1 Introduction

Year 2005 marks for the Laboratory of Computational Engineering (LCE) & Research Centre for Computational Science and Engineering (CCSE) the sixth and final year as a national Centre of Excellence with truly international staff of about 80 and of 10 different nationalities. Since the beginning of 2002 CCSE has operated an affiliate research unit called Advanced Computational Science and Engineering (ACSE) in Wolfson College of Oxford University with its own computing facilities, one part-time director and two full-time researchers. During this time it has also run Wolfson College visiting scholar programme for CCSE researchers to interact with various Oxford scientists in the fields of Theoretical Physics, Information Engineering, Neurocognitive Science, Materials Science, and Mathematical Biology. So far more than a dozen of CCSE researcher have visited Oxford thus fulfilling the role of international research training. The research of LCE, CCSE and ACSE has been multidisciplinary in nature and been carried out mainly in Computational information technology, Computational materials research, and Cognitive science and technology. In 2005 these activities have borne a lot of fruit: about 80 scientific publications of which more than 50 in high impact factor journals, and 8 PhDs of which one woman and one jointly with another laboratory.

This year also marks a key development in LCE’s nine year history at Helsinki University of Technology, namely that - for the second time - it was chosen by the Academy of Finland as the Centre of Excellence focusing now on Computational Complex Systems Research (CCSR) for 2006-2011. In addition, and also for 2006-2011 a continuation has been agreed for the Wolfson College affiliate unit - now focusing on Computational Complex Systems and Networks Research (CCSNR) - to operate with similar goals, with strengthened staff and with better facilities than the former ACSE. Since complex systems - be them physical, biological, cognitive, economical, or societal in nature - consist of interdependent elements showing self-organisation and emergent properties in their structure, function and response, a new research paradigm with holistic system level viewpoint is needed. This paradigm requires to combine physical, mathematical, biological, neurocognitive and social sciences together with computational modelling and analysis approach.

In recognition of this enhanced need for multidisciplinarity our new mission in Complex Systems Research consists of four focus areas: 1. Models & Methods, including Complex networks and agent-based models, Pattern formation in biological systems, Statistical and information theoretic modelling methods, and Brain signal analysis; 2. Engineered and Artificial Systems, including Engineered nanosystems and Modelling of learning and perception; 3. Cognitive & Social Systems, including Cognitive systems and Structure and dynamics of social network; 4. Computational Systems Biology, including Biomolecular modelling, Bioimaging, and Biospectroscopy. In order to achieve most from this type of interdisciplinary research the researcher themselves will jointly work in different focus areas.

Kimmo Kaski
Academy professor
2 Personnel

All the laboratory personnel can be reached by e-mail with address first_name.last_name@hut.fi. More complete contact information can be found from the laboratory web page http://www.lce.hut.fi/. List of the personnel in the laboratory:

Professors
- Jääskeläinen Iiro Professor
- Kaski Kimmo Academy Professor
- Lampinen Jouko Professor
- Sams Mikko Academy Professor
- Tulkki Jukka Professor

Adjunct Professors (Docents/Visiting Professors)
- Abraham, Douglas Prof. (Oxford University, UK)
- Alexandrov Yuriy Prof. (Russian Academy on Sciences, Russia)
- Barrio Rafael Prof. (Universidad Nacional Autonoma de Mexico, Mexico)
- Haraldsson, Gudmundur Prof. (University of Iceland, Iceland)
- Kertész Janós Prof. (Technical University of Budapest, Hungary)
- Landau David Prof. (University of Georgia, USA)
- Lehtokangas Mikko Docent (Tampere University of Technology)
- Mouritsen Ole Prof. (Southern Denmark University, Denmark)
- Oresic Matej Docent (VTT Biotechnology)
- Manna Subhrangshu Sekhar Prof. (Satyendra Nath Bose National Centre for Basic Sciences, India)
- Rauschecker Josef Prof. (Georgetown University, USA)
- Parkkinen Jussi Prof. (University of Joensuu)
- Rissanen Jorma Prof. (IBM Research Center, Almadena, USA)
- Räihä Kari-Jouko Prof. (University of Tampere)
- Stenholm Stig Emeritus Prof. (Kunglika Tekniska högskola, Stockholm Sweden)
- Sutton Adian Prof. (Imperial College, London, UK)
- Tirri Henry Prof. (University of Helsinki)

