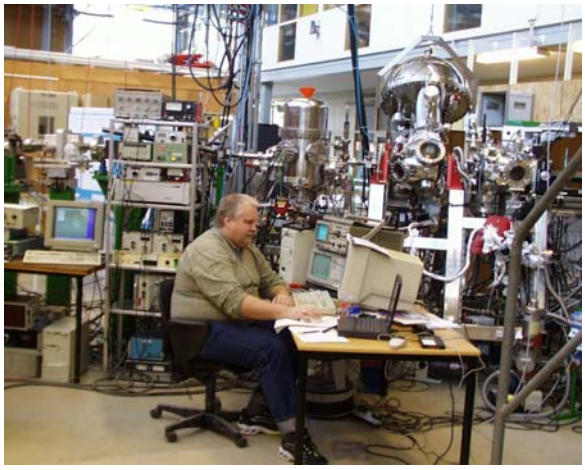
- selection of the experimental objects,
- wide variability of the experimental conditions,
- multisided (systems) approach.

The experimental objects of the group are, by their nature, insulators. They differ from thoroughly examined semiconductors by a wide band gap (or forbidden band). Such materials are usable even at temperatures, considerably higher than the room temperature. The objects under investigation are mostly fabricated at the Institute, by the group members, applying high temperature techniques.

As to the experimental conditions, the energy of influencing quanta or electrons can be varied in wide limits (from X ray region to infrared diapason, energy of electrons from some electron volt to the energies characteristic to the accelerators, 300 keV), temperature of the object (from the cold near absolute zero up to temperatures of incandescence), pressure of the ambient gas from an ultra high vacuum up to normal conditions etc.

Periodically the members of the group pay research visits to the accelerator centres in Lund and Hamburg, where they irradiate objects with synchrotron radiation, electromagnetic radiation, emitted by super-high-speed (relativistic) electrons, revolving in the accelerator, called synchrotron. From the wide spectrum of this radiation monochromators separate beams of certain wavelength to irradiate objects. Varying the wavelength, one gets the excitation spectra of luminescence, efficiency spectra of defect generation etc. The laboratory of X-ray spectroscopy, belonging to the group, carries out investigations on the frontier of atomic physics and solid state physics, uncovering the processes, encompassing cores of the crystal-forming atoms, e.g. creation of relatively high energy electron excitations – X ray excitons. Besides the visible and invisible emissions significant additional information on the objects is obtained from the electron spectra – energy distributions of the electrons, emitted from an irradiated solid. Just now at the Institute is established a new laboratory, that of the electron spectroscopy. A contemporary electron spectrometer, Gamma-data-Scienta SES100 has already arrived.

Systems approach means, in simple words, that different characteristics of the same object are juxtaposed, but also the variation of characteristics in the series of similar objects (e.g. KCl, KBr, KI) is examined.



The scientists of the Institute working at the MAX-lab – the synchrotron centre of the University of Lund.

The phenomena, discovered former by the group members, the photon multiplication[3] and transformation of electron excitations into lattice defects, are now futher examined in detail.

The both phenomena open new aspects of interaction of radiation and matter. Different generation modes of the both phenomena are scrutinized. These phenomena open also new application possibilities: the first one for construction of new types of luminescent lamps and display devices, the second one – in improvement of radiation sensors and dosimeters and in the search and design of radiation proof materials. The group is actively examining these possibilities and has real progress in the field. Namely, by the photon multiplication effect the use of toxic mercury vapours in the luminescent lamps can be avoided, replaced by discharges in argon or xenon. Thus, more environment benign devices can be fabricated. Further, the efforts are made to design bioequivalent luminescent dosimeters for fast neutrons. The fluxes of fast neutrons are generated by nuclear reactors and nuclear explosions. The harmful for the tissues effect of different radiations, e.g. gamma radiation and fast neutrons, is quite different. It is not simply proportional to the radiation energy, absorbed in the matter, the neutron damage is far more serious. The dosimeters just in use are not bioequivalent.

Radiation proof materials are needed, among other demands, for the crystal optics, applicable in the beams of ultraviolet lasers: under certain circumstances laser radiation also wrecks a crystal lattice.

The researches have been done by the contracts with the Canadian Space Agency and the European Commission (aimed at the means to enhance the radiation sustainability of the materials for laser techniques). The results, gained in tight collaboration with Czech and Italian physicists are in use by some European enterprises, fabricating sensitive radiation sensors (scintillation counters), used also in the medical diagnostics – in the computer tomographs.

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[3] The photon multiplication is a process when in response to one exciting photon two or even several luminescence photons are emitted, i.e. the luminescence quantum yield exceeds a unity.

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CENTRE OF EXCELLENCE IN CHEMISTRY AND MATERIALS SCIENCE

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Centre of Excellence in Chemistry and Material Science (CECM) simultaneously includes also EC Centre of Excellence of Photovoltaic Materials and Devices for Solar Energetics (Prof E.Mellikov).

The Centre of Excellence in Chemistry and Materials Science is formed on the basis of six highly qualified research groups of the Department of Chemistry of University of Tartu and three research groups of the Faculty of Chemistry and Materials Technology of Tallinn Technical University in order to concentrate and integrate the so far existing, already internationally acknowledged research and development potential of Estonia in the interdisciplinary field of chemistry and materials science. That would greatly help to reach the major goal of significantly intensifying and better focusing the efforts to study and develop the new, effective, cheap and environmentally friendly materials for the photovoltaic and electrochemical power devices (solar and fuel cells, Li-ion batteries, supercapacitors), stereoselective catalysis, for the design of bioactive compounds and drugs, sensors and radiation detectors for the environmental analysis, and new technology for production of rare earth metals.

Major direction of the R&D work of CECM:

- theory of chemical reactions and its applications (M.Karelson);
- acid base equilibria and their contemporary applications (I.Koppel, P.Burk, I.Leito);
- the research and development of semiconductor compounds- type PV materials and electroconductive polymers for creation of materials for solar energetics and technologies (E.Mellikov, J.Krustok, M.Altosaar);
- bioactive compounds and their implication in drug design and proteomic analysis J.Järv, A.Rinken, A.Uri);
- new methods for synthesis of chemical compounds and their technological applications (U.Mäeorg, A.Uri, T.Rodima);
- new materials and technologies for novel, highly-effective power sources (fuel cells, Li-ion batteries, supercapacitors; E.Lust, J.Tamm, I.Koppel);
- the study of properties, structure and applications of multilayered conductive polymers (A.Öpik, K.Lott);
- novel materials and methods of analysis and their applications in environmental monitoring (dosimetriy electrochemical materials and biosensors analysis and certification of materials (I.Leito, M.Kerikmäe, L.Paama, M.Danilkin, T.Tenno, K.Tammeveski);
- nanostructural materials and high-temperature interfacial and solid state electrochemistry (E.Lust, J.Tamm);
- photoluminescence in ternary composite semiconductor materials (J.Krustok);
- chemistry and technology of monograin materials (E.Mellikov, M.Altosaar);
- novel solar cells (E.Mellikov, T.Varema, M.Altosaar);
- the basic and applied studies of materials based on nano and submicron films (M.Krunks, J.Hiie);
- metrology and quality assurance in chemistry: applied research and providing related services for the community (I.Leito);
- new technologies of production of rare earth metals and their derivatives (M.Karelson);
- the applied nanotechnology studies in materials science (M.Kerikmäe, M.Danilkin);
- the development of new technologies of proteomic study in cooperation with international chemical and biotechnology companies (J.Järv, A.Rinken).

The personnel of CECM consists of more than 90 teachers (incl. 4 members of the Estonian Academy of Sciences and 9 ordinary professors) and researchers and ca 70 doctoral students.

The current annual financing of the Centre from domestic and international sources is around 40 MEEK (ca 2.5 MEUR). In 2003 the investments into infrastructure and instrumentation exceeded 14 MEEK (ca 0.9 MEUR).

During the period 1998-2004 the co-workers of CECM have had or have over 50 grants from Estonian Science Foundation, over 10 EC projects (FW5, FW6, etc) 15 targeted financing or postdoctoral projects from the Ministry of Education and Science or ESTAG and numerous contracts and other support from Estonian (e.g., AS Silmet, AS Elcogen, etc.) or foreign private sector (e.g. Schenten Glasgroap, Bruker AXJ, Aqua Consult GmbH, Svenska Superfarad AB, Dow Chemical Co., etc.).

For the same time period over 500 peer-reviewed publications, monographs or their parts have been published (incl. over 70 during the year 2003), 10 patent applications filed (or approved), four co-workers of CECM (I.Koppel, E.Mellikov, J.Järv, M.Karelson) have been awarded the Estonian State Prize and 43 Ph.D. dissertations defended (incl. 20 persons during the years 2003–2004).

The following most outstanding results of the R&D work of CECM should be mentioned:

- the development of new principles of the design of superstrong superacids and -bases and its applications for the creation of components of highly effective stereoselec-

tive catalysts and electrochemical power sources,
- the development and study of the limits of applicability of new methods of computational chemistry for the description of technological processes,
- the creation of new materials for solar energetics, their study and applications,
- the studies for the design and working out of novel effective fuel cells and supercapacitors,
- the studies on the mechanism of action and applications for the drug design of bioactive compounds (receptors, proteins, enzymes),
- the development of novel materials and analytical methods and their applications in the environmental protection and monitoring (thermoluminescence detectors, biosensors) and also in the analysis and certification of materials.

INFRASTRUCTURE AND EQUIPMENT

The CECM has in its disposal the laboratory complexes in the Chemistry Building of UT at Jakobi 2 St. and in the VB block of the Main Building of TUT.

The major research and synthesis facilities and instrumentation and the respective modern software is eather available at CECM. (GC-MS spectrometers, SEM/EDSI EBIC instrumentation, titration equipment, pH meters, complex for ionizing radiation measurements (Cole/Parmer), electron beam evaporator, magnetron sputtering devices, FT IR spectrometer, UV/VIS spectrometers, HPLC instruments, professional Mbraun (dry)gloveboxes, Silicon Graphics, Sun and IBM work-stations, GC instruments, ion-chromatographs, beta-counters, ultrasonic baths, centrifuges, separation columns, freezers (-78°C), software (Gaussian03), Spartan02, Jaguar 3.5 Turbomole 5, NWChem 4.0, etc., cell harvester (Brandel), laminar flow box, cell culture room, high-temperature ovens, TLD dosimetric complex, rotating ring-disc electrode measurement system PINE, chronocoulometer, potentiostat/galvanostat PAR, conductometers, impedance measurement systems, various potentiostats and polarographic analysers (9), AFM, STM and EPR spectrometers, spectrofluorimeter, X-ray diffraction and electron microscope JEOL-JSM-35CF, BET-system, *etc.*) or at our collaboration partners in. Estonia or abroad.

In particular, these latter include: high-power and solid state NMR equipment and FT TOF/ MALDI (Tallinn, National Institute of Chemical Physics and Biophysics), FT ICR spectrometers for the study of gas-phase ion-molecules reac tions (U of Nice, U of Kyushu, CSIC, Madrid) etc.

In its turn, the CECM research facilities are used for collaborative applied and developmental by personnel of the collaboration partners of CECM.

The instrumentation of the working groups of the Faculty of Chemistry and Materials Technology of University of Tallinn has had extremely intense upgrading, especially in the year 2003 when over 11 MEEK (0.7 MEUR) were used for that goal.

CECM has very extensive collaboration contacts with numerous (over 100) partners of R&D cooperation from Europe, United States, Japan, Australia, etc.

STRUCTURE AND REACTIVITY OF CHEMICAL COMPOUNDS AND THEIR APPLICATION FOR DESIGN OF ADVANCED MATERIALS AND TECHNOLOGIES

MAJOR DIRECTIONS OF R&D WORK

- The design of neutral superacids and – bases, the "limits of growth" and potential applications.
- The least-coordinating anions, ionic liquids and their applications for the Li-ion batteries and supercapacitors.
- The experimental and computational study of acid-base equilibria in the gas phase and nonaqueous solution.
- The study of the influence of the electronic structure and solvent on the properties of chemical compounds and materials.
- The study of the interactions between alkali-metal cations and Lewis bases.
- Metrology and quality assurance in chemistry.
- Novel methods of analysis and their applications.

MAJOR RESULTS

1. The new principles of the design of the superstrong Brønsted acids were worked out by generalization and significant development of the so far existing methods for the design of superacids. It was found that the design of the least-coordinating and least-basic anion should be performed in such a way where besides the incorporation of the strongly electron-acceptor and highly polarizable substituents in the immediate vicinity of the acidity center of the neutral acid and the very extensive delocalization of the negative charge the emerging anion lacks the π-electrons as well as lone- electron pairs. On top of that, it is highly desirable that the anion of the superstrong Brønsted acid should have rather high symmetry (e.g.,-icosahedral) and that the delocalization of the negative charge should take place according to the mechanism which corresponds to the concept of three-dimensional sigma-aromaticity.
   These principles suggest the design of the new superstrong superacids (e.g., on the basis of the derivatives of $CB_{11}X_{12}H$ closo-carboranes (see Fig.1), where X stands, e.g., for the halogen or CF_3 group) whose superacidity is expected to exceed that of the sulfuric acid by 70 to 80 powers of ten!
   These results are of great importance for the design and creation of the components of the highly effective electrochemical power sources (Li-ion batteries, supercapacitors, fuel cells), stereoselective, recoverable, environmentally friendly and water-resistant catalysts for the organic synthesis, for the design of new ionic liquids for the "green chemistry", etc.
2. The study of the dependence of the superbasic properties of phosphazenes, phosphorus ylides and some other superbases on their electronic structure helped to clarify the general regularities which determine the basicity of the Brønsted superbases. In a similar way to the case of Brønsted superacids, the "limits of growth" of the basicity of superbases as potentially important modern synthetic and analytical reagents, were studied.
3. Very often, the acid-base properties depend very significantly on the solvent effects. The latter can strongly change the relative order of acidity or basicity of the compounds studied as well as the intensity of acid-base interactions. Therefore, in case of different synthetic, technological and analytical applications it is extremely important to know the quantitative aspects of the dependencies of the acid-base equilibria upon the properties of the solvent. This research group has developed very extensive unified acidity-basicity scale in the dipolar solvent-acetonitrile and the so-called ion-pair basicity scale in the low-polarity solvent – THF.
   First time ever, the present group succeeded to work out the spectrophotometric technique to establish an extensive acidity scale in apolar solvent – heptane. The lipophilic superbasic titrant t-BuP_4 (see Fig.2) was used as a titrant which, upon protonation recovers the bulky cation which is soluble in nonpolar solvent, is characterized by a very extensive delocalization of its positive charge and by very weak interaction with the conjugated anion of the Brønsted acids.
4. Several important regularities which characterize the intensity of the interaction between alkali-metal cation (e.g. Li^+ cation) and Lewis' bases depending on the nature of the neutral and anionic bases and upon the electronic structure of the Lewis' base were established.
5. Several procedures for the quality assurance, validation of methods, for the evaluation of the uncertainty of measurements and determination of the criteria for traceability of results, new reference materials as well as for the interlaboratory tests were worked out.

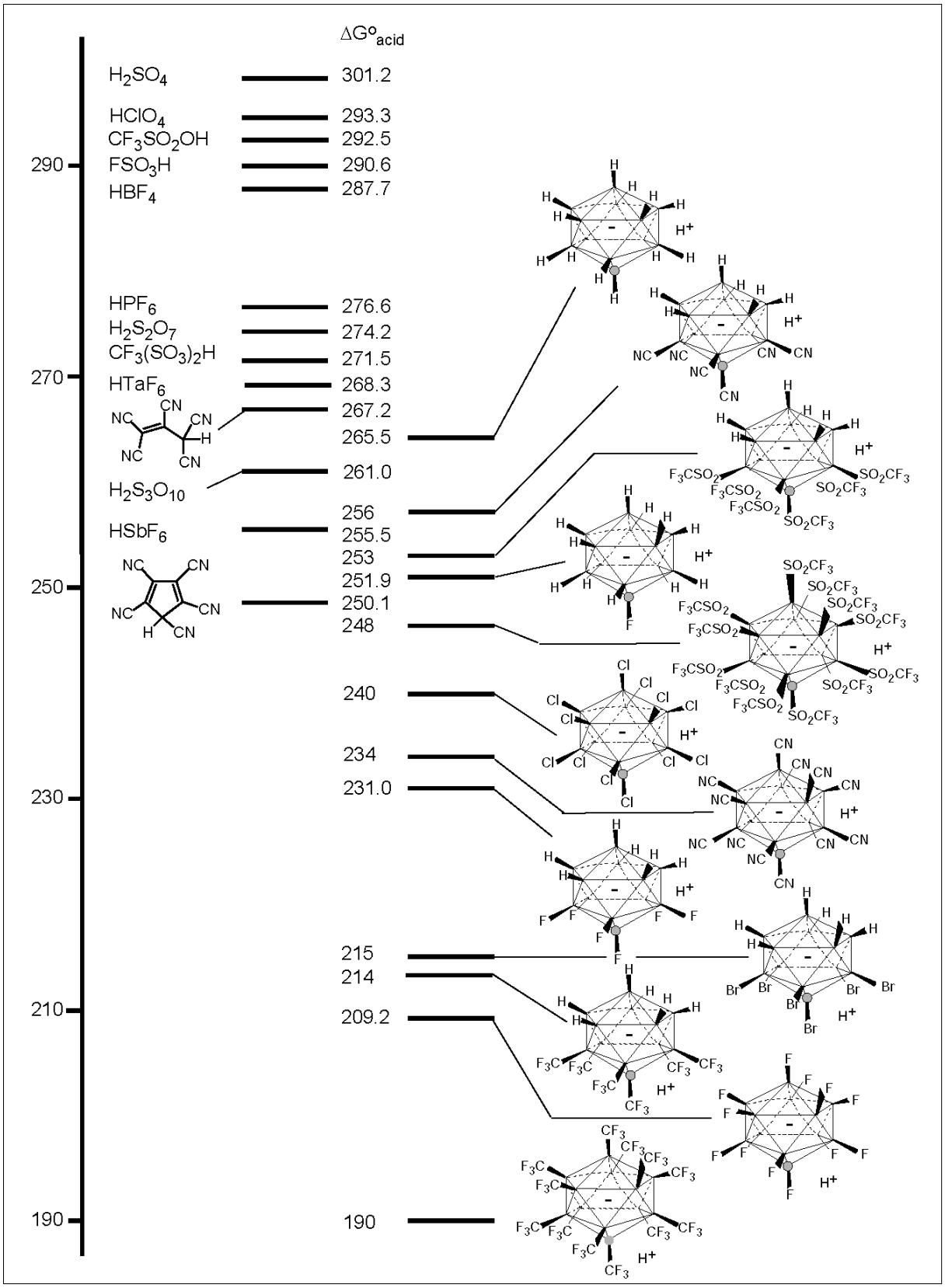

Fig. 1.
Gas-Phase Acidity (ΔG^{o}_{acid}, kcal/mol) Scale of Neutral Superacids. Acidity Increases Downwards.

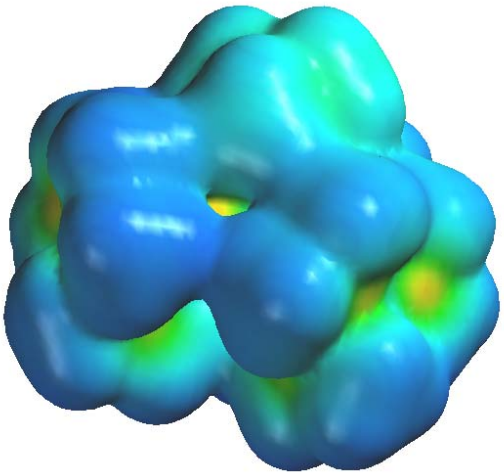

Fig. 2.
Molecule of the Lipophilic Superbase *t*-BuP_4.

During the last five years the research group has published ca 70 fullsize papers. Eleven PhD dissertations were defended during the same period of time.

The research group has very close and extensive collaboration with R&D partners from the USA, Japan, Germany, Spain, France, Australia, Sweden, Russia, Ukraine, etc.

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Abboud, J.-L. M., Koppel, I. A., Alkorta, I., Della, E. W., Müller, P., Davalos, J.Z., Burk, P., Koppel, I., Pihl, V., Quintanilla, E. Stereoelectronic, strain and medium effects on the protonation of cubylamine, a Janus-like base. Angew. Chem. Int. Ed. 42/20, 2281-2285 (2003).

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CHEMISTRY, PHYSICS AND TECHNOLOGY FOR PHOTOVOLTAIC SOLAR ENERGETICS

Research is concentrated to the fundamental studies of different inorganic PV materials (cadmium telluride (CdTe), copperindium-diselenide ($CuInSe_2$) type materials) and electroconductive polymers and technologies their formation with the aim of getting new fundamental knowledge about above-given materials and develop new design cheap devices for PV energetics.

The biggest attention is given to the fields of studies where members of the research group have long-time experience and know-how.

1. Photoluminescence studies of different CIS type materials $CuInS_2$, $CuInSe_2$, $CuInTe_2$ and $AgInTe_2$ (see Fig 3). During the year 2003 $CuInTe_2$, $AgInTe_2$ and other materials with different stoichiometry were grown in laboratory and used by us for description of all PL peculiarities in these materials. It was shown that the recombination model, which we have used for other highly doped ternaries holds also for $CuInTe_2$. and their phonon replicas.
   As a result we proposed a defect model for $CuInTe_2$. At the moment the similar studies will be performed for $AgInTe_2$. Lot of experimental work was done to study behaviour of Na and K in $CuInSe_2$. It is known that especially Na plays a essential role in $CuInSe_2$ based solar cells, but there are lot of speculations about it. We used a highly sensitive PL method and showed that the complicated solid solution of Na (or K) with $CuInSe_2$ is formed on the surface of samples. Methods of capacitance spectroscopy and especially admittance spectroscopy are used for investigation of properties of developed by our group solar cells. Preliminary studies have given a lot of information about recombination processes near the junction region of solar cells.
2. Regularities of formation thin films in magnetron sputtering process and in processes of chemical and electrochemical deposition. The main aim of studies is to investigate processes of formation different absorber, buffer and electrode layers by above-mentioned methods with aim of production of thin films with tailored technical parameters for their further use in different type solar cell structures.

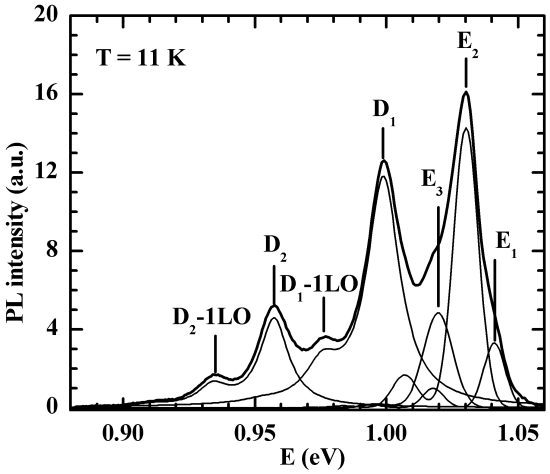

Fig. 3.
PL spectrum of $CuInTe_2$.

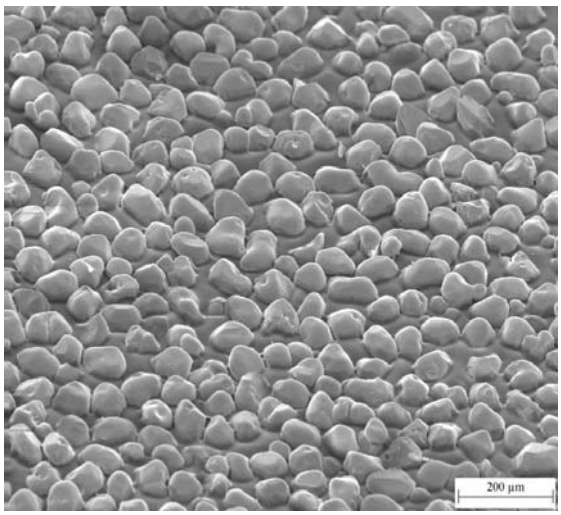

Fig. 4.
SEM photo of surface of monograin layer solar cell.

3. Scientific foundations for technologies of formation nano- and microcrystalline powders of different CIS type materials. Additionally to studies of kinetics and mechanism of recrystallisation of different CIS materials in different fluxes investigations of influence of different technological parameters and dopants to the properties roentgen-phosphors are performed.
4. Development and investigation of photovoltaic structures with conductive polymers in different sandwich configurations, for example:
   glass/ITO/CISe/PANI/Ag,
   glass/ITO/CISe/PPy/Ag,
   Cu/CIS/PPy/i-ZnO/n-ZnO,
   Cu/CIS/PEDOT-PSS/i-ZnO/n-ZnO,
   Cu/CIS/PEDOT-PSS/Graphite_dot,
   Cu/CIS/PEDOT-PSS/Au (semitransparent)
   and Cu/CIS/PEDOT-PSS/Au (grid).
5, Development of solar cells in new design. Regularities of different processes of formation solar cells in developed by us new design on the base of monograin layers (Fig. 4) are under investigation. The developed technology is protected with patents in more than 20 countries. The research and development activities are supported and co-financed by the foreign company. There is permanent interest to the developed technology by different other foreign companies due to perspectivity of monograin layer solar cells for niche and architectural applications.

Results of research performed during the year 2003 are published as 17 papers or accepted for publication papers in international journals and 2 patent applications are under finalization. Development contract with Scheuten Glasgroap had successful continuation during the period. 4 young members of project research team were gone through the training in well-known European universities in this year. During the next year the training of as minimum 6 young scientists is planned. Members of the team are participating in three EU FW5 RTD projects.

Co-financing of research and development activities from industry and European Commission has been about 12 million Estonian crown during the year 2003. About 11 million EEK is invested into the infrastructure of laboratory mainly in use of finances of the group.

At the moment about 95 % of laboratory equipment is not older than 4 years. The new unique scientific equipment purchased during the year 2003 includes high resolution scanning electron microscope LEO35 with EDS and EBIC possibilities, electron beam evaporator, high preciseness spin coater, spectrometer Autolab 306, ultrahigh vacuum equipment, etc.

EC financed EU FW RDT projects in the field of group RTD activities: EU RDT projects NNE5-2001-00544 The European Polymer Solar Battery, NNE5-2002-00017 Materials and Technologies for Photovoltaic Applications from Estonia; NNE5 –2002 "Accompanying Measures for Co-ordination of NAS and European RTD Programmes on Photovoltaic Solar Energy".

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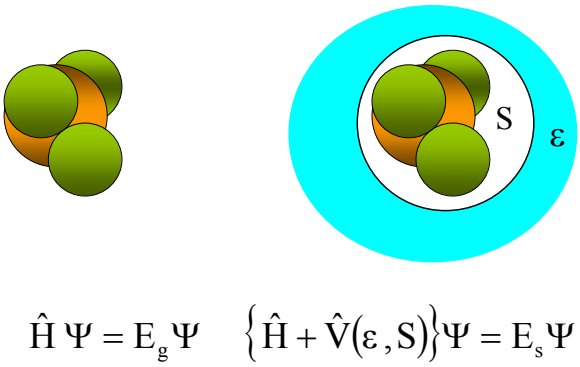
THEORY AND MODELLING OF COMPLEX MOLECULAR SYSTEMS

The contemporary chemical and biotechnology, the development of novel materials and medical drugs, and many other research areas require the knowledge of reliable data about the intrinsic structure and properties of chemical compounds and complex molecular structures. Precise *ab initio* methods based on quantum theory are mostly applicable for relatively small molecules in the gas phase. Almost all industrial chemical processes and all chemical reactions in living organisms proceed, however, in disordered condensed media such as the solutions, membranes of polymers. The intermolecular interactions in these dense systems may significantly affect the electronic structure of compounds and thus their physical properties or chemical reactivity. Notably, many novel technological processes and biochemical reactions are also so complex that their *ad hoc* description is virtually impossible.

Therefore, one of the most important areas of modern theoretical chemistry is the development of alternative approaches for the adequate description and reliable prediction of molecular structure and properties in complex dense molecular systems. The more promising within such approaches appear to be the quantitative structure-property relationships (QSPR) and the application of various artificial intelligence methods. The recent achievements of the theoretical chemistry group at the Centre of Excellence are indeed connected with the development of novel methodology and software for the predictive QSPR and the quantum chemical description of molecules in dense disordered media (Fig. 5). The original expert system based on theoretical molecular descriptors and the met-hods describing the interactions with solvent reaction field have been successfully employed for the prediction of physico-chemical, technological and biomedical properties of a large variety of complex molecular systems. The methods developed have allowed to obtain robust models for the prediction of the density, solubility, refractive index, dielectric permittivity, the boiling, melting and flash points, and other properties of technological importance of structurally variable chemical compounds. The use of novel molecular descriptors and docking calculations have revealed intricate details of the drug-receptor interactions, the affinity and specificity of new medical drug candidates (see Fig. 6).

The group has extensive ongoing international collaboration with more than 20 institutions around the world, including such top research centres as the Florida Center for Heterocyclic Compounds (USA), Jülich Research Centre (Germany) or Mario Negri Institute (Italy).



$$\hat{H}\,\Psi = E_g\Psi \qquad \left\{\hat{H} + \hat{V}(\varepsilon, S)\right\}\Psi = E_s\Psi$$

Fig. 5.
Simple self-consistent reaction field model for the description of the electronic structure of a molecule in a surrounding medium S with dielectric permittivity ε.

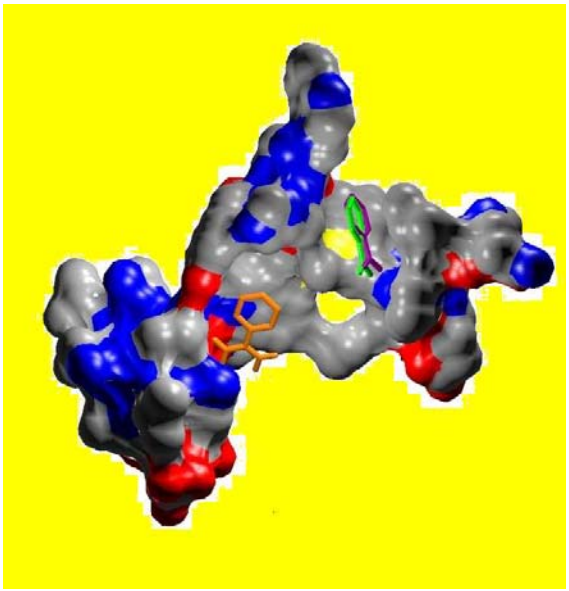


Fig. 6.
Computer modelling of the aromatic compound docking with Transcription factor Malt domain III protein.

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THE ELECTRICALLY CONDUCTIVE POLYMERIC MATERIALS IN MULTILAYER STRUCTURES: CHEMISTRY AND TECHNOLOGY

The aim of work of group is the investigation of the fundamental properties (the defect structure, conductivity mechanism, kinetic properties of the materials doping process) of ECP and A_2B_6 semiconductive materials. Our results permit to conclude that combined method for composite coatings formation onto varies light transparent substrates by electrochemical polymerization of PPy from solutions containing of high-temperature doped PPP particles gives the opportunity to improve the structure, morphology and electrical properties stability of prepared structures. By this way we extend the possibilities for development in technologies of inorganic-polymer composites and multilayer structures based on photoactive A_2B_6 type materials. One of the possibilities to improve of mechanical properties of electrically conductive polymers is the combining of PPy with classical insulating polymers as polyethylene, polypropylene and others. The aim of our investigations is prepare electrically conductive composites PE(polyethylene)/ $PPy(Cl)_{chem}$ and to investigate the redox prope rties of these materials by cyclic voltamperometic technique. The highest electroactivity and electrochemical stability was still found for materials, doped with small anions as Cl^- and NO_3^-.
Technical parameters of semiconductor materials are strongly influenced by defects. Due to necessity of tailoring properties of materials used in our development activities during the last year the chemical diffusion coefficient D as a function of temperature and components vapour pressure was investigated for undoped ZnS and CdSe monocrystals at high-temperatures between 750-1150^{0}C. It is found, that the dominative defects in the diffusion process are the double ionized Zn and Cd atoms. The defect structure of CdSe:Al, CdSe:Ga, CdSe:In, ZnSe:In, ZnS:Al, ZnS:Ga and ZnS:In was analyzed by the high-temperature conductivity method.

The electroneutrality condition $n = [D^{\bullet}]$ was found as the dominative for achievement the high n-type electrical conductivity.

Hybrid organic-inorganic structures based on n-CISe/p-ECP (ECP = PANI and PPy) heterojunctions were prepared using electrochemical and casting techniques and characterized for PV application. The studies confirm that a n-p barrier is formed between the n-CISe and p-ECP layers. The cell improvement due to the illumination during the PPy electrodeposition of the buffer layer is shown. The studies prove also that the deposition of a thin PPy film onto CIS potentiostatically under white light illumination at low potentials is preferable for producing the PV structures. A new approach to prepare

Cu/CIS based solar cell using an organic buffer layer of PEDOT-PSS was studied. The optimal conditions for spin-coating of high-quality thin PEDOT-PSS films with a good adherence to the surface of polycrystalline CIS are determined.

In cooperation with Budapest Technical University the investigations for development of DNA-biosensors based on electrically conductive PEDOT is started. The PEDOT thin films doped with (PSS^-) and $Fe(CN)_6^{4-}$, (FCN^{4-}) anions were prepared by the electrochemical syntheses method. Prepared structures are characterized by AFM, EQCM and SECM techniques.

EC financed EU FW RDT projects in the field of group RTD activities: EU RTD projects NNE5-2001-00544 The European Polymer Solar Battery, NNE5-2002-00017 "Materials and Technologies for Photo-voltaic Applications from Estonia".

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INTERFACIAL AND SOLID STATE CHEMISTRY AND APPLIED ELECTROCHEMISTRY

MAIN RESEARCH DIRECTIONS

- Electric double layer structure at Bi, Cd and Sb single crystal faces.
- Adsorption kinetics of organic compounds at Bi, Cd and Sb single crystal faces and at carbon electrodes.
- Influence of geometric and energetic inhomogeneity of surface on the adsorption characteristics of various compounds (see Fig. 7 and 8).
- Influence of crystallographic structure of the solid surface on the kinetics of various electrochemical reactions (cathodic hydrogen evolution, electroreduction of oxygen, complex anions, cations and organic compounds).
- Electrochemical behaviour of nanoporous carbon electrodes (Fig. 9) and supercapacitors (cooperation with Tartu Technologies Ltd.)
- Electochemical reactions at solid oxides and electrochemical characteristics of solid oxide fuel cells (cooperation with AS Elcogen) (see Fig. 10).

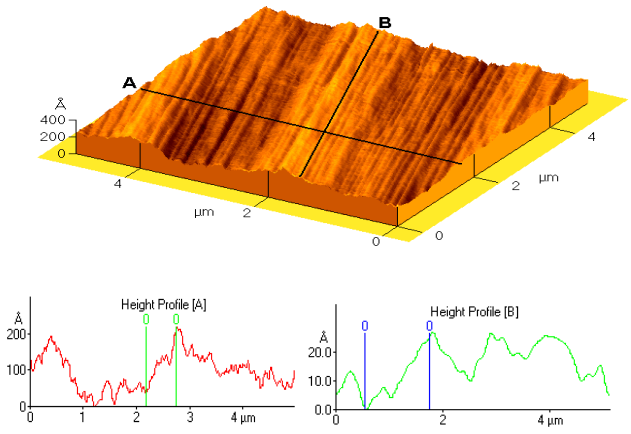

Fig. 7.
Surface structure of Sb(III) electrode cut at the room temperature.

- Electrically conducting polymers and quantum chemical calculations by following methods:
  - ✓ molecular mechanics,
  - ✓ semi-empirical: AM1, PM3,
  - ✓ *ab initio* HF: 3-21G…6-31++G**,
  - ✓ density functional: B3LYP,
  - ✓ perturbation theory: MP2.

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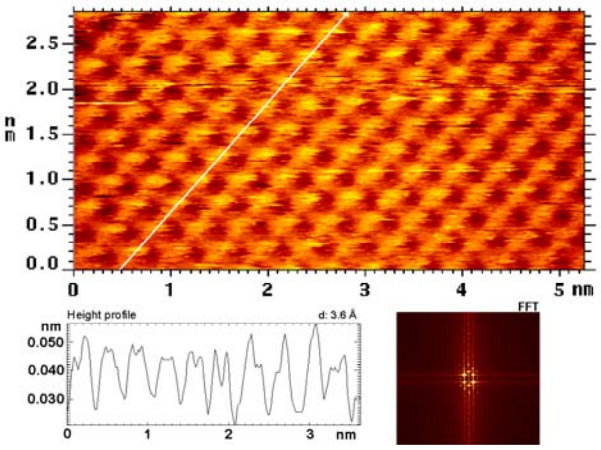


Fig. 8.
UHV-STM atomic resolution image, selected surface profile and fast Forier transformation image for Sb(111) surface cleaved at temperature of liquid N_2.

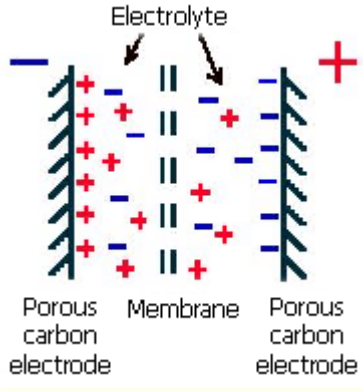
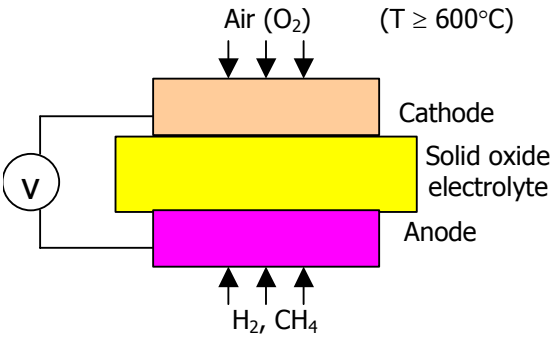


Fig. 9.
Double layer capacitor.



$O_2 + CH_4 \rightarrow$ fuel cell$\rightarrow CO_2 + 2H_2O$

Fig 10.
The general scheme of solide oxide fuel cell.

TARGETED SYNTHESIS OF COMPLEX MOLECULES AS NOVEL MATERIALS AND BIOACTIVE COMPOUNDS AND DEVELOPMENT OF APPROPRIATE THEORETICAL CONCEPTS

The objectives of this topic can be achieved through coordinated activity of the group members working in different research areas: fine organic synthesis, targeted design of novel compounds and contemporary biochemistry and moelcular biology. Such multi-level research is supported by cooperation with other groups within the Center of Exellence, and has yelded the results summarized below.

New biomimetic compounds, consisting of stuctural elements of nucleic acids and peptides and linked by various spacers of different structure have been synthesized as ligands targeted against nucleotide receptors, specifically against the P2Y1 subtype of these receptors. Several nucleoside-peptide conjugates were synthesized as bi-functional inhibitors of protein kinases.

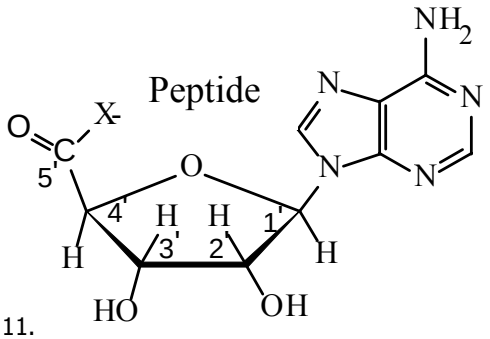


Fig. 11.
The general formula of protein kinase bi-functional inhibitors, where X stands for a linker group between nucleoside and peptide parts.

Further the influence of pegylation of these compounds upon their activity and cell-penetrating ability was studied. It has been found that pegylation increased stability of these compounds in living cell, as is typical for biomimetic molecules. In paralel to synthetic work and activity assay also the kinetic mechanism of enzyme inhibition by these compounds was initiated, characterizing their interaction with the free enzyme and the enzyme-substrate complexes. In addition to these novel compounds several peptide and PNA series were tested as intracellular. A new non-peptide ligand of melanocortine receptor has been characterized and more systematic study of this ligand has been started.

For advancement of the methods of design of new bioactive compounds our investigations into kinetic mechanism of ligand binding with G-protein coupled receptors were continued. The model of non-exclusive binding of agonists and antagonists with these receptors was developed and compared with the concepts of allosteric ligand binding with the 7TM recepors. The effect of different G-proteins on ligand binding at m2 muscarinic receptors was investigated and influence of some pathologies on properties of dopaminergic receptors was discussed.

In parallel with bioactivity studies several synthetic approaches were introduced, including new reagents and their applications for synthesis of hydrazines with four different substituents. These methods provide new perspectives for preparation of bioactive compounds, including azapeptides. Modulation of chemical reactions by ultrasound seems to be a perspective approach for working out new selective synthetic methods. Kinetic studies on Grignard reaction with silanes in diethyl ether and ether-toluene mixtures and definition of the role of specific solvation in these processes has widened perspectives of practical application of these reactions, including modified technologies for bulk chemical industry.

As a new trend, investigations were initiated in preparation and study of smooth siloxane surfaces for AMF visualization of immobilized biopolymers, important step for design of molecular chips and related technologies.

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ANALYTICAL AND ELECTROCHEMICAL METHODS OF ANALYSIS AND THEIR EXPLOITATION IN ENVIRONMENTAL MONITORING

MAIN RESEARCH DIRECTIONS

- Development of biosensors for environmental monitoring,
- Mathematical modelling of biosensors,
- Development of short-term method for estimation of oxygen demand of wastes and wastewaters,
- Study of oxygen mass-transfer through surfactant films,
- Characterization of nanostructured and chemically modified electrodes.

One of the objectives in the frames of the research was to study the adsorption of surfacetants on the liquid-air interface at various surfacetant concentrations in solution. A special device based on electrochemical oxygen sensor has been designed in order to determine the oxygen permeability through the interface.

The modelling of experimental results enabled us to characterise the adsorption phenomena and the state of molecules on the gas-liquid surface. The mass transfer through air-water interface depends on amount of surfactant on the interface as well as on the structure of a surfactant molecule. The device can be used for the determination of the air-water interface oxygen permeability of natural waters and wastewaters and for the evaluation of effectiveness of aeration processes in wastewater treatment plants.

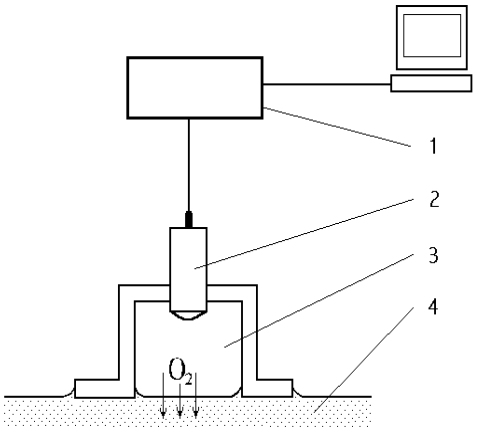

Fig 12.
Measuring device for the determination of O_2 mass-transfer through air-water interface: 1- oxygen meter, 2- oxygen sensor, 3- gas chamber, 4- solution.

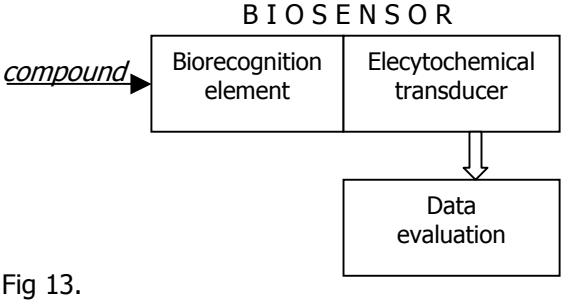

Fig 13.
Biosensor's operational principle.

To work out applications for environmental technologies in express analysis the biosensors

based on different biologically active components (microorganisms, various enzymes) were studied. Also the characteristic parameters of processes, connected with biologically active compounds, but also the calculations of these parameters from the electrochemical biosensor output signal were studied. The elaborated tyrosinase-based biosensor can be used for the determination of carbaryl. It was found that carbaryl acts as an inhibiting substrate towards tyrosinase and it is necessary to use a combination of two independent calculated parameters for the determination of carbaryl in the concentration range 0.1- 20 mg/l. Biochemical oxygen demand (BOD) sensor designed by the work group, can be used to determine the BOD values of inflows of different wastewater treatment plants. The traditional BOD_7 analysis needs 7 days incubation period, but with BOD-sensor BOD_7 can be evaluated over 1 hour.