Secretaries
- Järvenpää Aino
- Lampinen Eeva

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- Ala-Korpela Mika Ph.D.
- Andersen Tobias Ph.D.
- Brandt Sami Dr. Tech.
- Bunker Alex Ph.D.
- Engelhardt Peter Ph.D.
- Frydrych Michael Ph.D.
- Heikkonen Jukka Dr.Tech., Academy Fellow
- Karttunen Mikko Ph.D.
- Linna Riku Ph.D.
- Möttönen Riikka Ph.D.
Ojanen Ville  Ph.D.
Róg Tomasz  Ph.D., Marie Curie Fellow
Saramäki Jari  Ph.D.
Stimson Lorna  Ph.D.
Szelestey Peter  Dr.Tech.
Tiippana Kaisa  Ph.D.
Töyli Juuso  Ph.D.
Valpola Harri  Dr. Tech., Academy Fellow
Vehtari Aki  Dr. Tech.

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Kostiainen Timo  M.Sc.
Kumar Udyant  M.Sc.
Kumar Vibhor  M.Sc.
Kumpula Jussi  M.Sc.
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Kumpula Linda
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Lankinen Niko
Lilja Ville
Lindroos Virpi
Malkamäki Kaisa
Mannari Ville
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Pihlström Kim
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Toivanen Mika

Trainees
Hartikainen Maria
Kaarela Ilari
Koskentalo Katri
Sandholm Niina
Vanhatalo Jarno
Vanhatalo Maija
Yli-Krekola Antti
3 Teaching

LCE’s curriculum consists of four major subjects which can also be taken as minor subjects:

- Computational Engineering
- Cognitive Technology
- Computational Systems Biology
- Neuroinformatics

The major subjects can be studied in the following Degree Programmes:

- Electronics and Electrical Engineering
- Communications Engineering
- Bioinformation Technology
- Computer Science and Engineering

Courses taught in 2005

Spring 2005

- S-114.101 Cognitive neuroscience (3 cr) L
- S-114.102 Philosophy of technology (2 cr) L (Connet course)
- S-114.150 Computer Simulation in Engineering and Economics (2-4 cr) LV
- S-114.155 Business game (2 cr)
- S-114.204 Modelling of perception (3 cr) L
- S-114.220 Research Seminar on Computational Science (3 cr) L
  Topic: Neurorobotics
  Topic: Complex networks
- S-114.240 Seminar on computational engineering (2+2 cr) V
  Topic: Computational/experimental methods in understanding biological systems
- S-114.250 Special topics in computational science (4 cr) L
- S-114.326 Physics IV (S) (3 cr)
- S-114.401 Semiconductor Quantum Structures (4 cr) L
- S-114.426 Physics IV (Sf) (4 cr)
- S-114.510 Computational systems biology (3 cr)
- S-114.610 Special Course in Bayesian Modeling (2-5 cr) L
- S-114.710 Perception and production of speech (4 cr) L
- S-114.720 Systemic Psychophysiology (1 cr) L
- S-114.760 Emotions and communication (4 cr) L
- S-114.771 Memory and Learning (2 cr) L

Autumn 2005

- S-114.1100 Computational science (5 cr) L
- S-114.1310 Introduction to Modelling and Information Theory (3 cr)
- S-114.1710 Cognitive Neuroscience (4-5 cr)
- S-114.2500 Basics for Biosystems of the Cell (5 cr)
- S-114.2502 Seminar on Computational and Cognitive Bioscience (3 cr)
- S-114.2601 Introduction to Bayesian Modelling (5 cr)
- S-114.2720 Perception and Action (4-6 cr)
- S-114.3200 Special Course in Computational Engineering I (6 cr) P
- S-114.4220 Research Seminar on Computational Science (3-6 cr) P
  Topic: Modeling in spatial epidemiology and spreading of contagious disease
Courses that can be taken any time

- S-114.2801 Neuroinformatics (5 cr)
- S-114.3215 Special Project in Computational Engineering (3-8 cr)
- S-114.3520 Special Project in Computational systems Biology (3-7 cr)
- S-114.4771 Special Project in Cognitive Science and Technology (3-7 cr)P
- S-114.4772 Individual Studies in Communication and Cognition (1-9 cr)P

For more information see publication: Study Programme, Helsinki University of Technology, or the www-page http://www.lce.hut.fi/teaching/.
4 Theses

Doctor of Science / Philosophy
- Tobias Andersen Model-based assessment of factors influencing categorical audiovisual perception
- Anu Huttunen Analysis and optimization of photonic crystal components for optical telecommunications
- Jani Lahtinen Statistical Inference and Random Network Simulation
- Ville Ojanen Neurocognitive mechanisms of audiovisual speech perception
- Klaus Riederer HRTF Analysis: Objective and Subjective Evaluation of Measured Head-Related Transfer Functions
- Peter Szelestey Computational modelling of fracture and dislocations
- Marko Sysi-Aho A game perspective to complex adaptive systems
- Toni Tamminen Models and methods for Bayesian object matching