The research group has worked out a special device and method of measurement for the determination of short-term biochemical oxygen demand. Method enables to estimate the biodegradability of wastewater components and relative amounts of fast and slowly biodegradable components of wastewater. The fast determination of biodegradability of wastewaters is a very important aspect to assure the efficiency of wastewater treatment processes. The method is also applicable to study the characteristics of active sludge and biodegradability of different substances, for example phenolic compounds.

There has been an increasing interest in the study of chemically modified electrodes. These can be used in various devices, including electrochemical biosensors. We have used the diazonium salt reduction method for the covalent attachment of quinones to carbon electrodes. These quinone-modified electrodes show a high electrocatalytic activity for the two-electron reduction of oxygen to hydrogen peroxide. Carbon electrodes grafted by quinones are good electrocatalyst candidates for the electrochemical production of hydrogen peroxide.

Chemical modification of surfaces is also a powerful means to design indicating electrodes of controlled electrochemical properties for biosensors. For instance, we have successfully employed the gold electrodes with covalently immobilised cytochrome c for the electrochemical detection of superoxide ion (O_2^-).

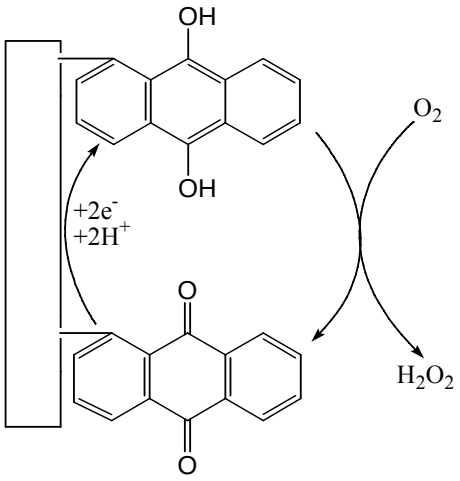

Fig. 14.
Electrochemical synthesis of hydrogen peroxide on an anthraquinone-modified carbon electrode.

Nanostructuring of electrodes offers a unique opportunity to alter the electrocatalytic properties of catalytically active materials on various supports. Even submonolayer amounts of catalysts on inert supports can significantly alter the electrochemical behaviour of these electrodes. The research under this task was aimed at establishing a relationship between the electrocatalytic activity of nanoscale catalysts and their surface structure.

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THEORY, DESIGN AND EXPLOITATION OF RADIATION DETECTORS AND LUMINESCENT MATERIALS

Our research group has being matured for more than 20 years in studies and development of luminescent materials. We carry out both fundamental and applied research in the field.

We have a long-term co-operation with Synchrotron Radiation Laboratory of Physics Faculty of MSU and Physics Chair of MUCTR. This co-operation enables us to access unique scientific instruments like synchrotron radiation sources and quantum magnetometer.

Our research work involves solid state chemistry, solid state physics, radiation damage, material science, and also development of equipment. We apply different techniques in our studies: luminescence, thermo- and optically stimulated luminescence (TSL and OSL), optical-, radio-, and gamma-resonance spectroscopy, magnetic measurements, chemical preparation and analysis of luminescent materials.

The fundamental research includes studies of intrinsic and impurity defects, interaction of defects, mechanisms of luminescence and energy transfer.

The investigation of intrinsic and impurity defects in Alkaline Earth Sulphides (AES) and Oxides (AEO) is carried out to create connection between fundamental studies concerning solid state chemistry and physics and luminophor applications. For this purpose a new method of synthesis of AES and AES luminophors in sulphur vapours is worked out. Also, the plastical deformation and radiation damage are studied in connection with intrinsic defects and their properties. Both plastical deformation and neutron irradiation were found to damage crystal lattice through displacement of dislocations, with intrinsic defects being generated in the regions where dislocations cross each other. The ionic processes are going in the damaged crystal lattice at lower temperatures compared with the processes in the unbroken lattice. This means that the restoration of the damaged lattice at heating is also carried by moving dislocations transporting intrinsic and impurity defects.

We have accomplished extensive EPR studies of V centres, F centres, cation and anion vacancies in AES. The results are published in papers.

When studying chemical and physical mechanisms of defect generation, a particuar interest is turned to a problem of formation of impurity ion pairs and complex centres containing impurity defects and intrinsic lattice defects. The problems of charge, energy transfer, and luminescence efficiency are also investigated.

Our resent results on synthesis of luminescent materials with controlled impurity arrangement and improved energy transfer mechanisms open a good possibility to work out new luminescent materials. New infrared-sensitive luminophors are presently being developed and studied. These new materials are promising for future technologies of information storage and displaying. We study two different kinds of luminophors: new storage OSL (optically stimulated luminescence) luminophors and dosimeters, and also new infrared-sensitive upconversion luminophors.

We also do investigations and applied works in the field of thermoluminescent dosimetry. Various TLD (thermoluminescent dosimeter) materials were subjected to optical stimulation, and possibilities were estimated to check the dose by means of OSL measurements. The well known TLD (thermoluminescent dosimeter)-material $Li_2B_4O_7$:Mn was studied for the light-induced energy storage. The influence of reducing and oxidising environment, and also the role of some impurities was investigated. The titanium complex with oxygen is the most probable sensitising agent causing the light-sensitivity of $Li_2B_4O_7$:Mn-based TLD.

Exhibition in Spain, September 2003, and our TLD sorting gauge.

Fortunately, the comp-lex is destroyed at elevated temperatures yet suitable for pellets sintering. The technology of TLD sintering is now essentially improved to avoid light-sensitivity.

The new technology of synthesis of AES-based luminophors and TLD calibration is supported by our studies in the field of automation and remote control systems. The remotecontrolled programmable technological equipment is already functioning in our laboratory: automated furnaces with loading hands, which are programmed for thermal treatment of materials step by step. Also, we have computer-driven sorting gauges for TLD pellets. Our rotary sorting gauge and TLD pellets were demonstrated at the industrial exhibition hold in parallel with International conference on scintillators and luminescent materials SCINT 2003 in Valencia. Our production has attracted the attention of foreign specialists in the field.

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CHEMISTRY AND TECHNOLOGY OF NANOCRISTALLINE AND SUBMICRONIC FILMS

The research under the proposed project is to develop high-effective nanocrystalline and submicronic films for photovoltaics, dielectrics and phosphors by cost-effective chemical methods. The farther scope is to contribute in making solar energetics competitive as a energy source. To reach this purpose the cost of energy produced is one of the limiting factors and therefore low cost solar cells must be developed. Principally the problem could be solved using as small as possible amount of materials, consequently thin film solar cells prepared by cost–effective chemical methods. In the present study chemical spray pyrolysis, chemical deposition, sol-gel technique and growth from molted salts will be applied to produce thin films. In the part of fundamental research the studies on the formation chemistry of compound semiconductors and dielectrics (CdTe, $CuInS_2$, $CuInSe_2$, InxSyOz, Zn(O)S, TiO2, ZrO2) and determination their properties by physico-chemical methods will be carried out. The development of well-grounded chemical technologies needs the further studies on the thermoanalytical behaviour of novel metal-organic precursors and phase equilibrium in the system Cd,Zn-Te,O-Cl,I. The applied research part includes physical studies on the growth and properties of nano and submicronic films prepared by chemical methods. Photovoltaic solar cell structures will be prepared and characterised. The new constructions of photovoltaic devices will be developed.

The investigations are performed in 3 main research fields.

FORMATION CHEMISTRY OF THIN FILMS BY CHEMICAL METHODS

1. Formation chemistry of SC buffer and absorber materials in spray pyrolysis process, including reactions in spray solution, structure and thermal behaviour of intermediate complex compounds as precursors for spray pyrolytic process to establish the best film deposition procedure routes and to find out the limitations for film properties. For example, the structure structure of metal chalogenide thiourea complex compounds Me(tu)nXm.yH2O (Me=Cd,Zn,Cu, X=Cl,Br; n=1,2,3, m=1,2 y=0,0.5,1) as model compounds for pyrolysis process of metal sulfides is studied by XRD, RAMAN and FTIR, their thermal decomposition by TG/DTA/DTG and TG/EGA methods.
2. Phase equilibrium in Cd-Te-O-Cl system by thermoanalytical methods to model recrystallization processes of CdTe in presence of CdCl2 and oxygen with the aim to work out the best routes to prepare high efficiency CdTe/CdS solar cells.
3. Formation of metal oxides and forming thin film properties in sol gel process using different metal alćoxide precursors, gelating agents and solvents, following processes during thermal treatments by thermo-analytical methods.

THIN FILMS BY CHEMICAL METHODS

1. The growth and properties of $CuInS_2$ (CIS) on flat and porous window layers (ITO, TiO_2, ZnO). It is shown that growth on ITO electroders is similar to that on glass substrates. ITO could be used as ohmic contact, growth on porous TiO_2 leads to the oxida- ion of CIS on TiO_2/CIS interface, growth on ZnO depends on the orientation of underlayer. CIS crystallite size is inversely dependent on the orientation rate of metal oxide underlayer.
2. Growth of CIS films with large crystallites. 2 preparation routes were used: Cu-rich spray solutions and recrystallization of nanocrystalline films. XRD, SEM, EDS and che- mical analysis methods were used for characterization and it is found that the use of Cu-rich solutions and recrystallization in presence of Cu_xS phase leads to In-rich films with mean grain size of one micron.
3. Electrical properties of sprayed CIS films (resistivity, conductivity type, concentration of carriers) by thermopower, 4 point and C-V measurements on CIS/Al Schottky barriers and p-n junctions. CIS films from stoichiometric and Cu-rich solutions show p-type conductivity. The conc. of majority carriers 1xE17 cm-3. Resistivity is higher in the case of In-rich solution used.
4. The formation and properties of TiO_2 films by sol gel spin coating and spray processes are studied. The structure of the films was characterized by FTIR, FTIR, AFM, optical properties by ellipsometric and electrical properties by impedance measurements. The technological parametres leading to dense (n=2.3) anatase films with high dielectric permittivity (e=75) have been established. The development of flat and nanoporous TiO2 films by sol gel as n-type window layers for SC.

CHARACTERIZATION OF PV STRUCTURES PREPARED BY CHEMICAL METHODS

The study of output parametres and characterization of TiO_2/buffer/CIS and ZnO/buffer/CIS solar cells prepared by chemical methods. By all layers sprayed SC the efficiency of 2.4 % is reached. The use of buffer layer in TiO_2 based solar cells effectively supresses interface recombination according to I-V measurements. By V_{oc}=f(T) measurements is confirmed that interface recombination, as the limiting factor of solar cell performane, could be decreased using In-S buffer layer.

The reasearch work is a international collaboration between TTU and Helsinki University, Helsinki TU, Uppsala University, Kiel TU, Durham University, research institutions of Germany and Netherlands – HMI, ECN.

There are working 1 visiting PhD student, 4 PhD students, 1 master student under the project, PhD students are worked at 2 universities abroad, participating 1 one summer school in year 2003.

EC financed EU FW RDT projects in the field of group RTD activities: EC projects HRPN-CT-2000-00141 "ETA solar cells" and NNE5-2002-00017 "Materials and Technologies for Photovoltaic Applications from Estonia"; WTZ projekt EST 02/001 "Low-cost processing of high-k dielectric thin films".

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The Centre of Molecular and Clinical Medicine was established in 2001 to raise the level of Estonian medical research and to concent-rate the skills and funds in a selected cutting-edge areas of medical research, neuroscience in particular.

The Centre brings together ten of the best pre-clinical and clinical research groups from the University of Tartu into a consortium where the combination of high-standard theoretical and applied biomedical research as well as clinical research has been well achieved. In 2002 the scientific quality of the Centre was assessed and we received the highest possible rating 5,0 from European Commission in Call for Accompanying Measures for East-European Centres of Excellence recognized as a NAS Centre of Excellence.

The general mission of the Centre is to perform internationally recognized research in medicine, particularly in order to reduce the burden of neurological diseases, mental illness and beha-

vioural disorders (as separated entities or complex chronic diseases) through research on brain, mind and behaviour.

Main research directions:

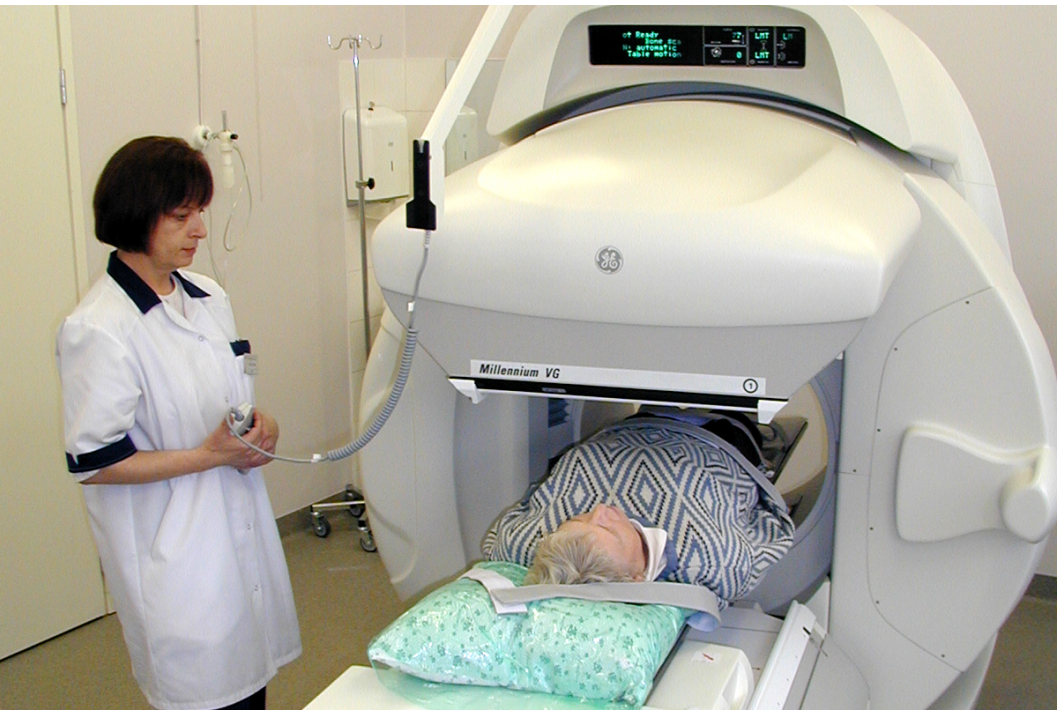
- Genetic, biochemical, and physiological factors contributing to mental and behavioural disorders (role of neuropeptides in behavioural and mental disorders, eating disorders, genomics of behaviour and mental disorders).
- Mechanisms of target destruction in neurodegeneration and neurodegeneration associated chronic diseases (brain bioenergetics, oxidative stress, neuroimmunology and inflammation).
- Interaction between genes and the environment in neurological diseases.
- Development of new therapies for neurological diseases (neuroprotectants, neuronal stem cells, probiotics).

During last five years our scientists have published more than three hundred of articles in international peer-reviewed journals and as chapters of books. Among them are papers in highly ranked journals as, Proceedings of the National Academy of Sciences of USA, Journal of Cellular Biology, Nature Biotechnology, FASEB Journal, American Journal of Human Genetics, Journal of Neuroscience, Circulation Research, Journal of Clinical Psychopharmacology, Journal of Clinical Endocrinology and Metabolism, American Journal of Pathology, Investigative Ophthalmology and Visual Science, Biochemical Journal, Neuropharmacology, Pain, Neuroscience. Several scientists are acting also as an independent expert for EC Research Directorate, Finnish Academy and INSERM.

Research in Centre is sponsored mainly by Estonian Ministry of Education and Research, Estonian Science Foundation, Estonian Technology Agency and European Commission (EC). During last five years the staff of the Centre has been holding approximately 60 different research grants or contracts including more than ten grants from EC. Currently the Centre is involved in 4 EC projects (QLG3-CT-2000-01405 Cystatin B and myoclonic epilepsy, QLK3-CT-2002-02114 European network to develop new therapeutic strategies for Parkinson's disease using lentiviral vector technology, QLK1-CT-2001-00135 Functional assessment of interactions between the human gut microbiota and the Host and QLG1-CT-2002-90390 Integration of Estonian medical science into the European Research Area: towards a healthier society) and in one Wellcome Trust sponsored research project.

The Centre uses several animal models for characterization of human diseases.

Centre's researches identifying target molecules for nervous system disorders.



The Centre has well-developed facilities to diagnose various disorders of nervous system.

The Staff of the Centre consist of roughly 80 staff scientist excluding postdoctoral fellows, PhD students and technicians The Centre is involved in two PhD students teaching schemes (incl. Graduate School), being the most relevant training site for PhD students in medical sciences as well for PhD students in Neuroscience (altogether 40 PhD students). Currently more than a half (approximately 2/3) of the Estonian Ph.D. in medicine have come from groups joined to the Centre as well as most of the postdoctoral fellows work or have been working in these groups.

Several prominent European scientists are giving seminars or lecture courses in topics where our competence needs to be strengthened. From 2003, with the financial help of EU, several specific training and exchange programmes were initiated to meet the scientific needs of the Centre by organising the hands-on courses involving the emerging neuroscience and related methods.

The Centre is based on the infrastructure of the Biomedicum of the University of Tartu (8000 m^2) and the nearby located Clinics of Neurology, Psychiatry and Pediatrics (400 m^2). The Biomedicum was built in 1999 in order to establish the most contemporary centre for biomedical research in Estonia. As a result, the research groups of the Biomedicum are equipped with most modern equipment giving a good basis for the fulfilment of the GLP rules. This includes also more expensive equipment like mass spectrometer, flow cytometer, QPCR, laser confocal and electron microscope and stereology system for 3D brain analysis. There is also a modern animal house with readily adjustable conditions for animal experiments that meet the needs of researchers and animals. In parallel our clinical departments have invested 5 million Euros for imaging equipment required for clinical neuroscience.

Several SMEs collaborate with research groups of the Centre and from years 2004-2005 there will be a new building for the Tech-

nology Institute associated with the Biomedicum. Research groups in the Centre have also access to methods, facilities and equipment from other departments of the University of Tartu including the Institute of Molecular and Cellular Biology. We can use the services of the Central Laboratory and Pathology Service of Tartu University Clinics, but also services of the Library and Computer Centre. There are also excellent accommodation facilities for students and visitors (700 places) since autumn 2002.

BIOENERGETICS

The main focus of current research is to understand the mechanisms of intracellular regulation of mitochondrial function in living cells in health and disease. The work includes the following components:

- Characterization of the relationship between mitochondrial energy producing function and expression and compartmentalization of pro- and anti-apoptotic proteins in the brain, cardiac and skeletal muscle cells *in vivo*.
- Experimental studies of mitochondrial – cytoskeletal interactions in the cells in vivo, molecular characterization of proteins controlling mitochondrial position in the cells, characterization of the outer membrane properties of mitochondria and the study of modulation of genes related to mitochondrial – cytoplasmic crosstalk in heart failure and neurodegenerative diseases.
- Studies on bioenergetic aspects of pathophysiology of cardiovascular and neurodegenerative diseases: those related to perfusion problems (ischemia, ischemia-reperfusion, hypoxia) in the vascular system, and those related to alterations in the cells – mitochondrial neuropathy and myopathy – will be studied in combined clinical and experimental research.

RESEARCH DIRECTIONS

- Experimental studies on the mechanisms of Starling's phenomenon. The effects of variation in muscle and sarcomere length on the function of complexes between mitochondria and ATPases (intracellular energetic units – ICEUs) are studied.
- Identification of the proteins associated with cytoskeleton that determine the mitochondrial localization and tissue specificity of regulation of mitochondrial respiration in oxidative muscle cells. The cDNAs, exclusively specific for oxidative muscles are isolated and expressed in an eukaryote system. The recombinant proteins obtained will be used in the reconstitution experiments, with estimation of their regulatory influence on mitochondrial respiration.
- Elaboration of the mathematical models to quantitatively describe the transfer of compartmentalized energy transfer in muscle cells in healthy and pathological conditions. The data obtained from the abovementioned experiments are analysed with a purpose to develop and improve the quantitative models, in collaboration with the Institute of Cybernetics, Tallinn.
- Clinical Studies. Estimation of the possibility that the ICEUs represent the targets in ischemic injury, heart failure and neurodegenerative myopathies. The atrial specimen received from patients during cardiac surgery and the preparations of skeletal muscles from patients with coxarthrosis, traumatic injuries and neurodegenerative muscle diseases are studied with respect to structure and function of ICEUs, to define alterations in mitochondrial respiratory chain, in interaction of kinases with oxidative phosphorylation, and in channeling of adenine nucleotides between mitochondria and ATPases.

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BIOCHEMISTRY

Recent decade is characterized by tremendous increase in biomedical and clinical interest in oxidative stress (OS). Prolonged high-grade OS, expressed via excess of ROS, abnormal lipid peroxidation, severe modified LDL, proteins and DNA, has one of the key-positions in the development and progression of Alzheimer's disease, parkinsonism, premature aging, stroke, ischemic or traumatic damages of brain, arteriosclerosis, ischemia/reperfusion damages, etc. The OS-related fundamental-clinical projects (project ASSER, study of antioxidants, protector-molecules, protective mechanisms, probiotics, metabolites) will have impact on both understanding of adaptive mechanisms of human organism and regulation/suppression of high-grade OS. Eventually, this knowledge allows work out effective and optimal schemes for prophylaxis and treatment. Due to above mentioned reasons the main focus of our current research are OS and diseases – molecular mechanisms, proteomics, peptidomics and metabolomics.

RESEARCH DIRECTIONS

- Studies of adaptive roll of low-grade oxidative stress.
  At the moment the emphasis is on studies regarding protective manipulations against ischemia/reperfusion damage.
- Studies of high-grade OS-caused damages and diseases, neuroprotectivity and designing, synthesis and investigation of neuropeptides (incl. neuroprotective compounds).
  We are planned to continue: 1) the design and synthesis of novel peptidic/non-peptidic protector-molecules and study their effects *in vitro* (ROS scavenging ability, effects on different cellular signaling pathways in normal brain, in Alzheimer's disease brain, etc.) and *in vivo* (stroke model on rats, Parkinson disease model on rats, etc.); 2) proteomics – to study novel proteins or different expression of proteins/peptides in different knockout mice brain regions and postmortem Alzheimer/Parkinson disease brains using MALDI-TOF technique, sequence unknown peptides and proteins from brain tissue preparations using CAF (chemically assisted fragmentation) MALDI-TOF technique; 3) peptidomics – to study antioxidative and other properties of different peptides (GSH analogues, CCK and its analogues, peptides occurring after trypsination of different proteins etc.); the synthesis of novel PNA oligomers targeted to the different neuropeptide receptor mRNAs; the synthesis of cell penetrating PNA constructs and measurement of their antisense activities *in vitro* and *in vivo*; to study SNPs of different genes involved in neurodegenerative diseases using MALDI-TOF technique; 4) metabolomics – to study different expression of endogenic biomarkers in neurodegenerative disease patients using MS/MS technique. This all allows develop the OS-based model of neurodegeneration.

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IMMUNOLOGY

The Immunology Group focuses on characterization of antigenic target molecules and immunological reactions towards these targets in model autoimmune and microorganisms-induced inflammatory disorders. The general aim is to get new information about the antibody-mediated and cellular mechanisms of autoimmune disorders and to develop novel serological and molecular methods to characterize the immune responses in these disorders. One of the practical goals of the research group is to establish novel immunological diagnostic and therapy-monitoring tests usable in different clinical settings (close collaboration with different research groups and autoimmunity reference laboratory at the Tartu University Clinics).

RESEARCH DIRECTIONS

- Studies of autoantigenic targets in steroidogenic and nervous tissues
  The goal is to explore the molecular cloning and proteomics methods in the characterisation of autoantigenic molecules participating in the destruction process of steroidogenic and nervous tissues, to develop novel autoimmunity study methods based on the use of these autoantigenic molecules and their epitopes. Special attention is paid on the characterization of autoimmune targets in polyendocrinopathies.
- *HLA*, *CTLA-4*, *INS* polymorphisms in the development autoimmunity and diabetes.
  The goal is to study the role of polymorphisms of *HLA, CTLA-4* and *INS* genes and different enterovirus strains in the development of immune reactivity against pancreatic tissue and in the natural history of diabetes and related diseases.
- Autoimmune mechanisms in coeliac disease.
  In close cooperation with clinical departments autoimmune mechanisms of intestinal mucosa injury and other tissues are studied.
- Role of B and T cell immune reactions in the development of autoimmunity
  The goal is to specify characteristic cellular immunity y changes in different types of tissue specific autoimmunity (Down syndrome and *B. burgdorferi* infection are used as models).
- Role of *Helicobacter spp*. in the development of liver autoimmunity
  The aim is to characterize *Helicobacter hepatis* and other *Helicobacter* spp. related immune reactions in liver autoimmunity (primary biliary cirrhosis in particular) using our long-lasting competence on *H. pylori* and gastritis studies.

PUBLICATIONS

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HUMAN GENETICS

The main aim of our new current research is to get new knowledge on human neural stem cell biology, and the possibilities to use them for the therapy of neural diseases. The conditions of isolation, propagation, integration, and differenttiation of neural stem cells are investigated using morphological characteristics, the expression of cell surface antigens, transcription-, replication, -and reparation factor genes, extracellular matrix proteins, etc., karyotype, and biological activities. The objects of the study are neural stem cells, which are isolated from normal and genetically defective foetuses. Parallel the same characteristics are investigated in sphere forming brain tumour (glioblastomas) cells according to the hypothesis that at least part of brain tumours might be arisen from preexisting neural stem cells. Also the characteristics and factors influencing development of neuromuscular diseases and mental retardation are our traditional research fields.

RESEARCH DIRECTIONS

- Studies of human neural stem cells.
  At moment the emphasis is on studies of the expression of certain transcription-, replication-, reparation factors, and some RNA-binding proteins in neurospheres, and in the cells differentiated from them. The creation of 2D-electrophoretic database for human neural stem cells has been started.
- Studies of neurospheres generated from glioblastoma biopsies.
  The neurospheres have been generated from glioblastoma biopsies, and the study of differentiation of neurospheric cells is in progress. The cloning of neurosphere cells has been started, and several clones generated to study the nature of cellular heterogeneity of neurospheres, and other differentiation problems.
- Studies of disease related gene mutations and chromosome aberrations.
  We have identified several unique chromosome aberrations as causes of mental retardation, and infertility, and also some gene mutations and polymorphisms which are either the causes of certain eye diseases (gelatinous drop like corneal dystrophy) or the factors or modifiers of diseases susceptibility (cataract, glaucoma, diabetes).
- Studies of neuromuscular diseases.
  The study of different factors influencing regenerative possibilities of human muscle cells in different muscle diseases is in progress.

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CHILD NEUROLOGY

The aims of our study group are:

- to investigate the prevalence and incidence of several chronic and degenerative disorders (diseases) in children and adolescents;
- to determine possible pathogenetic and risk factors;
- to find possible preventive tools. Chronic and degenerative disorders in children and adolescents have great impact on the development of child and on quality of life.

The most vulnerable systems in this age group are the immune-, endocrine- and nervous system. Therefore we have aimed our studies particularly on these fields. At first we need to know the epidemiology of these diseases. This knowledge will help to plan medical care and further research on this topic.

RESEARCH DIRECTIONS

- To investigate specific immune-response and molecular mechanisms in common chronic diseases such as in asthma and juvenile idiopathic arthritis (JIA).
- To investigate the influence of the several external factors and molecular mechanisms in the development of autoimmune diseases, such as celiac disease, type I diabetes and JIA.
- To investigate the phenotype-genotype correlation in most common neuromuscular diseases (X-linked Muscular Dystrophies, Spinal Muscular Arophy), in Angelman and Prader-Willi syndromes, and cystic fibrosis. This knowledge may lead to new methods for treatment and management to increase the surveillance and to improve the quality of life (including gene therapy).
- We have started population-wide analysis of all patients with 21-hydroxylase deficiency (21-OHD) in Estonia.
- To investigate the mechanisms influencing the oxidative stress in term and preterm babies born with caesarean section, in asphyxia. We have aimed to find out preventive methods and early intervention tools.
- To investigate the epidemiology and risk factors of childhood stroke (included neonatal stroke), and cognitive development of children with stroke. To investigate the cognitive development of children with epilepsy .

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MICROBIOLOGY

The main research focus of our research is to test the interactions between pathogenic microorganisms, indigenous microflora and human physiological functions. The aim is to find out possibilities for influencing the pathogenesis of infections and some non-infectious chronic diseases by improving the human microbial ecology. The development of probiotics and suitable prebiotics for human healthy use has been ongoing.

RESEARCH DIRECTIONS

- Human microbial ecology and the possibilities for influencing it in pathogenesis of most spread chronic diseases in Estonia.
  The investigations of microbial ecology and possibilities to influence it are conducted in two directions: a) for chronic infectious diseases as *H. pylori* infections, recurrent UTI, chronic prostatits and tonsillitis, and b) for chronic non-infectious diseases as allergy and arteriosclerosis as a putative basis for degenerative diseases. The antimicrobial and antioxidative probiotics and suitable prebiotics are applied.
- Elaboration of methods for microbiological and molecular monitoring of drug-resistance in *Helicobacter pylori* and formation of genobank for *Helicobacter pylori* strains.
  Assessing the mechanisms of resistance to metronidazole and clarithromycin in *Helicobacter pylori* strains by microbiological and molecular methods. Developing molecular methods for detection of *H. pylori* in fecal samples, providing the mass-screening of population and modulation of antimicrobial and probiotic treatment of *H. pylori* infections.
- Antibiotic use and resistance of *S. pneumoniae* and *H. influenzae* in Estonia.
  Estimation of a link between antibiotic consumption and AB-resistance of respiratory pathogens in Estonian children.
- Hepatitis C – molecular-biological and hepatictis A – molecular-epidemiological investigation in Estonia.
  To determine the profile of antibodies against linear and conformational epitopes of viral structural and nonstructural proteins (C, E1, E2, p7, NS2, NS3, NS4A, NS4B, NS5A, NS5B) in chronic C hepatitis patient.s
- Estimation *in vivo* probiotic activity of the DNA-tagged lactobacilli to uro-pathogenic *Escherichia coli* in mouse models.
  The aim of the current project is to construct molecular tagging methods of lactobacilli with probiotic properties.
- Functional Assessment of Interactions between the Human Gut Microbiota and the Host (EU 5FWP Grant QLRT-2001-00135).
  The principal intention of the EU AND MICROFUNCTION project is to determine, through mechanisms of effect, the influence that probiotics, prebiotics and synbiotics can exert on gastrointestinal health.
- Lactobacilli probiotics as functional food.
  The aim of the project is to perform applied research for development of probiotic productions (biotherapeutic capsules, yoghurt, cheese) on the basis of the original *Lactobacillus fermentum* ME-3 strain of Tartu University. The patent application PCT /EE02/ 00006/28.06.2002 describes the claimed health promoting properties by lactobacilli strain with antimicrobial and antioxidative properties.

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NEUROPHARMACOLOGY

Our research interest is focused to the study of pharmacology of neurodegenerative and affective disorders. Neurodegenerative diseases are a heterogenous group of disorders that typically have adult onset, progressively debilitating and often fatal. Abnormal neuronal death is the major feature of these diseases. Neurodegeneration might be restricted to the distinct regions of the central nervous system or distinct neuronal populations, but in some cases they could affect simultaneously several regions of the central and peripheral nervous systems. Neurodegenerative component has been shown to be present also in several affective disorders. Our recent studies as well as many others suggest that abnormal activation of apoptosis might be a major contributing factor to the cellular loss in neurodegenerative diseases. On the basis of these studies pharmacological approaches aimed to prevent, retard or compensate abnormal neuronal death are extensively explored.

RESEARCH DIRECTIONS

- Neuroprotective therapies.
  We have studied the possibility to use the modulators of metabotropic glutamate receptor the ischemic damage mediated in part by glutamate and the mechanisms of dehydroepiandrosterone. In co-operation with other European scientists and in the framework of the EU grant we are studying how the mutations of certain genes lead to these diseases and how this could be prevented.
- Neurogenesis and its pharmacological regulation.
  Recent studies have also demonstrated that some specific regions of the adult brain contain stem cells that have the capacity to proliferate and differentiate into neurons. Another strategy to cure neurodegenerative diseases is, therefore, directed toward enhancement of the restorative capacity of the brain via activation of neurogenesis We are studying the possibility to enhance normal neurogenesis and thereby enhance the capacity of the brain to restore neuronal populations.
- Pharmacotherapy of mood disorders.
  Among several neurotransmitter systems involved in the pathophysiology of depression and being affected by antidepressants the serotoninergic system seems to be of great importance. Our research is focused on the elucidation of the role of selective serotonin receptor subtypes in the mechanisms of antidepressant action. This approach is aimed at the development of the most effective and selective drugs, which could be used in the pharmacotherapy of mood disorders.
- Mitochondrial component of neuronal death.
  Although it is generally assumed that most energy required in neurons is provided in the form of ATP by mitochondria, relatively little is known about the functioning and regulation of the intracellular energy transfer mechanisms responsible for delivery of that energy throughout the neuronal body. Here we would like to find answers for following questions: How the neuron adapts to increased local energy need? Could the energy transport in neurons be facilitated by energy transfer shuttles? Is the mitochondrial traffic and docking regulated by local energy deficit? In what extent the generation of new mitochondria is directed by energy deficit? Whether the abovementioned processes are impaired in certain neurodegenerative diseases?

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NEUROPHYSIOLOGY

The research interest of a group is focused to the study of molecular mechanisms of emotional and neurodegenerative disorders. Emotional disorders represent the most common psychiatric sufferings in the modern society. The development of modern neurobiology and molecular biology offers the unique possibilities to compete these disorders. The screening of new target genes linked to emotional disorders and the subsequent development of animal models will help us to develop more effective preventive strategies and new avenues for the treatment of emotional disorders. In the field of neurodegenerative disorders the research group established the collaboration with the Leuven Catholic University (Professor Veerle Baekelandt) to participate in the EU 5th Framework project "(N)EUROPARK". The general objective of the project is the development and testing of new therapeutic strategies for Parkinson's disease (PD), based on the understanding of the role of the PD associated genes α-synuclein and parkin in neurodegeneration.

RESEARCH DIRECTIONS

- Molecular mechanisms of emotional disorders.
  The studies are performed in the preclinical and clinical level. The aim of clinical studies is to establish the link between the single nucleotide polymorphisms of "classical" and neuropeptide neurotransmitters, and emotional disorders (anxiety and mood disorders). We established a strong association between the haplotypes of proopio-melanocortin and cholecystokinin1 receptor genes, and depressive disorders. In the preclinical studies we perform the experiments to reveal the gene expression profiles in the "emotional" brain of rodents due to the anxiogenic manipulations. We detected two new targets from these animal studies – wolframin and limbic system associated membrane protein (LSAMP). The next step is the development of mice lacking wolframin and LSAMP gene. Also we are planning the characterrization of the function of these two proteins.
- Molecular mechanisms of neurodegenerative disorders.
  In collaboration with the spin-off company Visgenyx Ltd. we develop the new animal models of PD. This approach is based on the knowledge that the defects of certain genes can cause the inherited forms of PD. The genes of interest are following: α-synuclein, parkin and DJ-1. Currently our research group is involved into the development of mice having α-synuclein gene point mutation. Also we prepare the genetic constructs to knock-out parkin and β-synuclein genes.

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NEUROLOGY

The main focus of our current research is to guarantee the validity basic research stemming from clinical data which requires high-quality standardized clinical characterization of individual patients. This would allow the creation of clinical data banks, registers and banks of biological samples, which will be used by our internal research team as well as by collaborating basic research groups.

The enhanced development of the molecular neuropathology is urged by the clinical need, as the adequate neuropathological diagnosis is the only way to diagnose exactly e.g. in case of brain tumors and neurodegenerative diseases. As a feedback to the clinitian it improves professsional skills and also helps to choose the right treatment options. Therefore, the work of the research group of molecular neuropathology is of higher priority.

RESEARCH DIRECTIONS

- Clinical epidemiology of neurological diseases. Quality of life.
  The research is focused on systematization and modelling of databases — Parkinson's disease, Alzheimer's disease, epilepsy, vascular diseases of the nervous system, myotonias, myasthenia, gliomas, spastic paraparesis. The research is focused also on fundamental and applied studies for clinical application of molecular mechanisms of neurodegeneration and neuroprotection for diagnosis and therapy. This includes new treatment strategies (cell therapy, brain stimulation etc) and specific diagnostics for early detection and therapeutic monitoring of neurodegenerative diseases. As a long-term project we are willing to start collecting CNS tissue samples from patients with clinically well-characterized neurodegenerative diseases (Alzheimer's disease, Parkinson's disease).
- Molecular neuropathology and mechanisms of glioma invasion.
  The focus of research is molecular neuropathology and mechanisms of glioma invasion. Cell-matrix interactions are of key importance for determining the invasive properties of tumor cells and clinical outcome. A bank of specimens of human gliomas is generated and characterized expression patterns of key matrix proteins and proteases/inhibitors regulating matrix metabolism.
  Currently, our aim is to set up intracranial glioma models in mice in order to test novel antitumor compounds (such as mutant anthrax toxins) in experimental therapy.
  A comprehensive expression mapping of tPA, neuroserpin and plasminogen in normal human CNS using tissue arrays and analysed the expression of plasminogen activators and several metalloproteinases in mouse model of multiple sclerosis, experimental autoimmune encephalomyelitis is performed. The results of the project are expected to be useful in practical morphological diagnostics of brain tumours, in prognostic evaluation of glioma patients and in developing new strategies for treatment of human gliomas. In addition, these studies should give additional insight into the role of extracellular proteases in the normal developing and adult central nervous system

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PSYCHIATRY

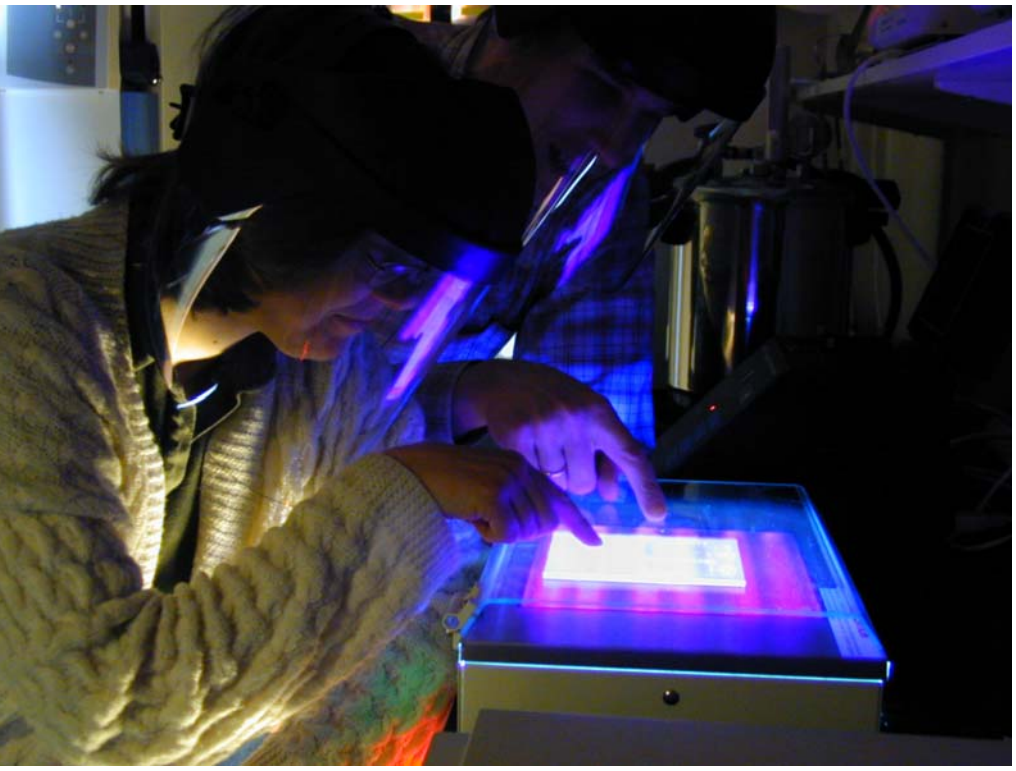
Research focus is epidemiology and pathological mechanisms of anxiety disorders, mood disorders and schizophrenia. The work of the research group of psychiatry is focused on the epidemiology as well as on the role of genetic variability in the manifestations of psychiatric disorders and psychobiological markers of morbidity and treatment response in mental disorders.

The following main directions of research in psychiatry are included:

- epidemiology and psychosocial factors of mental disorders;
- biological markers of schizophrenia, mood and anxiety disorders; relationship of genetic variability to psychiatric disorders and personality traits;
- pathogenesis and prevalence of sleep disorders.

RESEARCH DIRECTIONS

- Epidemiology and psychosocial factors of mental disorders.
  In the field of epidemiology we studied the prevalence and psychosocial background of depression in general population, insomnia, social phobia, and psychiatric disorders in children and adolescents. A self-rating Emotional State Questionnaire (EST-Q) was developed as a screening method for epidemiological studies and for detecting clinically important symptoms of depression and anxiety in primary care.
- Biological markers of schizophrenia, mood and anxiety disorders; relationship of genetic variability to psychiatric disorders and personality traits.
  In collaboration with a Canadian group we introduced cholecystokinin tetrapeptide (CCK-4) challenge as a model to study the neurobiology of panic attacks in humans. Also this experimental approach was used in study of functional influence of serotonin system on the panic. In collaboration with Kuopio University Hospital and the Department of Radiology of the Tartu University Clinics we have conducted the SPECT stu-dies of serotonin transporter in patients suffering from anxiety disorders. In collaboration with the Departments of Physiology and Biotechnology of the University of Tartu we have started with a large genotyping project to establish the relationship of genetic polymorphism to the expression of mood and anxiety disorders.
- Pathogenesis and prevalence of sleep disorders.
  In the topic of sleep research we started to use digital polysomnography that increased the possibilities for sleep research and was applied for the purposes of clinical diagnostics. The main research directions in this field were diagnosis and treatment of sleep apnea and sleep disorders related to psychiatry.



The Centre is frequensly organizing practical courses on molecular medicine.

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The centre has been established as the Centre of Ecology at the Faculty of Biology and Geography, University of Tartu. The Vegetation Remote Sensing and Boundary-Layer Energetics group from Tartu Observatory and the Sustainable Forestry group from the Estonian Agricultural University associate with the centre externally from the University of Tartu. The key research within the centre is to concentrate on two major themes — material cycling and species diversity. These two themes are tightly linked with mutual ties to bio-productivity, and because both utilise spatially organised data sets and analytical tools, their applications usually encompass important spatial dimensions. Local expertise in the fields of carbon and mineral cycling in ecosystems and bio-diversity is anecessity because Estonia has signed several relevant international agreements (e.g., Rio convention, Kyoto protocol) and sustainable development is keystone to the developmental strategy enforced by Estonian legislation. Fulfilment of these agreements and strategic goals is possible only with the assurance of local expertise and qualifications. The centre is supported by leading Estonian scientists in these fields. The mission of the centre is to develop applications that support sustainable development and nature conservation in Estonia. To achieve the primary strategic goals of Estonian R&D the most crucial development of the centre would entail an improvement in standards and in international scientific competitiveness, and an improved infrastructure for a modern scientific environment. Additionally, it is important to create a scientific community of suffi-

cient size and intellectual scope to train competitive PhD students and specialists effectively. During the last 5 years almost 30 students have completed their PhD studies at the groups of the centre.

Short-term research goals, based on current research within individual groups, include: investigation of the scale-dependence on the formation of animal and plant diversity, investigation of the carbon budget of natural and semi-natural plant communities, improvement of remote sensing methods to characterise plant communities, and the development of sustainable forestry technology in Estonia.

Applied research in the centre is based on ongoing research within the groups of the consortium. The most promising directions of the current applied research are:

- Investigation of key processes and most relevant factors determining the nutrient removal efficiency of constructed wetlands for wastewater treatment and riparian buffer zones. Creation of a GIS-supported model for placing and delineating the constructed wetlands in different landscape conditions.
- Providing technology for sustainable management of Estonian forests.
- Conservation of endangered plant and animal species and restoration of extinct populations.
- Elaboration of the optimal management regime for diverse semi-natural grasslands and methods of restoration of overgrown grassland communities.
- Development systems supporting spatial decisions for analysis of regional development and regional planning in Estonia for sustainable development.
- Elaboration of quantitative remote sensing methods to estimate vegetation parameters of ecological importance.

APPLIED ECOLOGY

General topic of the research is related to scaling leaf level photosynthetic properties to canopy level production. The research involves studies in photosynthesis acclimation within canopies, canopy growth, relationships between water and carbon exchange at the leaf and canopy levels. The main aim is to understand environmental and plant level limitations that constrain total photosynthetic productivity. The group is interested also in the impact of elevated CO_2 and ozone on photosynthesis and growth. Recently, a study on carbon storage pools in Estonian natural and semi-natural communities was launched.

We have constructed a photosynthesis scaling model for single canopy layer (O. Kull). This model allows to simulate the functioning of a canopy dependent on environmental conditions and plant growth-form. The underline experimental studies showed that during an acclimation of the leaf photosynthetic apparatus to light conditions, the proportion of the light harvesting part changes in relation to the rest of the photosynthetic apparatus, and also that the energetic cost of a leaf mass unit changes simultaneously. Plasticity of the photosynthetic apparatus (e.g. the possible range of acclimation) is in shade-tolerant species, characteristic for a stable developed community, wider than in light-demanding early-successional species.

Investigations on influence of plant hydraulic parameters on photosynthetic performance (A. Sellin, A. Sõber, K. Aasamaa) showed that leaf hydraulic conductance and stomatal conductance were higher in more vigorous trees and in branches growing under better light conditions. About half of leaf hydraulic resistance is regulated by light availability, leaf water status and abscisic acid content through rapid physio-

logical reactions whereas the stable part of leaf hydraulic resistance is correlated with anatomical parameters of both leaf apoplast and symplast, revealing that this part of hydraulic resistance is a consequence of long-term acclimation to prevailing environmental conditions.

In co-operation with Michigan Technological University and Finnish Forest Research Institute we have studied combined effects of elevated CO_2 and O_3 on aspen (in USA) and birch (in Finland) clones with different sensitivity to ozone (A. Sõber, O. Kull, I. Tulva, P. Mänd). Although elevated CO_2 caused partial stomatal closure, it did not lead to decreased sensitivity of trees to ozone. Under some circumstances, clones that were considered ozone tolerant, showed ozone sensitivity under elevated CO_2 environment. Both, effect of CO_2 and O_3 increased with the duration of fumigation. However, these effects strongly interacted with nutrient status and radiation environment of leaves.

We are involved in EC Framework projects VULCAN and EUROFACE where global climate change impact on European ecosystems are studied (O. Kull, P. Mänd, L. Hallik, I. Tulva, E. Eensalu).

The laboratory is equipped for basic sample manipulations (drying, weighing, cutting etc.) and for some simple chemical analyses (e.g. chlorophyll). More complicated chemical analyses are usually ordered from bigger specialised laboratories. A special laboratory is equipped for plant gas exchange and water relations studies. The equipment consists a self-designed gas-exchange system where leaf CO_2, H_2O, O_3, light and temperature environment are controlled and gas exchange can be measured with LI-COR 6262 analyser. This laboratory is also equipped with pressure-bomb system to study hydraulic conductivity and plant water status. We have two porometers (Delta-T, UK and LI-COR) to measure stomatal conductivity in field and SF-2000 sectrometer with integrating sphere (Ocean Optics, USA) to measure spectral properties of radiation and leaf reflectance. Portative chlorophyll fluorescence system PAM-2000 (Walz, Germany) and CO_2 porometer CIRAS-2 (PP-Systems, UK) are used for field and laboratory measurements. Hemispherical imaging system WinScan based on Nikon digital camera and software provided by Regent Instruments (Canada) is used for measurements of gap fraction and structure of leaf canopies. Set of PAR, temperature and humidity sensors as well as R:FR sensors (Sky Instruments, UK) in conjunction with Delta-T DL2 data-loggers is used for monitoring of microclimate within canopies. Currently, two canopy access towers are installed in Järvselja study area.

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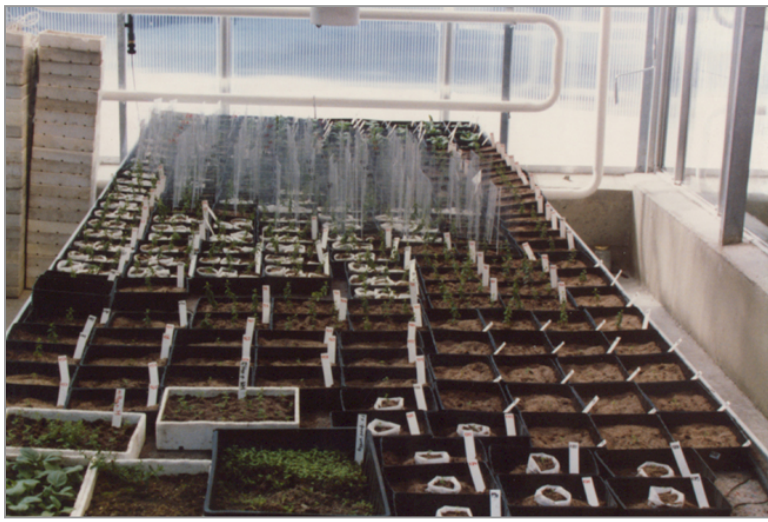
PLANT ECOLOGY

The research by the group of plant ecology has mainly been focussed on the study of the patterns of plant diversity and on the processes behind the patterns. There is a significant natural variation in plant diversity, e.g. diversity of arctic tundra and tropical rain forest differ several times. Variation of almost the same magnitude can also be observed even within a relatively small region. In Estonia, for example, plant diversity in calcareous forest communities exceeds several times plant diversity in dry boreal forests on acidic soils. In addition, biodiversity is influenced by various activities of the man. Continuing local and global extinction of species due to anthropogenic pressure was one reason why the so-called Rio convention about the protection of biodiversity was signed in 1992 on the level of governments.



In a minicosm experiment, it is possible to explain how do mycorrhizal fungi influence the outcome of resource competition between plants.

In the group of plant ecology, we have elaborated a general theory (so-called species pool theory), explaining the mechanisms behind diversity patterns. It is a synthetic theory, which takes into account processes on different scales (local biotic interactions, dispersal across landscapes, biogeographic history, evolution) and explains the actual level of biodiversity through the balance among different processes. The theory is novel in this respect that when explaining local patterns, it takes into account also the history of the particular ecosystem and dispersal of species in space and time.

Experimental research by the group has been directed towards explaining the particular role of different ecological processes behind the observed patterns of biodiversity. If one focusses on a particular plant community, one may ask why exactly those species coexist in given environmental conditions – is it a historical species assembly, that has developed during the thousands of years, or is it just a snapshot of a dynamic system, that is permanently changing due to species arrival and extinction? It was shown experimentally that actual biodiversity may be highly dispersal-limited. Dispersal, in turn, may be the function of both plant traits and the structure of the landscape around target community. The fate of any particular diaspore, however, is determined by the coincidence of several random factors like local weather conditions, biotic interactions and disturbances. Even more surprising was the result that almost 33% of the regeneration from seeds may rely not on the actual seed rain, but on the soil seed bank. These results deliver a clear message for biodiversity conservation – changes in environmental and management conditions are useless until the arrival of the diaspores has been guaranteed.

Another significant research topic of the group has been study of the role of microbial organisms in generating patterns of plant diversity. In particular, we have focussed on relatively poorly known but functionally important group of organisms – arbuscular mycorrhizal (AM) fungi. Those invisible organisms live in plant roots and support plants with mineral nutrients and water, while receiving carbohydrates from the plant. In the previous works, we managed to show that AM fungi influence the balance in plant-plant interactions and thus also the species composition of the whole plant community. Our recent activities are related to the study of the species composition of AM fungal communities in plant roots, since different fungal species may have a totally different effect – positive, neutral or negative – on the plant. AM fungal species in plant roots cannot be recognized on the basis of morphology and the only possible approach is to study the fungal DNA. Since the majority of AM fungal studies have been conducted either with cultivated plants, or in agricultural ecosystems, our focus has been on natural ecosystems, which are still much more common in Estonia than in the rest of Europe. We expect to discover interesting patterns when studying ecosystems under different human impact. Also, information about

the mutually beneficial or adverse relationships among AM fungal and plant species may be extremely important for restoration ecology – certain plant species may need specific fungal symbionts for establishment and growth.

The third direction of our studies has been the investigation toward understanding forces responsible for the structural variation of plant canopies. Quite surprisingly, majority of studies of canopy structure and leaf orientation have dealt with either agricultural plants or trees. Because of that, our studies on the forces determining structure of the herbaceous layer in multispecies grassland and forest communities have provided novel information. We have shown that the leaf orientation in a seminatural speciesrich grassland is a trait with high plasticity and depends on the whether conditions in any particular year. Also, we have shown that though the canopy structure in general can be described with the help of growth form spectra, since species-specific traits vary much more than previously assumed. Thus, one has to study species traits and their plasticity.

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ANIMAL ECOLOGY

At the moment the team involves six research scientists with a doctoral degree and 11 PhD students. Besides this, 18 master and bachelor students carry their research training at the group. The group runs entirely one and partly another target financing project from the Ministry of Education and Science, six grant projects from the Estonian Science Foundation and two applied research projects. In the last five years 4 PhD degrees were completed and more than 65 research papers were published in international journals with the peer review system, including such high-rated journals as Nature (1), Proceedings of the Royal Society of London (5), BioEssays (1). In 2001, the group received National Science Award from the government.

Recent research activity of animal ecology group involves field observations and experiments as well as laboratory studies with captive animals, and falls into the following areas of evolutionary animal ecology.

- Physiological and immunological ecology. In this field, spatio-temporal and individual variability of a large number of hemato-serological parameters in birds and their relationship with various components of fitness were studied for the first time in complex; primary experimental evidence for the existence of energetical cost of immune response in birds and insects was found, and trade-offs between immune response and certain life-history traits were demonstrated.
- Habitat selection and conservation biology. The effect of specific calcium limitation on various reproductive parameters of birds were for the first time experimentally demonstrated in naturally base-poor forest habitats; a series of original works were published on principles of habitat selection in some protected bird species, on possibilities for optimal combination of sustainable forestry and bird protection and on the state of biological diversity of some endangered taxonomical groups of animals in Estonia.
- Evolutionary ecology of insects. Major advances in this field have been made in studying direct and indirect effects of host-parasitoid interactions, effects of environmental factors on reproductive behaviour and population dynamics, and micro-evolutionary constraints on body size in insects.

Coccidian intestinal parasites have serious impact on health and sexual attractiveness of birds. To estimate infection intensity, MSc student Ulvi Karu analyses fecal samples from 52 greenfinches daily. These contain altogether about 16 000 000 oocysts of *Isospora lacazei*. Every day, Ulvi counts ca 20 000 parasites in the microscope.

Seminars of animal ecologists sometimes take place in a quite informal milieu – in the middle of nature. Their scientific value, however, does not suffer from this.

- Theory of sexual selection. Studies in this field have significantly advanced understanding of ultimate causes and mechanisms of attractiveness of carotenoid-based and other sexual traits in birds.

Within the Centre of Excellence, the group has the most productive co-operation with the groups of plant ecology and forestry (joint running of grant projects and applied research projects, joint PhD training) and the group of applied ecology (sharing scientific equipment).

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PHYSICAL GEOGRAPHY AND LANDSCAPE ECOLOGY

Main scope and objectives:

- analysis of changes of landscape pattern and material cycling with respect to significant changes of anthropogenic and natural driving forces in rural landscapes during last decades;
- creating a GIS-based simulation model and related scenarios based on information gathered during the fundamental research;
- quantitative assessment of the dynamics of climatic conditions and hydrological regime in Estonia regarding the global climate change;
- scenarios and decision support systems for implementation ecotechnological measures to control nutrient fluxes in sustainable catchment management;
- optimisation of design and management parameters of constructed wetlands for wastewater treatment and riparian buffer zones in terms of water quality and trace gas emissions.

The reserchers participate in target funded project of the Ministry of Education and Science, 4 Estonian Science Foundation grants and 5 EU 5 FP RTD projects. 8 PhD theses defended in 1998-2003 under supervision of team members.

Head of the group Prof Ülo Mander.

Results:

- empirical model of nutrient losses from catchments, based on land-use and soil structure, fertilization pattern and mean water discharge, that describes in smaller catchments about 95-99% of the variation of nitrogen losses and 69-93% of the variation of phosphorus losses;

- explanation of significant correlation between the changes in atmospheric circulation pattern and weather fluctuations in Estonia;
- optimisation of constructed wetlands for wastewater treatment for cold climate conditions; evaluation of the pattern of greenhouse gas (N_2O ja CH_4) emissions regarding the changing initial loading in constructed wetlands for wastewater treatment and riparian buffer zones; evaluation of the dynamics of nitrogen and phosphorus budget in treatment wetlands and riparian buffer zones.

Estonian Science Award in 2001 for series of scientific publications on "Changes in Agricultural Landscapes: Impact on Nutrient Cycling and Regulation by Ecotechnological Measures" in the field of agricultural research for the team of scientists: Prof Ü. Mander (team leader), senior researcher PhD Krista Lõhmus, senior researcher PhD Valdo Kuusemets, researcher PhD Hannes Palang and PhD student (that time) Ain Kull.

PUBLICATIONS

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GEOINFORMATICS AND CARTOGRAPHY

The group is based on Chair of Geoinformatics and Cartography of the University of Tartu (formed 10 years ago). Within the frames of ongoing scientific projects the following research is carried out:

- Wide analysis of the landscape parameters (with most applications in Estonia) based on different map layers, particularly on the database of square kilometer cells created by the group. The database is accumulatively filled with data useful for characterization of landscape values (plant cover, soil, fauna, water network, relief etc), meteorological parameters, tolerance and reaction of landscape to pollution, parameters of human settlement, land use etc., and

coming from different sources (maps, fieldwork, remote sensing). The database is open for use to other working groups.

- Outline, description and evaluation of valuable landscapes from cultural – historic, recreative, aesthetic and natural aspects according to the methods worked out by the group. Use of landscape resource is analysed in protected areas as well as conflicts between land reform and nature conservation as factors affecting living environment. Land use changes in Estonian cultural landscapes are modelled.
- Systems supporting spatial decisions are analysed as applicable for an analysis of regional development and regional planning of Estonia for sustainable development.
- Use of indicative parameters for spatial interpolation (for example probability of presence of plant and bird species depending on habitat parameters) is analysed. For evaluation of the precision and uncertainty of data analysis on smaller pixel size (ha or smaller if needed) are carried out. Possibilities for up- and downscaling of indicators are analysed.
- Physical-chemical parameters of subsurface and groundwater as affected by weather types and plant cover, and changes of plant cover pattern caused by changes in hydrological regime and nutrient runoff are analysed in detail. Based on the analysis, nutrient fluxes in catchment are modelled, combining dynamic modelling and GIS for predicting losses of nutrients under certain weather conditions, plant cover and land-use. The dynamic modelling is also used to analyse changes in nutrient fluxes as caused by climatic change and atmospheric pollution. Changes in landscape in general and changes of forest ecosystems in particular as caused by air pollution are modelled in detail.

The team has actively participated in development of the geoinformatic and mapping education in Estonia like developed theEstonia's School Atlas and the Estonian Geography Multimedia CD.

The members of the team are actively involved in graduate studies – over the last 5 years 2 PhD and 21 MSc projects have been completed, in near future 3-4 PhD students are expected to complete their thesis.

PUBLICATIONS

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GEOECOLOGY

The team of Geoecology at the Institute of Geology, University of Tartu focusses its research on the geological and geochemical processes of the surface rock/soil – water reactions, and on the geomorphological processes, determining and influencing the development of ecosystems.

Our primary aim is to assess the past and present soil-forming environments in interaction with the biosphere and atmosphere, which determines the elemental cycling, and retention and loss of nutrients in ecosystems. We model geoecological (geochemical, hydrogeological, palaeogeographic, etc.) processes of both, natural and anthropogenic factors of these processes, and provide a time-dimensioning of these processes in the past. Our research group has and will provide expertise into interdisciplinary research within the Centre on mineral weathering, hydrogeological-geochemical and landscape processes and will use the pertinent knowledge of other groups on the processes in biosphere, surface waters and soils.

At the moment the scientific team of the group involves 9 research scientist, 9 PhD students and 10 MSc students.

The group runs three laboratories: sedimentology-chemistry, X-ray diffractometry and ^{14}C-dating laboratory. All labs are renovated in 2003/2004. In 2003 a new Perkin-Elmer 2400 Series II CHNS/O Elemental Analyzer of the Centre was installed at the chemistry lab in

Institute of Geology. Also the group hosts sounding apparatus with acoustic and light signal for measurement of groundwater levels in boreholes, equipment for test-pumping and groundwater sampling, borehole fluid electric conductivity and temperature logging tools. In addition to this the group participates in a ICP-AES lab in co-operation with other research groups.

In last five years the researchers of the group have published 91 scientific research papers and within 6 PhD degrees were defended the same period. Current research funding of the group comes from Target Financing, Estonian Science Foundation grants and other research projects.

X-ray diffractometry laboratory at the Institute of Geology.

Geology – a young and promising group.

Our current research within the Centre of Excellence focusses on the interactions of the geological/geochemical and ecological processes. This work has initiated promising cooperation at the level of researchers and most importantly in graduate studies. Our running projects include:

- Landslide modelling and geohazard mapping in instable riverslopes of West-Estonian lowland.
- Hydrogeochemical studies of the potentially toxic elements in Estonian groundwater and their ecophysiological hazard and deleterious effect.
- Geotectonic land-uplift and sediment accumulation influence on reed-bed/meadow ecosystem development in West-Estonian wetlands
- Geochemical, mineralogical and hydrochemical studies and modelling of industrial wastewater interaction to characterise the pollution potential and long-term processes at solid waste disposal sites.
- Urban geology – interaction of geological-geotechnical and hydrogeological-geochemical processes in soft natural and anthropogenic soils in the cities.

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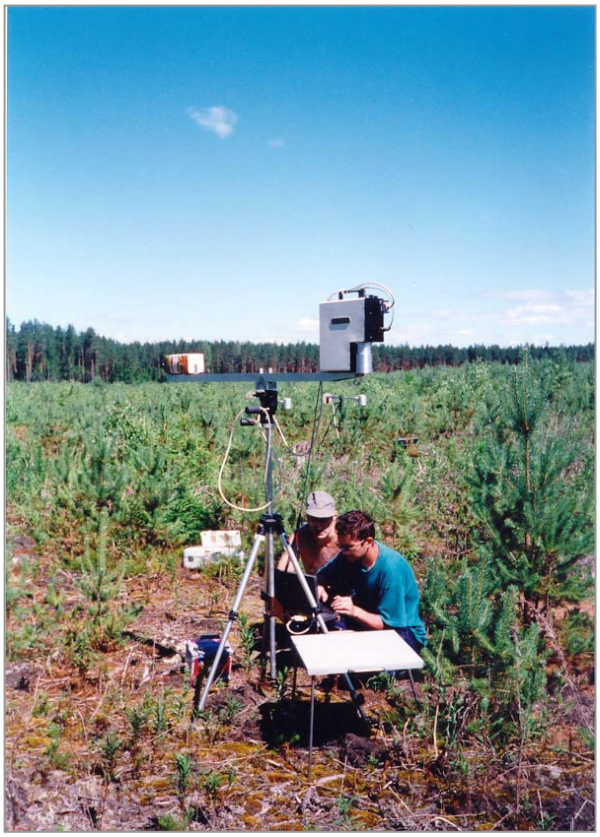
VEGETATION REMOTE SENSING

The main scientific problems are related to optical remote sensing methods and their application in vegetation studies: ecology, forestry, agriculture, landuse mapping and modelling of vegetation productivity. Remote sensing methods used by the group are suitable to analyse, upscale and integrate the knowledge obtained by the other groups of the Centre.

The research work by the group is much based on radiative transfer theory for vegetation founded by Prof. J. Ross whose book 'The Radiation Regime and Architecture of Plant Stands' (1981) has become a classical textbook in vegetation radiative transfer. Some analytical approximate formulas from the book are in use in the algorithms developed by NASA and other institutions in the USA to retrieve such products as vegetation leaf area index (LAI), absorbed photosynthetically active radiation (FPAR) from the measurements by multispectral and multiangular satellite systems MODIS and MISR. Based on the radiative transfer theory, different vegetation reflectance models have been developed by the group. Kuusk's homogeneous canopy reflectance model and forest reflectance models by Kuusk and Nilson (2000) are used by several European and US remote sensing teams to interpret remotely sensed data on vegetation. Kuusk (1998) was the first to apply the reflectance model inversion technology to retrieve vegetation parameters (LAI, leaf chlorophyll content, etc.) in a large area covered by a changes in land use (arable and abandoned Landsat TM image). Peterson and Püssa (2001) made quantitative analysis to estimate recent agricultural land, forests in Estonia from multitemporal Landsat TM images, since considerable changes have occurred in 1990-s after Estonia regained independence. Recently, several remote sensing application projects to monitor Estonian forest resources and forest cuttings were undertaken. The projects have been financed by Estonian Ministry of Environment.

Modern remote sensing technology provides different kinds of multispectral images, which are processed and interpreted by the group as results of physical measurements. In addition to the digital image analysis technology, the remote sensing team has to apply the atmospheric correction of the images. Ground-based spectrometric and radiometric field measurements as well as the structural measurements of vegetation also form an essential part of group's scientific activity (see the attached photo). To interpret the remotely sensed data, laboratory measurements of leaf optical properties and biochemical analyses are needed.



Field measurements by a GER-2600 spectrometer in a young stand at Konguta. Dr A. Kuusk and doctoral student M. Lang calibrating the spectrometer by a reference panel.

The team includes 5 scientists with a doctoral degree, 3 engineers, 3 doctoral students and several master students essentially support the research.

The remote sensing group has participated in several international projects, such as the Swedish remote sensing program RESE (Remote Sensing for the Environment) and VALERI (Validation of Biophysical Products from Large-Swath Sensors for Global Biosphere Monitoring). For the latter the forest region in Järvselja, Estonia serves as a test site.

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Kuusk, A., Nilson, T. A directional multispectral forest reflectance model. Rem. Sens. Environ. 72, 244-252 (2000).

Peterson, U., Püssa, K. Forest area and agricultural land use change in the Eastern Baltic region, IALE European Conference 2001, Development of European Landscapes, Conference Proceedings. Publicationes Instituti Geographici Universitatis Tartuensis. Tartu, 301-303 (2001).

SUSTAINABLE FORESTRY

The research group activities are focussed on the application of principles of sustainable and nature-friendly forestry. New applications in forest regeneration, silviculture, protection and utilisation are pursued. To provide ecologically based recommendations for forestry practice, sound research on productivity, nutrient cycling and biodiversity of forest ecosystems is needed, as well as adequate information on the dynamics of forest resources state, quality and increment. The fundamental research carried out by group is aimed at developing the yield and growth models, studying the forest ecosystem establishment on former fields and developing the survey methods for protected forests. Applied research is expected to provide recommendations for natural and artificial regeneration, close-to-nature cutting systems, management of protected forests and utilisation and valuation of Estonian forest resources.

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Kiviste, A., Alvarez Gonzalez, J. G., Rojo Alboreca, A., Ruiz Gonzalez A. D. Functiones de crecimiento de aplicacion en el ambito forestal. Kasvufunktsioonide rakendamine metsanduses. Institutio Nacional de Investigacion y Tecnologia Agraria y Alimentaria. Madrid, 190p. (2002).

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Kiviste, A., Nilson, A., Hordo, M., Merenäkk, M. Diameter distribution models and height-diameter equations for Estonian forests. Modelling Forest Systems, CABI Publishing, 169-180, (2003).

Nilson, A., Kiviste, A., Korjus, H., Mihkelson, S., Etverk,I., Oja, T. Impact of recent and future climate change on Estonian forestry and adaptation tools. Clim. Res. 12, 205-214 (1999).

Uri, V., Lõhmus, K., Tullus, H. Annual net nitrogen mineralization in a grey alder (*Alnus incana* (L.) Moench) plantation on abandoned agricultural land. Forest Ecol. Management 184, 1-3, 167-176 (2003).

Uri, V., Tullus, H., Lõhmus, K. Nutrient allocation, accumulation and above-ground biomass in grey alder and hybrid alder plantations. Silva Fennica 37, 3, 301-311 (2003).

THE CENTRE OF CULTURAL HISTORY AND FOLKLORISTICS IN ESTONIA

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THE STEERING COMMITTEE:
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Krista Aru (Estonian Literary Museum)
Cornelius Th. Hasselblatt (University of Groningen)
Pentti Leino (University of Helsinki)
Seppo Knuuttila (University of Joensuu)
Galit Hasan-Rokem (Hebrew University, Jerusalem)
Wolfgang Mieder (University of Vermont)
Vilmos Voigt (University of Budapest)

CCHFE was established in 2001. Its main task has been to evolve into a research centre capable of providing for the continuity and transmission of research done in the humanities, vitally important for the presence of national identity and the retention of social memory, for intellectual freedom and the all-embracing development of culture. The devices contemplated to meet this statutory goal are:

- Elaboration of strategies to preserve and use the communicative artefacts of the national cultural heritage.
- Activities in furtherance of the humanities-based information society, according to the needs of science and the society.
- More active than hitherto available, integration of top scientists of the countries bordering on Estonia (Latvia, Russia, Finland) into the research of points of contact and common elements of our cultural spaces (regarding both the periods and common features).
- Boosting of interdisciplinary scientific contacts and exchange, primarily between historians, sociologists, economists, and art critics.
- Promotion of spiritual culture, to give shape to scientific ethics and value criteria of the society.
- Development of a multilingual multimedia centre of the humanities.

The home institution of CCHFE is the Estonian Literary Museum, but its partnership programme involves scholars of stature in the humanities from the University of Tartu, from the Under and Tuglas Centre of Literature (UTCL) of the Estonian Academy of Sciences, from the Estonian Academy of Music, and from the Viljandi Cultural Academy. The centre includes about 40 individuals, half of them with a PhD and one-fourth students in a doctoral programme, mainly at the University of Tartu (ELM is not an educational institution and therefore does not provide graduate studies).

The work carried out is connected with 6 research themes with target-oriented financing by the Council of Scientific Competence, and with

15 grant projects of the Estonian Science Foundation. In the period of 2001–2004 CCHFE has been granted financial support by the state-financed programmes "Estonian language and national culture", "Estonian language and national memory", and "Scientific collections in the humanities and in the natural sciences".

Estonian Literary Museum is not only a research institution, but it has several national archives conglomerated round it. Research work is greatly enhanced by the fact that three fundamental archival units are situated under the same roof.

Those are:
THE ARCHIVE LIBRARY whose collections include more than 808 400 registered units (by Dec 31, 2003) – an archival library of great scholarly value, where most of the older printed matter ever published in Estonia and Livonia both in Estonian and German is represented;
ARCHIVES OF ESTONIAN CULTURAL HISTORY which include more than 300 000 archival units, among them collections of manuscripts, art, photos, tapes and films;
ESTONIAN FOLKLORE ARCHIVES, which include more than 5000 archival units of manuscripts, collections of photos, sound recordings and video recordings of nearly 20,000 archival units.

There are facilities for arranging conferences, working meetings, exhibits, and other academic or cultural events. To provide for the carrying out of research themes, experienced assistant personnel is made available. There are three net servers operating in the building (Haldjas, Ohto and Kirmus), the existing computer equipment is impressive and in good working order.

The research work carried out in ELM was evaluated, and credited with "excellent" by an international committee called by the Estonian Higher Education Accreditation Centre.

ELM is member of the International Council of Literary Museums (ICLM) bringing together literary museums of the world, and performs the tasks of a coordinator of research between literary museums in the 6-member council of the committee conjoining 358 members.

One of the leaders in Estonia of the UNESCO programme "Memory of the World" is the Archival Library of the Literary Museum. The folklorists of the Literary Museum are active participants in the international network of folkloristics: The Folklore Fellows, International Network of Folklorists and the International Society for Folk Narrative Research (ISFNR). Folklorists of ELM perform a leading role in the activities of the Baltic Institute of Folklore. The ethnomusicologists of ELM are members of the International Council of Traditional Music and in the European Seminar of Ethnomusicology. The scholars included in the centre of excellence of ELM participate also in the International Committee of Finno-Ugristics, in the International Organization of Folklore Festivals and Folk Art (CIOFF), in the European Folklore Institute, in the International Society of Semiotics, and in other international scholarly societies.

The most significant research results of the Estonian Literary Museum derive from the specific nature of this institution, as an association of archives and research units. The leading trends in the activities of ELM in the last decade, which also make for the activities of CCHFE and lay down its orientation, have been the following:

- Intensive activities in the field of digital media and data base: the publication of e-journals in folkloristics, and the digital publication of research works; the creation of database in folklore, folk music and literary history, the publication of e-anthologies of folklore, the ERNI project of literary history; data bases ELLEN, KLAABU, HERBA, etc.
- The publication of text critical editions of source material, fundamental for Estonian national culture: the correspondence of O. W. Masing, the dictionary of S. H. Vestring, the collected works of F. R. Faehlmann, etc.
- The continued publication of academic folklore editions in the series "Monumenta Estoniae Antiquae": proverbs and riddles, runic songs (*regilaul*), legends.
- Active research carried out in the folklore, traditional music, folk beliefs and ethnology of Estonians and other peoples.
- The restoration of the European context of Estonian culture: the assembling of the archives of Exile Estonians at the Archives of Cultural History, the publication of correspondence of special value (e.g. I. Ivask – A. Oras) and other non-fictional source material (diary of K. Ristikivi) in commentated editions.
- The research of history of literary institutions and groups, by applying the "dense" descrip-tion methods.
- Collection, research and publication of non-fictional memorised heritage of the people.

The most urgent tasks to be tackled by CCHFE from 2004 have been:

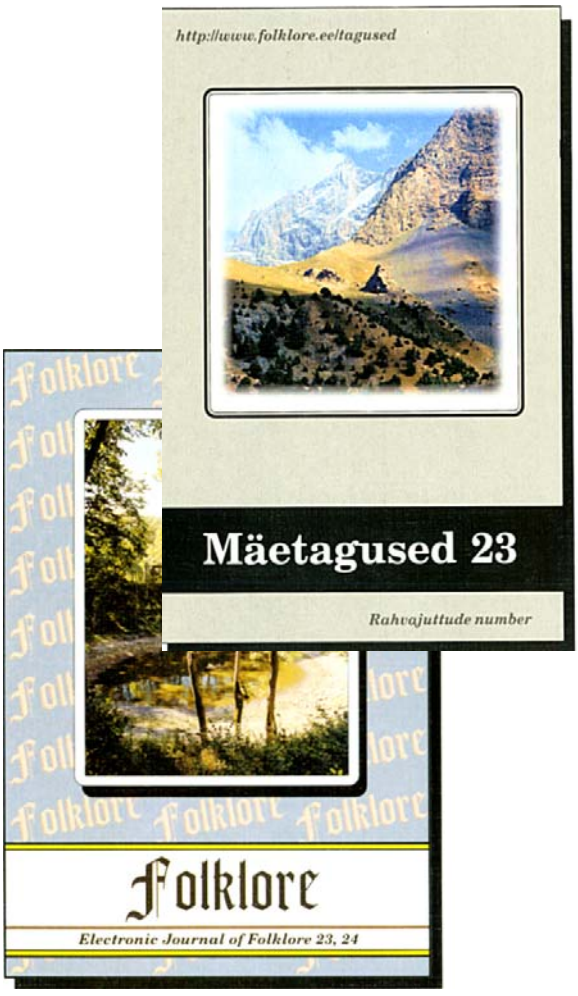
- The widening and consolidation of international cooperation, mainly: the compiling

and editing of the bibliography "Internationale Volkskundliche Bibliographie – International Folklore Bibliography – Bibliographie Internationale d'Ethnologie" (SIEF) that has been the responsibility of the Literary Museum since 2002 (editor-in-chief K.-M. Rooleid); the creation of a cooperation network of researchers of the cultural ideology and functional mechanisms of the Soviet period (partner institutions: A. Ahmatova Research Centre in St Petersburg, Lev Tolstoi Memorial Complex in Yasnaya Polyana, H. Heine Institut in Düsseldorf, Balzac Research Centre in Paris, etc.); the arrangement of the international Siberia-focused conference of anthropology "Generation P" on Oct 8–10, 2004 (partner: Max Planck Institute of Social Anthropology); development of the project "Music, National Identity, Ethnicity and Cultural Diversity in Europe" (partner: Tampere University) together with Lithuanian Academy of Music and Latvian Academy of Music; the final stage of the Balto-Finnic proverb project "Proverbia septentrionalia" in cooperation of the Finnish Literature Society and Joensuu University.

- Further efforts to digitalize cultural heritage and join the respective international projects: mainly, to create an environment that would make the collections of cultural heritage in the humanities available to the international research community, in accordance with the principles drawn in the eEurope 2002 Action Plan (2002) of the European Union; to provide necessary technical equipment for the digitalisation, collection, preservation, and utilization of archival collections; participation in the development of standards and norms for the presentation of digital information, in its contextual research and application of the meta data system. Furthermore, it is necessary to make sure that the accents and the availability level of the background investigation should correspond to the needs and requirements of the Estonian educational system. It is absolutely necessary that the cooperation mega project with the Finnish Literature Society to digitalize the runic songs and *regilaul* will continue in the future.

The work groups and partner members of CCHFE have been leading members in various scholarly events organized in Estonia during the period of 2001–2004, notably:

- an international conference to honour Oskar Loorits "Popular Religion and Folklore at the Turn of Millennium: Contemporary Research Methods" on 9–12 November, 2000 in Tartu;
- an international symposium "Sturm und Drang in Livonia. Patterns of riot – Der Sturm und Drang in Livland: Rebellionsmuster im Leben und in der Dichtung. J. M. R. Lenz 250 – K. J. Peterson 200" on 7–9 September, 2001in Tartu;
- "Sacred and Profane in the Dialogue of Cultures: Ritual and Generic Aspects" on 18–19 April, 2002 in Tartu;
- Pan-European conference "Cultural Context from the Archaeoastronomical Data and the Echoes of Cosmic Catastrophic Events" on 27–30 August, 2002 in Tartu, Viluste and Tõ-ravere;
- "Eros and Language: The Rhetorical Patterns of Translatability and Understanding" on 31 May till 2 June, 2002 in Käsmu;
- an international seminar "Popular Religion in Multiethnic and Multiconfessional Environment" on 6–7 December, 2002 in Tartu;
- the second international symposium of Baltic German literary culture "Hier ist woanders: Das baltische Welterlebnis der Keyserlings" on 18–21 September 2003 in Tallinn and Tartu.



The role in arranging international scholarly events has been remarkably active on part of the ELM Folklore Department and J. and R. Undusk from a partner institution (UTCL).

Since 1996 two peer reviewed e-journals in folkloristics have been published: "Folklore: Electronic Journal of Folklore" (http://www.folklore.ee/folklore) in English and "Mäeta gused" (http://wwww.folklore.ee/tagused) in Estonian. Articles in these journals are a contribution by international authors, the organizational and financial coverage and editorial work is provided mainly by the Folklore Department of ELM.

In addition to the activities on the level of working groups, an attempt of humanitarian integration centred around one wider research team is also planned. The theme selected is the relationship of culture with society, power and state, particularly the functioning of culture under the conditions of a totalitarian regime. There have been several conferences and seminars focusing on these topics, the main results since 2003 have been published in a series of so-called red annuals: "Power and Culture" (2003), "Internet Humour about Stalin" (2004), "Confor-ming Texts" (forthcoming in 2005).

THE CONTEXT OF CULTURAL HISTORY IN THE SOVIET ERA

This research group includes the theme leaders and researchers of the Archives of Estonian Cultural History whose research area covers the period. Included are also some researchers from the Estonian Archives of Folklore and external members from the Department of Estonian Literature of the University of Tartu.

In the study of the recent Estonian cultural history, namely that of the Soviet period, it would be rewarding to apply the complex approach of the new historicist method. There are favourable conditions for such research at the archives of the Estonian Literary Museum, because they include, in addition to personal collections on writers and cultural figures, also material of various institutions (the archive of the Writers' Union of Soviet Estonia and its Tartu Department, the archive of the journal *Looming*, the archive of the publisher *Eesti Raamat*, the literary archive of the daily *Edasi*, a.o.), a collection of life stories of Estonians, and the collection of oral tradition at the Estonian Folklore Archives.

RESEARCH OBJECTIVES

- To provide a "dense" description of processses and means by which the Soviet regime was internalized in the society, and how "the Soviet culture" was developed.
- To study the evolution of the Soviet ideological stereotypes in Estonia, and their persis-tence in the second half of the twentieth century.
- To investigate the emergence of possible resistance in Estonian folklore and exile literature to the paradigms established by the Soviet administration.

RESEARCH PROCESS

- In order to integrate separate investigations by historians, historians of culture, scholars of literature and art into various periods and aspects of the Soviet era, we have chosen the word "adaptation" as keyword, when raising the questions: How did artistic creators, how did government officials and other executive officers, how did people in general adapt to the social life that had changed ab-

ruptly? What were the possible adaptation strategies? What kind of concessions did the administration grant in various periods, what kind of concessions did the cultural intellectuals make? How was the nature of the new political power reflected in the works created in different periods? In order to find answers to these questions, a series of intra-institutional conferences was arranged in 2001–2002 "Signs of adaptation" (publication under the same title 2002), and "Adapting texts" in 2003–2004 (publication forthcoming). The same topics were discussed also at the annual conference of Kreutzwald Days, and at the seminars focusing on authors of the period (J. Kaplinski, P.-E. Rummo, E. Mihkelson).

- Additional material has been separately collected into the archives, while the most outstanding texts have been published (e.g. Karl Ristikivi's correspondence of 1938–1971; correspondence by Bernard Kangro and Gustav Suits 1944–1955; *Kirjad üle mere* by Mart Lepik).
- A new publication series was started in literature and cultural history *EKLA töid kirjandusest ja kultuuriloost*, where so far two books have been published (2002 and 2004).

MAIN AREAS AND TOPICS OF RESEARCH

- The comparative study of the reception of historical authors of stature (Kreutzwald, Faehlmann, and others) and their works (*Kalevipoeg*, a.o.) through literary history, but particularly their treatment in the Soviet period. Different strategies in the "adaptation" of Estonian literary classics: what were the cases of outright distortion, suppressing the truth and withholding of facts, what were the ideological underpinnings in various periods, etc. In connection with the celebration of Kreutzwald Year (2003) the history of Kreutzwald-research was re-evaluated, as well as distortions in the 20th century in the reception of the fundamental texts of the 19th century.
- History of the institutions of cultural history in Soviet Estonia: the Sovietization of the Estonian Writers' Union, the after effects of the Eighth Plenum of the Estonian Communist Party for the Estonian writers, history of the Estonian Literary Museum in the second half of the 20th century, purges and other restructurings in the Estonian Artists' Union and other organizations.
- Intellectual exchange of Soviet Estonian authors with exile Estonians: its nature in various periods; the analysis of interaction practice as it is reflected in non-fictional material (diaries, correspondence); the activities of Soviet Estonian administrators to hold in check and control that interaction; foreign relations of Estonian intellectuals, particularly interaction with the Finns.
- The aspects of gender studies, particularly the specific problems of creative women (e.g. innovative discussions of women writers in Soviet Estonia are written by E. Annuk as part of her doctoral dissertation).
- Further collection of Estonian life stories: a competition titled "The life of myself and my closest relations in Soviet Estonia and in the Republic of Estonia" was arranged in 2001, together with the society "Eesti Elulood"; in

M. Lauristin, R. Hinrikus and T. Anepaio on the Day of life-stories 19.03.2004.

2004 ended another competition "Life during the German occupation". The publication and research of that material is continued.

- Estonian folk tradition about the Soviet period, the so-called "oral history" in its various forms: research by M. Hiiemäe into the celebration of folk calendar festivities during the Soviet period, e.g. the celebration of Christmas.

INTERNATIONAL CONTACTS

Activities of Estonian intellectuals during the years when the Molotov-Ribbentrop Pact was in force have been studied together with German colleagues (conference in Flensburg in 2002, a publication is forthcoming). Researchers have attended several international conferences of semioticians, incl. Imatra Summer School. Seminars to introduce Estonian literature have been arranged in Finland together with the Finnish Literature Society and/or University of Turku (2000, 2003), and a seminar on women writers in Tartu (2002). Together with the University of Tartu, an international seminar to discuss women's life stories was arranged in Literature Museum (2002), which resulted in a publication "She Who Remembers Survives" (2004). In cooperation with the Department of Estonian Studies at the University of Toronto researchers have studied life stories and non-fictional texts of recent history. The next AABS (Association for the Advancement of Baltic Studies) confe-rence will take place in Toronto in June 2004, researchers of this work group being active in its organization.

PUBLICATIONS

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Hinrikus, R. (koost.) Eesti elulood III, Elu Eesti NSVs, EKM ja Tänapäev, Tallinn (2003).

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Olesk, S. Tõdede vankuval müüril: Artikleid ajast ja luulest. EKLA töid kirjandusest ja kultuuriloost 1. EKM, Tartu (2002.)

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Hinrikus, R. Deportation, Siberia, Suffering, Love. Kirss, T., Kõressaar, E., Lauristin, M. (Eds.) She who Remembers Survives: Interpreting Estonian Women's Post-Soviet Life Stories. Tartu: Tartu University Press, 62–77 (2004).

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Olesk, S. "Eestin Runottaren" aika. Ajan taju: Kirjoituksia kansanperinteestä ja kirjallisuudesta. Helsinki: SKS, 194–204 (2001).

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Sarapik, V. _topias and Islands. Sarapik, V., Tüür, K. (Eds.) Koht ja paik. Place and Location. Studies in Environmental Aesthetics and Se-miotics III. Tallinn, 107–128 (2003).

Veidemann, R. The formation of the Estonian nation from the semiotic aspect. Interlitteraria 5, Tartu, 87–101 (2000).

Veidemann, R. Hajoaako kirjallisuuden käsite? – Viron kirjallisuus vuosituhannen vaihteessa: Postmodernia ja modernia. SKS, Helsinki, 23-33 (2003).

RESEARCH GROUP IN MYTHOLOGY AND FOLK NARRATIVE

This research group consists mainly of scholars of the Department of Folkloristics of the Estonian Literary Museum, but it also includes folklorists, philosophers, and theologians from the University of Tartu, the Tallinn Pedagogical University and the Viljandi Culture Academy. The group aims to study topical issues in mythology and narratives, including the treatment of legends and tradition spread in virtual reality, their functions, behaviour, and dissemination strategies. The research work focuses on the changes and processes that have taken place in the Soviet and Post-Soviet period, focusing on the observation of key figures and their relation with earlier fixed stereotypes and models. Estonia's accession into the European Union has

introduced new topics of study – namely, the spread of global trans-national phenomena and their adaptation in lo-cal culture area, as well as manifestation of ethnic Estonian identity.

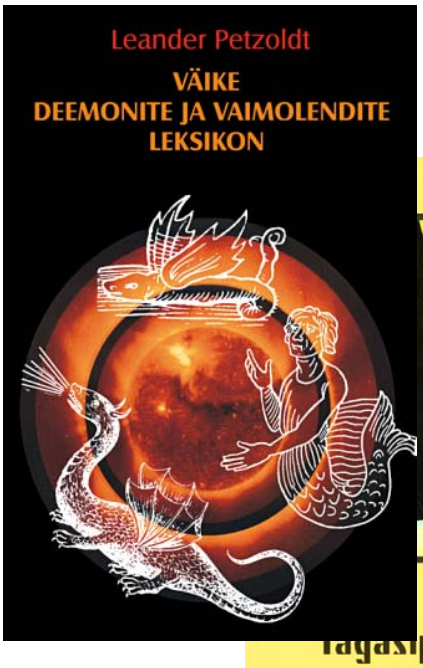
In addition to the publishing of electronic journals *Mäetagused* and *Folklore. Electronic Journal of Folklore* (see further in the preamble), the research group publishes the publication series *Sator. Artikleid usundi- ja kombeloost* and the bilingual publication series *Tänapäeva folklorist/ Contemporary Folklore*.

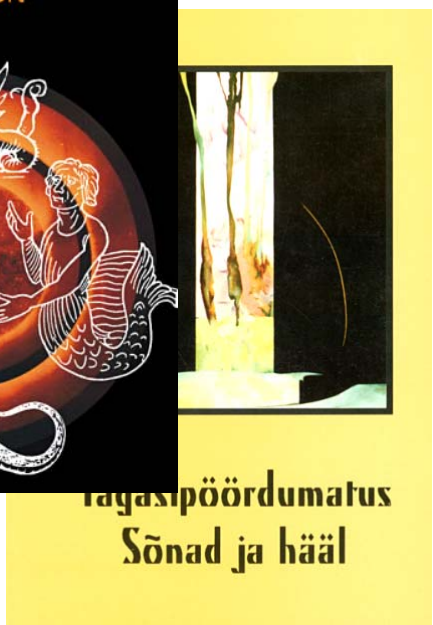
RESEARCH PROCESS

Investigation into modern research materials takes place through multiple-choice and open interviews with random or fixed samples. Week-ly seminars on mythology and narratology theo-ry are held regularly, translations of the works are available on the Internet (http:// www.folklore.ee/seminar). Traditional seminars on mythology are held each spring. Interdiscip-linary panel discussions and conferences are also organised. In addition to the international academic events, mentioned in the preamble, the group has organised several folkloric and interdisciplinary conferences, seminars, round-table discussions in Estonia, including applied e-conferences and tutorials (e.g. *Dialoog privaat-se ja avaliku elu vahel* 2002).

MAIN AREAS AND TOPICS OF RESEARCH

- The analysis of historical and modern outputs and constituents of legends. The observation of the legend genre in narratives, the continuance of the characteristic patterns of a living legend in modern culture and oral narrative history. The characteristic feature of a contemporary myth is the consistence and manifestation of narrative aspects in movies, cartoons, detective novels and other forms of mass culture. In addition, the consistence of the cognitive and explicatory aspect of legends associated with personal identity and national ideology, as well as the reflection of a legend as an aberration in pseudomythology, are also analysed. One of the new research trends is to observe how legends relate to stereotypes and basic emo-tions, like fear and shame. Studies into historical legends focus on comparative mythology, including the situational analysis characteristics of ethno-cosmology and the Balto-Finnic mythological creatures.
- The ritual institutions of tradition in multicultural environment. This study aims to explicate how ritual institutions are formed and modified, and their ideas are transcommunicated in the society influenced by multicultural media. The focus is on shamanic rituals and lore, groupings surrounding psychics and prophets and their activities, family rituals and religious rites. The topics also include ritual ceremonies associated with agriculture, herding, hunting and fishing, social and proprietary relations and strategies, especially among the small ethnic groups in Europe and Siberia; if possible, also the observation and interpretation of revived national movements are studied.
- Studies in narratology. The focus is on analysing the rapidly developing narratology studies in the world, investigating the regularities of traditional legend lore and personal experience stories (including spontaneous narration, the poetic and structural relations of narratives, the manifestation of oral history in narratives, fiction *versus* true life stories, narratives of borderline and risk groups). The topics include the proportions of mythological and historical motifs and contextual incidents in narratives and the role of the narrator in the formation of a story.
- Virtual communities and the level of heritage. One of the main topics studied is the affirmation strategies of small nations and their manifestations in modern media (manifestations of regional and family culture). The analysis of cyber lore (passwords, virtual cards, legends) and cyber philosophy





spread in the multi-media environment and the influence of traditional folklore on these phenomena. A more detailed analysis is made on three Estonian virtual communities with specific modes of expression, the ratio of real and virtual communication, folklore and language use. The formation of web groups and joint organised activities (e.g. Geocaching in Estonia) are also discussed.

INTERNATIONAL CONTACTS

This research group cooperates with international bibliographic publications *Internationale Volkskundliche Bibliographie = International Folklore Bibliography = Bibliographie Internationale d'Ethnologie* and *Demos*.

The group is involved in the following international projects: "Mythologia Uralica" (joint project for compiling glossaries in mythology: cooperation with Russia, Finland, Hungary); Joint Estonian-Finnish project "Epics Around the Baltic Sea"; Joint Estonian-Icelandic-German project "Sagas and Societies"; Joint project between the Nordic countries and Estonia "Masks and Mummers in the Nordic Countries" (2001–2003); Project with the University of Ulster and the University of Dublin "Mumming in Cross-Border and Cross-Community Contexts" (2002-2003).

The group has research contacts with the Max Planck Institute of Social Anthropology (Halle, Germany) in Siberian studies. Cooperation partners are also the Folklore and Ethnology institutions of Slovakian and Slovenian Academy of Sciences, research centres and organisations of Finno-Ugric studies.

The group also participates in the Folklore Fellows Network, the International Society for Folk Narrative Research (ISFNR), and Societé Internationale d'Ethnologie et de Folklore (SIEF). The Department of Folkloristics of the Estonian Literary Museum has a major role in organising the 14th World Conference of ISFNR (which will be held in 2005) in Tartu.

PUBLICATIONS

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Ventsel, A., Stammler, F. Between Neo-Liberalism and Dirigisme: Approaches to Reindeer Herding in Yamal and Sakha. Hann, C., and the "Property Relations" Group (Eds.) The Post-socialist Agrarian Question. Property Relations and the Rural Condition. I. Halle Studies in the Anthropology of Eurasia. LIT Verlag, Münster, 321–363 (2003).

RESEARCH GROUP IN THE THEORY OF RHETORIC AND PHRASEOLOGY

The majority of the group's membership consists of folklorists and phraseologists of Estonian Literary Museum. Besides, some scholars from UTCL working on rhetorical topics (J. and R. Undusk, et al.) are engaged as foreign members. In 2003 the group launched a new series *Reetor*, which will publish works on the minor forms of folklore, phraseology, theory of rhetoric and figurative speech, as well as folk humour and theory of humour.

MAIN RESEARCH OBJECTIVES

- The continued publishing of academic collections of the minor genres of Estonian folklore in the series *Monumenta Estoniae Antiquae*. In addition to five-volume *Estonian proverbs* (1980–1988), two volumes of *Es-*

tonian riddles, an analogous edition, were issued in 2001–2002. The third volume which includes scholarly overviews of the history of collecting and publishing Estonian riddles, their content and form, figurative and functional aspects, geographic distribution, equivalents of Estonian riddles in the tradition of the neighbouring Finnic, Baltic, Slavic, and Germanic languages as well as some other appendices will be published in 2005. The edition is based on a complete data bank that contains, in a typological arrangement, all hitherto recorded authentic texts of Estonian riddles, together with supplementary data (solution, time and place of recording, collectors, source abbreviations, cross-references between typologically compound forms, *etc*), and statistics. A paper version of *Estonian riddles* I–II was produced from this database via a computer program written particularly for this purpose. Next, an academic edition of Estonian proverbial phrases a. o. fixed expressions (idioms, similes, etc.) is planned to be compiled and published (see also the next section).

- Studying minor genres of folklore. In recent years the team led by Asta Õim has created an extensive database of Estonian proverbial phrases and phraseologisms, and the appurtenant user interface; software devices for processing the manuscript of corresponding academic edition will also be provided in the future (cf. the previous section). The mentioned data base allows to speed up and enhance substantially the research in phraseology, the principal current topics of which include the structure and figurative semantics of folk similes; categories and subcategories of proverbial phrases a. o. fixed expressions; occurrence and internal structure of particular thematic fields and conceptual clusters in phraseology; problems of developing specific software for serving phraseological corpora and databases.
- In Estonian paremiology the recent focal topics have been: relationships of different structural levels (syntactic – modal – figurative) and metaphor-theoretical aspects of proverbs, especially those emerging in animal metaphors. Two extensive monographic studies are currently in progress – one on typology and images of animal proverbs, the other on the history of collecting and publishing Estonian riddles.
- Theory of rhetoric and figurative language. This work is divided into two branches. One of them is to analyse the logical and ideological constructions and historical change of grand domains in language usages, the so-called discourses, practiced by our UTCL foreign members J. Undusk, E. Annus, *etc*. One of the aims of this work is to test the applicability of concepts entrenched in classical rhetoric or introduced by new rhetoric (like synecdoche, topos, oxymoron, enjambement, *etc*.) in contemporary research in culture typology and intertextual analysis. Literature, theatre, historiography, religious and philosophical texts, mainly descending from the Estonian and Baltic German cultural space of the 18th–20th centuries, but also on a temporally larger European scale – the broad variety of source materials have been and are being used as polygons of observation for these purposes. Another branch embraces the analysis and criticism of theories of figurative speech developed in modern (first of all, cognitive) linguistics and psychology, and evaluating their degree of applicability for explaining the imagery of proverbs, idioms, *etc*. A. Krikmann has done some research on these matters and held classes at the University of Tartu. Efforts will be made to integrate the cognitive and culture-theoretical viewpoints on figurative language and rhetoric, and make the existing results more comparable.

- Contemporary folk humour and theory of humour. As principal sources of study, both Estonian archive texts belonging to the older layer of folk jokes, as well as modern multilingual joke material obtained from the Internet are being used. L. Laineste has created a database of Estonian web jokes (*ca* 40,000 texts, plus supplementary data). Topics of active research include ethnic jokes in Estonia and on the international scale; poli-tical humour in the previous USSR (and the socialist camp in general) aimed at Stalin and other targets; contemporary trends of humour research and developments of humour theories (particularly the incongruence theory); the typology of classical ("Aarne-Thompson") jokes; structural differences and relationships between the older non-punchlined and newer punchlined jokes.

INTERNATIONAL CONTACTS

Jointly with the Finnish Literature Society and University of Joensuu, the follow-up volumes of the edition of shared proverbs of Finnic peoples have been prepared (the first volume, *Proverbia septentrionalia*, the output of a grand Finnish–Estonian project of 1960s–1980s, was published already in 1985, FFC no. 236). Members of the research group have participated in international conferences on paremiology held by the Institute of Lithuanian Literature and Folklore (2001 and 2004) and in annual conferences of the International Society for Humour Studies (2002 in Italy and 2004 in France). A. Krikmann is the editorial consultant of P*roverbium: Year-book of International Proverb Scholarship* pub-licshed annually by the University of Vermont (editor in chief Wolfgang Mieder); he also has lectured on various linguistic and folkloristic topics at the universities of Joensuu and Turku. J. Undusk (UTCL) has especially good connections with many European scholarly institutions (Institute of Literary Studies of the Hungarian Academy of Sciences, Stockholm University, The Herder Institute in Marburg, J. W. Goethe-University in Frankfurt am Main, etc); he has also been a recipient of many foreign grants and awards.

PUBLICATIONS

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RESEARCH GROUP IN POETICAL AND MUSICAL FOLKLORE

This study group consists of researchers of the Estonian Literary Museum and members of teaching staff of the University of Tartu and the Estonian Music Academy in Tallinn. They have obtained their PhD degrees in different disciplines, such as musicology, psychology, linguistics, and cultural anthropology.

This kind of interdisciplinary background makes it possible to apply multiple methods to the study of poetical and musical folklore, e.g. those from sociology, cognitive science, acoustics, and linguistics, as well as to integrate research of music, verbal texts, and context in which the two occur.

RESEARCH PROCESS

AUDIOVISUAL MATERIAL IS RECORDED DURING FIELDWORK AND THEREAFTER ARCHIVED

↓

QUALITY OF THE RECORDED MATERIAL IS PROCESSED
BY A SOUND ENGINEER, IF NECESSARY

↓

THE MATERIAL IS MADE ACCESSIBLE FOR RESEARCH

↓

THE MATERIAL IS ANALYZED, PROVIDED WITH COMMENTARIES AND PREPARED FOR FURTHER PUBLISHING BY RESEARCHERS

↓

RESULTS:
PUBLICATIONS, CONFERENCE PAPERS
AND UNIVERSITY COURSES

↓ ↓

ADDRESSEE *A*: (scholarly community)
ADDRESSEE *B*: (general public)

→ students ←

Ethnomusicological research requires sophisticated hard- and software in its every stage. Fieldwork is carried out generally using digital recording techniques. Estonian Folklore Archives continue to use the SAWPro software. Digitisation and restoration of earlier recordings, including those on wax cylinders from the early 20th century, are currently in progress using the Cool Edit and Virtos Denoiser software.

ADDRESSEES OF RESEARCH WORK

A part of research results is directed to the scholarly community working in the field of ethnomusicology. Another and a more extensive part of results which is related to the culture in a broader sense, is intended for the general public. Students represent a sort of interface between the two groups. Members of this study group deliver courses in various Estonian universities: the University of Tartu, the Estonian Academy of Music, the Viljandi Culture Academy as well as in the Heino Eller Tartu High School of Music and abroad.

MAIN RESEARCH PROBLEMS

✔ What is the role of traditional music in the preservation of national identity?
Can possible shifts of identity be detected in traditional music, which might be explained by the globalisation of the contemporary world?

✔ How are changes in musical tradition perceived and defined by active carriers of traditional music as well as by its consumers?

RESEARCH RESULTS AND OUTPUT

- A publication series called *Töid etnomusikoloogia alalt* (Working Papers in Ethnomusicology) was started in 2002. This series is expected to become the main output of the study group, directed to both addressees: scholars and the general public of Estonia. The first three issues deal with the functions of traditional music and with changes in its perception in contemporary society. Similar problems have been dealt with by the study group members in their other publications. Those scholarly publications are accompanied by audio CDs and video recordings.
- Visual sound reproduction techniques form a necessary tool to be used both in the restoration of old recordings as well as in research. The so-called spectrographic representation of sound was made available already after World War II; today it is accessible via specialized computer hard- and software like CSL (Computerized Speech Laboratory), Multi-Speech, Praat, etc. Sound analysis is used by the study group members in order to investigate the temporal structure of traditional music, changes in the sound quality due to bimusicality of certain tradition carriers, and properties of different vocal techniques. The latter question is important for both theory and pedagogical applications in the training of singers.
- A recent study by Jaan Ross and Ilse Lehiste demonstrates how in the old Baltic Finnic folksongs, the so-called runic or Kalevala songs, speech and music as two separate sound systems mutually influence each other under conditions of co-existence. Triinu Ojamaa has studied different segmentation principles of the Samoyed musical tradition to be found in Siberia, and showed that cultural background plays a role in determination of how to divide a continuous acoustical signal into culturally relevant units. This kind of research has at least a double function: to mediate a particular musical tradition to the general ethnomusicological audience as well as to look into more fundamental laws of how speech and music are interconnected within the framework of singing, in other words – to try to answer the question of what singing actually is.
- Alongside with the studies of music, some members of the group (Liina Saarlo and Mari Sarv, both doctoral students at the University of Tartu) also do research into the verbal texts of folksongs. The subject of the thesis by Mari Sarv is the regional characteristics of poetics in old Estonian folksongs,

which concentrates on metrical and verse structural characteristics of this tradition. Her research is related to previously referred studies on text-and-tune relationship in the runic songs.

INTERNATIONAL CONTACTS

Research of the study group "Poetical and musical folklore" generally follows the trends common to ethnomusicological studies in other European countries, regarding both methods and content. This has facilitated our integration into international research projects as well as professional organizations, such as the European Society for the Cognitive Sciences of Music, the European Seminar in Ethnomusicology, etc. Since 2003 the study group has participated in the project called "Citizens and Governance in Knowledge-Based Society" under the section "Music, National Identity, Ethnicity and Cultural Diversity in Europe". This project is aimed at coordinating research on popular music across Europe. In addition to the studies on authentic folk music, it focuses also on country music, jazz and rock, which from the Estonian perspective has been rather unusual. As to the cognitive musicology, the study group has in recent years developed contacts with the Department of Speech, Music and Hearing at the Royal Institute of Technology in Stockholm, Sweden, with the Pavlov Institute of Physiology in St. Petersburg, Russia, and with the Ohio State University in Columbus, USA.

T. Ojamaa and J. Ross, Conference on Interdisciplinary Musiocology, Craz, 15.-18.04.2004.

PUBLICATIONS

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CDs and CD-ROMs

Discovering Siberia: Songs of the Forest Nenets. Music of the Finno-Ugric Peoples 1. Koost. ja toim. T. Ojamaa. Tartu (2002).

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CENTRE FOR DEPENDABLE COMPUTING

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Centre for Dependable Computing (CDC) unites scientists from different institutions sharing common research interests and working on common themes following a jointly agreed research plan. In fact, the associated research groups have for years constituted an informal research network that, depending on the prevailing political and financial situation, has worked together organising all-Estonian seminars, conducting projects for supporting computer science higher education (TEMPUS projects) or running international winter schools for graduate students. Establishing a centre of excellence enabled a more systematic consolidation of these efforts. The research plan of the Centre is in agreement with the plans of the participating institutions.

The Centre involves scientists from seven institutions:

- Institute of Cybernetics at TUT (IoC),
- Dept. of Computer Science, TUT (CS/ TUT),
- Dept. of Computer Control, TUT (CC/ TUT)
- Dept. of Computer Engineering, TUT (CE/ TUT),
- Institute of Computer Science, University of Tartu (CS/UT),
- Tartu University Inst. of Technology (TUIT),
- Cybernetica AS (CybAS).

The Centre is coordinated by a Research Council, consisting of the leaders of its research groups and the head of the Centre. Strategic supervision is in the hands of an international Advisory Board of four renowned European scientists: Prof Reino Kurki-Suonio, Tampere University of Technology, Finland; Prof Kim G. Larsen, Aalborg University, Denmark; Prof Reinhard Wilhelm, University of Saarland, Germany; Prof José Oliveira, Universidade do Minho, Braga, Portugal.

RESEARCH PLAN

The research topics of CDC grouped by research areas for the closest years are:

MATHEMATICAL FOUNDATIONS & PROGRAMMING LANGUAGE TECHNOLOGY

- Type-theoretic and category-theoretic studies of (co)inductive types and (co)recursion schemes.
- Algebraic and categorical semantics of intermediate and modal logics, with applications to programming languages;
- Proof-theoretical studies on constructive set theory, Martin-Löf type theory, and explicit mathematics.
- Development of methods for static analysis and abstract testing methods based on abstract interpretation.

- Development of program transformation methods for strong functional programming languages; specifically deforestation, supercompilation etc.
- Development of methods for stack code validation and type checking in stack-based languages.

FORMAL METHODS IN SOFTWARE ENGINEERING

- Development of structural program synthesis methods for systems with distributed architecture.
- Integration of different program synthesis paradigms (deductive, inductive, transformational synthesis).
- Automatic theorem proving and its application for verification of hardware.
- Development of formal specification, verifycation methods and tools combining deductive and algorithmic techniques.
- Integrating formal verification with techniques allowing extending the size of systems that can be verified.
- Time-aware, interaction-based computational models for timing and behavioural analysis.

TRUST AND CONFIDENCE

- Development of efficient techniques for public key distribution and certificate validation (both on-line and off-line). Efficient protocols for long-term preservation of validity confirmations.
- Secure and auditable queries from public databases and registries.
- Time-stamping schemes, their security and efficient implementation.

DESIGN AND TEST OF DIGITAL SYSTEMS

- Development of new methods of modelling physical defects and logic faults to increase the quality of testing of today's complex digital systems.
- Development of new hierarchical diagnostic models of digital systems and highly efficient algorithms for test generation, fault grading and design error and fault diagnosis.
- Development of new efficient design methods based on new paradigms like SOC, co-design, and oriented to testability and built-in self-test criteria.

The research activities of the research groups of CDC are primarily funded from the governmental budget for basic scientific research (target financing) or grants from the Estonian Science Foundation, in total 7,08 million Estonian crowns in the year 2003. The research groups of CDC are also participating in a number European projects funded by the 5th Framework Programme of the EU. At the current moment (Nov. 2003), five EU projects are running:

Thematic network IST-2001-38957 APPSEM II

Thematic network IST-2001-33123 CoLogNet

Accompanying measures project IST-2001-37592 eVikings II

Accompanying measures project IST-2000-30193 REASON

Accompanying measures project IST-2001-35174 OpenEvidence.

Improving the effectiveness of doctoral PhD studies in computer science is a strategic objective of the CDC. The Centre is annually organizing winter and summer schools for PhD students in computer science with lecturers from abroad. The Centre is also in charge of several series of all-Estonian seminars (computer science theory days, formal methods seminar days etc.) as well as master classes of invited foreign lectures.

In 1998-2002 the following young scientists defended their doctoral degrees under supervision of members of CDC: S. Tupailo (Stanford U., 1998), T. Uustalu (KTH, 1998), A. Buldas (TTU, 1999), H. Lipmaa (UT, 1999), V. Vene (UT 2000), P. Ellervee (KTH, 2000), O. Sokratova (UT, 2001), J. Raik (TTU, 2001), A. Kuusik (TTU, 2001), J. Willemson (UT, 2002), P. Laud (U. des Saarlandes, 2002), M. Brik (TTU, 2002). Currently, 24 PhD students are being supervised by members of CDC.

An overview of the scientific results grouped by the research groups is presented in the following sections.

The main research directions of the group are logic and algebra as the foundational disciplines of theoretical computer science, and programming language theory (semantics, design, implementation). More specifically, the group is focusing on structural proof theory and type theory, categorical logic, ordinal analysis, algebraic combinatorics, semiring theory and algebraic automata theory, programming language semantics and programming language implementation, program analysis, incl. type-based methods, semantics-based program manipulation, language-based security.

MAIN RESULTS

A number of new results has been obtained in the theory of inductive and coinductive types, monads and comonads, with applications to modularity in representing and reasoning about syntax and computations with effects and to type-based termination: A novel structured recursion scheme based on a comonad and a distributive law has been formulated which makes it possible to treat a variety of standard structured recursion schemes as instances of one generic scheme. A general account has been given of the so-called Mendler style of formulating structured recursion schemes where the totality of the function being defined (termination of the program) is ensured by the polymorphic type imposed on the scheme. A strong generalization has been given for the theorem by Adámek and colleagues on non-well-founded term algebras as free completely iterative monads. CPS and monadic translations have been defined for languages with inductive and coinductive types. Frameworks for representing and reasoning about syntax with variable binding have been studied for non-well-founded syntax and explicit substitution. A fixed-point-theoretic construction has been given for calculating the coproduct of two ideal monads. This construction enables one, e.g., to calculate the combination of the monads capturing non-determinism and probabilistic choice.

A novel definition of secure information flow has been given which is based on computational rather than information-theoretic independence of the public outputs of a program from its secret inputs. It has been shown how to analyse a program for security in a language

From the 8th Estonian Winter School in Computer Science (EWSCS'03) at Palmse.

with an encryption operator and how to analyse a program for relative security (security on the assumption that some of the outputs of a program are non-secret).

A method for exact static analysis of multi-threaded programs has been developed which avoids state space explosion by use of global invariants. The method has been implemented in a prototype for validation of avionics software.

Several constructive foundational mathematical theories (constructive set theory, Martin-Löf's type theory) have been shown to be realizable into Feferman's explicit mathematics.

A number of results has been obtained on rewriting on semirings and the algebraic theory of automata.

The group initiated the Estonian computer science theory days that have been held twice a year since autumn 2002. In 2004, two international events will take place in Estonia organised by members of the group: the IST TN APPSEM II 2nd Annual Meeting, APPSEM 2004 (Tallinn, 14-16 April 2004) and the 5th International Summer School and Workshop on Advanced Functional Programming, AFP 2004 (Tartu, 16-21 August 2004).

Cooperation partners: Ludwig-Maximilians-Universität München, INRIA Sophia Antipolis, Universidade do Minho, University of Leicester, University of Nottingham, Universität des Saarlandes, Universität Trier, University of Calgary, University of Leeds.

Research team: Tarmo Uustalu, Peeter Laud, Jaanus Pöial, Olga Sokratova, Mati Tombak (prof), Sergei Tupailo, Varmo Vene; Reimo Palm; Härmel Nestra, Ahti Peder, Tiina Zingel (PhD students).

PUBLICATIONS

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FORMAL METHODS IN SOFTWARE ENGINEERING

To meet the high requirements on the reliability of complex systems and to speed up productivity of software development teams, methods for getting provably correct programs are needed. Formal proof theory provides a basis for two different approaches to correct software development: program construction (program is derived from its specification) and program verification (program is proven to meet requirements of the specification). In practice, a variety of combinations of these two diametrically opposed approaches is used.

The main aim of this research is studying logic, algebra and systems theory based methods for proving properties and synthesising programs and systems, and also studying properties of the proof methods themselves. Current rese-

arch is addressing developing techniques and tools applicable for obtaining both transformational and reactive (embedded) systems.

The rapidly increasing number of embedded and distributed computer applications has revealed the need for development of new models of computing based on concept of non-linear time. The software-intensive systems are often operating in incompletely known environments, in an interface between natural and artificial world that is not always predictable in the phase of system development. Introducing time to computer science in a sufficiently sophisticated form has become essential for verification of timing properties of such systems. Research of this team is also focused on formal description and analysis methods of time-sensitive multi-agent systems, and on methods for assessment of structural and behavioural properties of time-sensitive software.

The research team has competence in the areas of proof theory and automated theorem proving, program synthesis, timed and hybrid automata, compositional program verification, correctness by construction techniques, and application domains such as mechanical engineering and control.

SYNTHESIS OF PROGRAMS

A common formal basis for representing semantics of computations both at the level close to hardware primitives, and at the level of software components is presented. This logic is expressive enough for describing, first, the structure of hierarchical configurations and, second, dataflow both at signal and object level. It is sufficiently efficient for synthesis of large configurations and algorithms from their high-level specifications.

Automatic knowledge based program construction based on declarative description of ontology of a problem domain has been investigated. An algorithm for coding sequential programs by real numbers was developed together with a method of transforming a task for program synthesis (on a first-order computational model) into an optimisation problem. This is an inductive approach based on the idea to search for the optimal program from among all possible sequences of relations of the computational model using genetic programming techniques. Actually, the same computational models by Tõugu are used for specification of problem ontology that are utilised for knowledge representation in structural program synthesis (deductive approach). We believe that combining these two types of techniques might provide more general and effective procedures to automate software development. This would simulate human reasoning where deductive inference steps are interleaved with drawing conclusions from samples of experimental data.

A new architecture of the system for synthesising distributed programs for GRIDs was developed (Fig. 1). This research is motivated by utilisation and developing further existing paradigms (program synthesis using intuitionistic propositional calculus, Java language etc.) by increasing their performance via parallel computing.

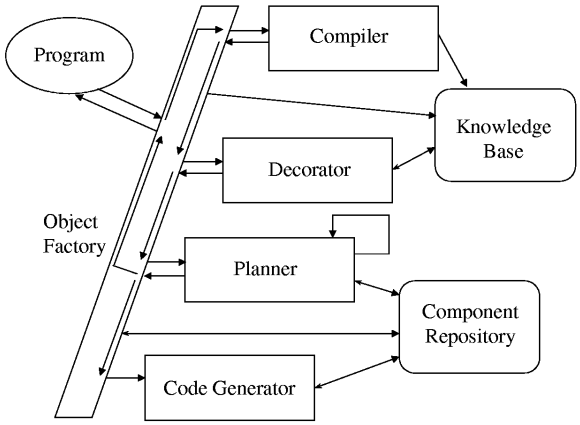

Fig. 1.
Modular structure of the distributed program synthesizer.

Co-operation partners: Royal Institute of Technology in Stockholm, Norwegian University of Science and Technology, Stanford University.

MULTIAGENT SYSTEMS

Theoretical studies aim at developing time-sensitive interaction-centred model of computation, the experimental studies focus on the development and assessment of pilot applications as multi-agent systems. Time models and time-sensitive ontologies of agents have been of prime interest. Interactive computations, roles of (intermediate) interaction were analysed in temporal aspects. Software architecture of time-aware agents was designed and implemented in C# for .Net. A generic collection of map agents has been implemented as a pilot application. Another prototype system – compiler agents for proactive translation – is under development.

Towards the fault-tolerant parallel computing models a fault-tolerant communication model for parallel computation package DOUG (Domain Decomposition on Unstructured Grids) has been developed. This prototype implantation has been successfully used in stability assessment of flow simulation with the Navier-Stokes equations.

Co-operation partners: University of Lübeck, University of Bath, Pennsylvania State University, University of Toulouse.

VERIFICATION OF HYBRID DYNAMIC SYSTEMS

New methods have been proposed for construction of finite models for first-order predicate formulas describing real-time systems. New techniques for proving non-derivability have been found and implemented in the automatic theorem proving system Gandalf. The continuously developing module of the abovementioned theorem prover won the yearly international contest of proving systems held as a part of the CADE-19 conference in Miami.

A representation of taxonomies has been developed that allows using an inference engine for classical logic for systems verification and solving queries in semantic web.

The first prototype system has been implemented that is able to extract facts and rules from the specifications of correctness of the systems and in several semantic web languages, translating them into first-order logic. The representation of taxonomies used allows to increase efficiency of inference engines if certain classes of subproblems are recognised in a particular context and the system can reuse the corresponding solution strategies.

Co-operation partners: Chalmers Technical University, Danish Technical University, Ålborg University.

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The main goal of the research is to develop and analyze security solutions for electronic documents and databases, as well as to study theoretical limits of cryptographic security measures.

TIME STAMPS

Methods have been studied for producing reliable proofs that an electronic document was created at certain time, without assuming the presence of unconditionally secure third parties.

Main results: (i) It has been shown that construction of systems for proving the creation time of electronic documents (so called time-stamping schemes) in which the proofs are verifiable off-line is possible. (ii) Upper bounds for efficiency have been proved in several practical cases. (iii) A prototype-service for such a time-stamping scheme has been developed that accounts for all practical aspects related to such services. Hence, the applicability of such services has been proved in practice as well.

A large fraction of electronic data, in addition to cultural or esthetical value, also has an evidentialry value. Electronic data are sometimes used as proofs of events or facts. In order to guarantee the reliability of such proofs, data must be obtained from reliable sources and the origin of data should be verifiable (and sometimes provable).

Time stamps guarantee one aspect of reliability – the verifiability of creation time. A time stamp is a confirmation (or proof) that an electronic data item existed at certain time. The results obtained by the research group in the last five years show that such proofs are possible without involvement of trusted third parties. At the same time, the system still remains efficient enough for practical implementations.

Interesting theoretical results have been obtained about the limits of mathematically provable security properties of time-stamping schemes. It turns out that, without adding additional checking procedures to time-stamping systems, there exists no formal proofs that a time-stamping system is secure, based on collision-resistance of the cryptographic hash function used in the system.

SECURE DATABASES

It has been studied to what extent and how it is possible to protect data in databases, assumed that the holder of the database is not completely trustworthy.

Results: (i) It has been proved that one can construct secure databases that enable so called undeniable proofs. The holder of such a database cannot give contradictory replies to queries, so that the replies at the same time have correctly verifiable cryptographic codes.

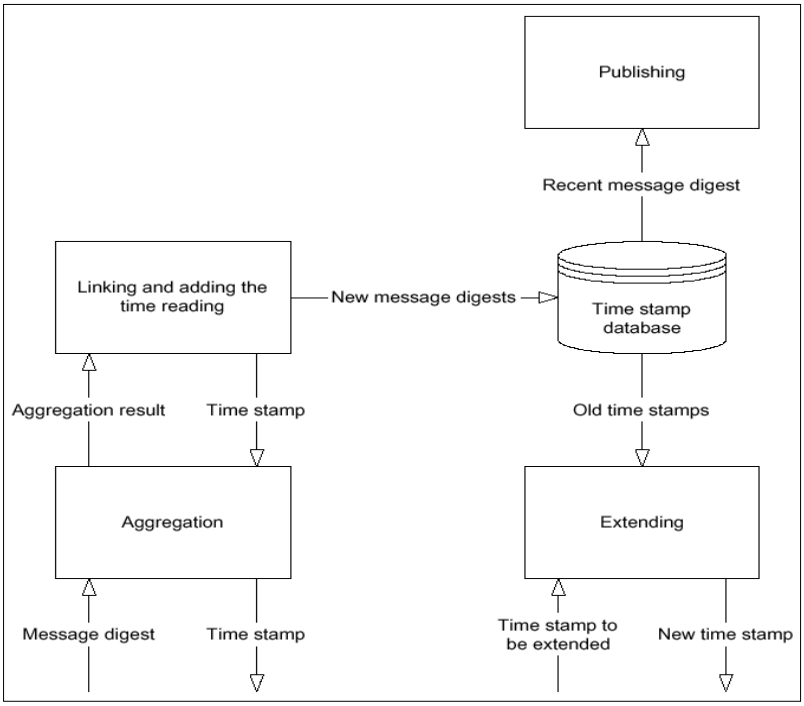

Figure 2.
General scheme of a time-stamping service that enables off-line verification.

(ii) A practical security solution has been developed, based on both the secure database and the time-stamping technologies.

The security of databases and registries does not mean just the aspect of confidentiality – data must be readable only for authorized persons – but also the aspect of integrity – a reply of the database to a query must be provably authentic and reflect the actual content of the database at the moment of receiving the query.

The necessary cryptographic protocols were developed two years ago by the researchers of this group. The security of the protocols was also proved using methods of computational complexity theory.

Theoretical results have been applied in the development of a practical database security solution X-road, which is widely used today in the Estonian public sector to facilitate co-operation of state-level databases and registers. The X-road system has received high grades and awards at international level.

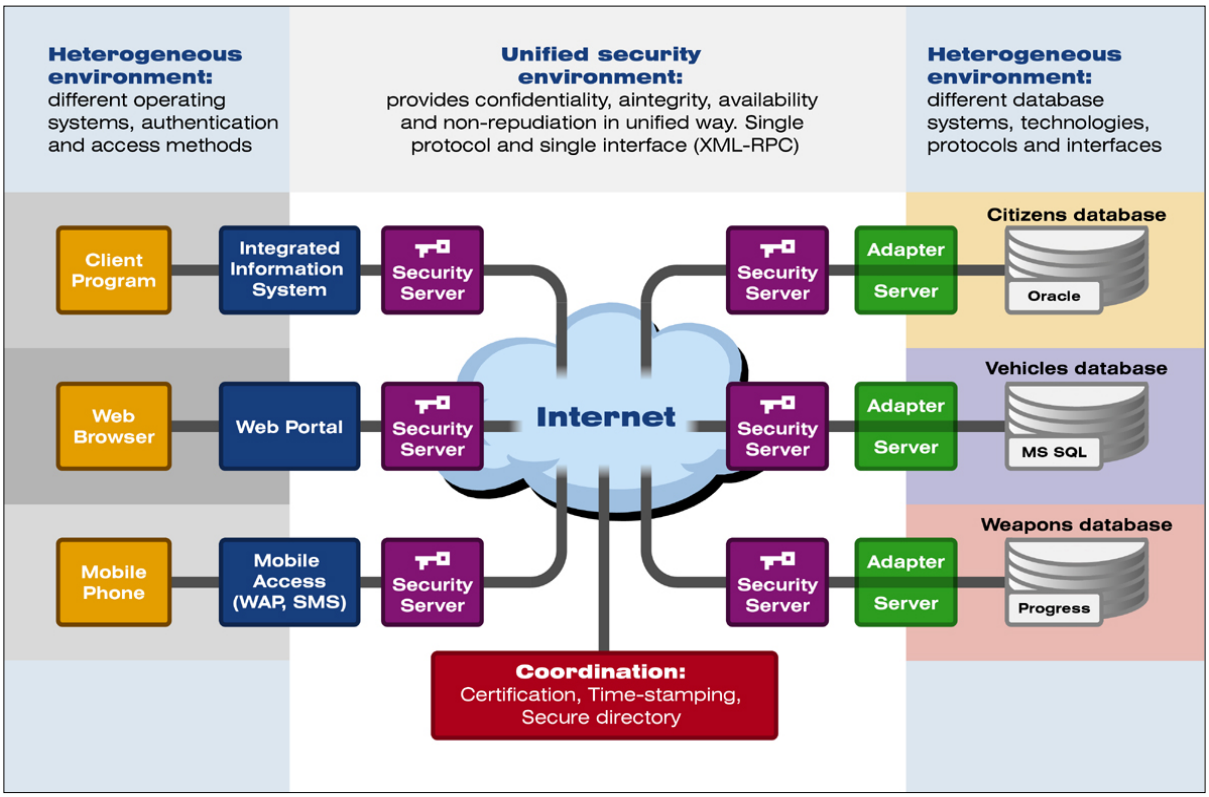

Fig. 3.
General scheme of the X-road secure database system.

Often, it is necessary that the authenticity of the reply stays verifiable for a certain period of time after its creation. For example, such a requirement is important, if the replies are used as legal documents. In addition to external threats (such as hackers) one must account for a possible misbehaviour of the database holder. Also the holder is capable of modifying records in the database, as well as reply to queries incorrectly.

The newest cryptographic methods enable us to set certain limits to the misbehaviour of database holders. Namely, they cannot give contradictory replies (with respect to certain semantics that the records of the database define).

Co-operation partners: Helsinki University of Technology.

Research team: Ahto Buldas, Peeter Laud Jan Willemson; Sven Laur, Meelis Roos, Jelena Zaitseva (PhD students).

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DESIGN AND TEST OF DIGITAL SYSTEMS

The scientific goals of the research group are closely related to the most highly recognized guidelines for design and test solutions of "The MEDEA Design Automation Roadmap". MEDEA (Micro-Electronics Development for European Applications) is a part of the pan-European EUREKA network for cooperative R&D in computeraided design (CAD) and design automation. The team is involved in design and test of digital systems, self-testing and fault tolerance. The main objective of the research is to develop new efficient methods for modelling, design and test of digital systems to guarantee the efficiency, high quality and fault tolerance of systems in the conditions of ever increasing complexities. To achieve this target the team has competence in and is actively working on the following more specific problems: diagnostic models for digital systems, automation of test program generation, fault simulation and fault diagnosis in digital systems, physical defect oriented fault analysis, decompositional design and design error diagnosis in digital systems, analysis and partitioning methods for hardware / software codesign, and development of unified representation of systems for control and memory intensive applications.

MAIN RESULTS

A novel diagnostic model for digital systems based on decision diagrams (DDs) has been introduced into the theory of testing. The new model affords generalization of testing problems allowing uniform formal handling of systems on logic, procedural, functional as well as behavioural levels. Introduction of the new class of structurally synthesized binary DDs (SSBDDs), as well as discovering several interesting properties of SSBDDs afforded to increase the efficiency of algorithms for test generation, fault simulation, and fault diagnosis.

A new hierarchical approach to test generation for digital systems based on using the DD-model was proposed. Combining the high-level efficiency of solving complex deterministic search problems and medium-level accuracy of fault "transportation" analysis with low-level exact fault activation allowed to reach high efficiency and high quality in test generation.

A uniform approach to solving logic tasks of digital test was developed. The basis of this approach is the diagnostic model in form of structurally synthesized binary DDs (SSBDDs) that differently from the common BDDs preserve the structural features of gate-level circuits in the model. This feature made it possible to solve numerous logical tasks of a digital test like test generation, multi-valued simulation, timing simulation, and fault diagnosis at the macro level (instead of the gate level), which allowed to reduce the complexity of the model and to speed up the algorithms. Based on the SSBDD model the conception for a diagnostic software Turbo-Tester was developed and implemented as a set of different diagnostic tools: test generation, fault simulation, and testability analysis.

A new approach to increase the speed of high-level simulation of synchronous digital systems was developed based on using High-Level DDs

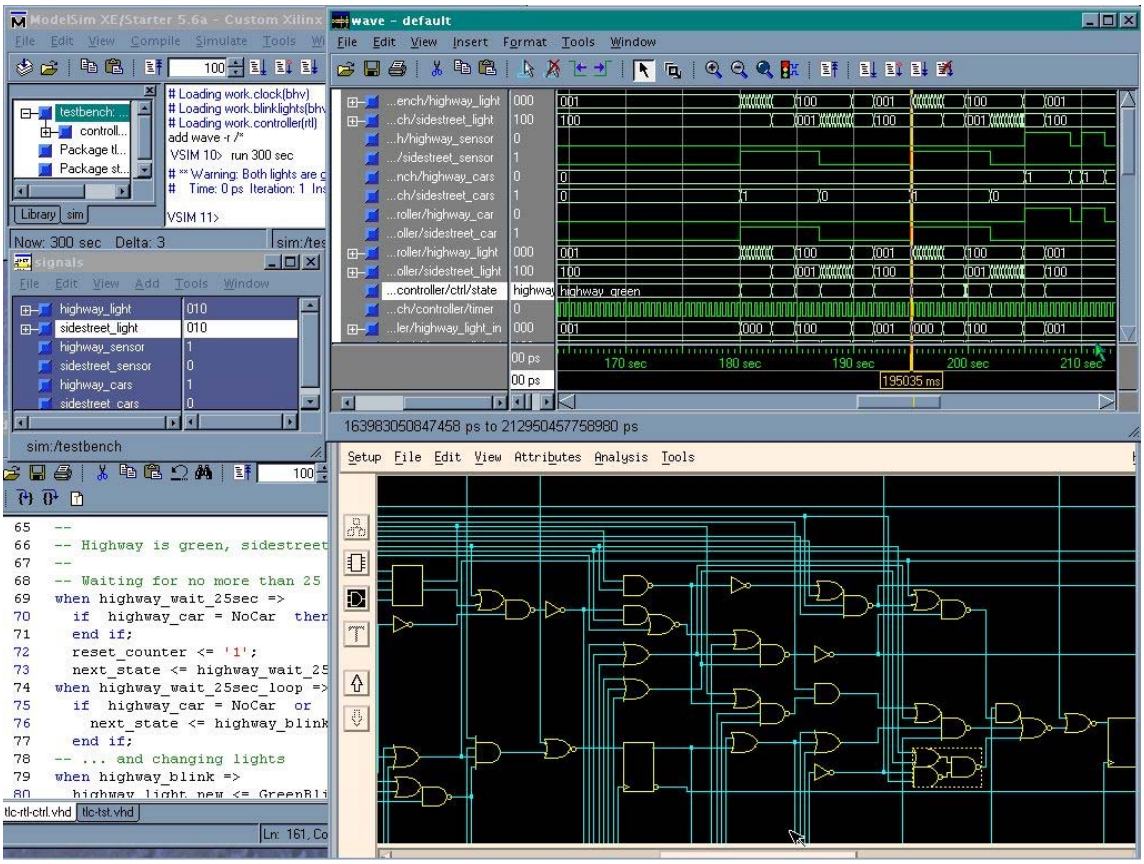

Fig. 4.
Modern environment for designing digital circuits.

(
HLDDs). HLDDs appear to be an efficient and compact representation of the system beha-viour for the high-level cycle-based simulation. In order to fully exploit the advantages of HLDDs new simulation algorithms combining forward event-driven and recursive back-tracing techniques have been proposed. Experimental results carried out on real case examples de-monstrated the gain in simulation performance of the proposed approach.

A new conception to defect oriented fault ana-lysis in digital systems has been developed. The new approach allows the first time to handle in a regular way the defects that increase the number of states in the circuit. By introducing the concept of functional faults, uniform met-hods for defect-oriented multi-level fault simu-lation and test generation were proposed. The new conception allows coping with the problem of creating high accuracy test patterns in the conditions of continuously increasing complexi-ties of digital systems.

New analysis and partitioning methods for HW/SW codesign were developed. They target control intensive applications, and allow more efficient partitioning than universal methods. The methods were used in the designing of a cryptographic processor. A prototype tool was implemented which incorporates the partitio-ning methods.

A new unified internal representation for control and memory intensive applications was develo-ped. The internal representation allows the analysis and synthesis tools to exchange infor-mation without loss of specification details. It is input language independent and allows hetero-geneous specification of digital systems. The first version of a prototype tool, which uses this internal representation, was implemented at KTH (Sweden). New methods are being added to the tool currently at TTU.

E-learning. A new conception of a training sys-tem for teaching design and test of electronic circuits was developed and implemented. A set of tools was designed for exercising design, test and diagnostics related problems in digital sys-tems. Access to the tools via Internet makes it easy for students from foreign universities to use the e-learning environment at any time in any place. At the present moment the set of test

tools developed by our group has been used in nearly 90 institutions from more than 30 countries worldwide.

Research team: Raimund Ubar (prof), Marina Brik, Peeter Ellervee, Margus Kruus, Jaan Raik, Aleksandr Sunditsõn, Kalle Tammemäe; Margit Aarna, Eero Ivask, Artur Jutman, Helena Kruus, Aimar Liiver, Elmet Orasson (PhD students).

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