M.Sc. - Diplomas
- Topi Hurtig Multimodalisen informaation hyödyntäminen reitinopastusdialogissa (in Finnish)
- Jörkki Hyvönen An efficient library for simulating complex networks
- Laura Kainonen Usability evaluation of the graphical user interface of the lawful interception network element
- Jaakko Kauramäki The effects of attention on neural tuning
- Kaisa Kautto Uniform point distributions and their duals on closed, positively curved surfaces
- Jussi Kumpula Current-induced heating in a ballistic nano-conductor
- Maria Lahdenperä A tool for predicting protein-protein interactions through cross-species comparisons
- Taina Lehtimäki Improving Eye Movement Control in Young Readers
- Tapio Nieminen Reconstruction methods in cryon electron tomography
- Janne Ojanen Minimum description length principle in denoising
- Pasi Ritaluoto Electron transport through quantum point contacts
- Iina Tarnanen Electroencephalography in 3-T Magnetic Resonance Imaging Scanner
- Mika Toivanen Simulation of Lactococcus lactis metabolic networks
- Teemu Tuulari Taikkaavaisuuden kuormituksen vaikutus puheen audiovisuaaliseen havaitsemiseen (in Finnish)
- Johanna Tervala Tarkkaavaisuuden kuormituksen vaikutus puheen audiovisuaaliseen havaitsemiseen (in Finnish)
- Saku Vainio Lyhyimmän polun laskenta laajalla tieaineistolla (in Finnish)
- Petri Vormula Tietämyksen hankinta ja tiedon esittäminen nosturin taajuusmuuttajien ja anturitietojen aikasarjadatasta (in Finnish)
5 Research Projects

5.1 Computational Information Technology

Modelling complex systems to the accuracy that allows predicting the outcomes of the studied system in certain conditions poses a difficult measurement and estimation task. Purely reductionist modelling of even modestly complex systems is impossible: a litre of ideal gas would require knowing the positions and velocities of the order of $10^{23}$ particles; modelling brain functions on the level of single neurons would require knowledge of each neuron function and all the connections, which is out of reach both due to measurement and computational limitations. Such systems can be modelled using statistical approach, where individual unknown constituents of the system are replaced by their probability distributions, and the models operate on average values or other statistical quantities.

Purely probabilistic treatment of the modelling task leads to the Bayesian approach, where probability distributions are used to represent uncertainty due to stochastic elements (aleatoric probability), and also due to not knowing the actual values (epistemic probability). Consequently, the result of the analysis is the posterior distribution of the end variables, given the observed variables and prior assumptions that represent the knowledge before the data is observed. The approach requires integration over high-dimensional distributions, which has made the approach practical only for simple models and distributions. The recent increase in computing power, together with some advances in theoretical and numerical methods, has made this approach feasible in a large set of complex tasks. For example, this approach yields statistical analysis tools for artificial neural networks, which are flexible models but difficult to control and analyze by other statistical or machine learning techniques.
5.1.1 Bayesian Modelling and Application Areas

Our research concentrates on hierarchical Bayesian modelling, developing methods for measuring the performance of the models, and developing efficient Monte Carlo techniques.

Application areas include statistical modelling problems especially in health care data analysis, object recognition and computer vision, inverse problems in brain imaging, and intelligent human-machine interfaces.

**Bayesian Methodology**

Researchers: Aki Vehtari, Simo Särkkä, Jouko Lampinen, Toni Auranen, Aapo Nummenmaa, Elina Parviainen, Jaakko Riihimäki, Jarno Vanhatalo

The main research areas of the Bayesian methodology group are model assessment and the estimation of predictive performance, the elicitation and inclusion of structural information, and advanced dynamic models (see following chapters for case examples). Another important methodological research topic is how to elicit the expert knowledge and transfer it to a probabilistic model in application problems. Examples of important model concepts used are:

1. Hierarchical models; which can handle various nested structures in the data and specify a partial lack of knowledge in a controllable way
2. Non-parametric models; which can be used when the particular functional model of the phenomena can not be specified unambiguously
3. Dynamic models; which can model dynamics in the phenomena studied
4. Inverse models; which can be used to infer the possible causes given the outcomes when we already have accurate forward model describing what the outcomes would be if we would knew the causes; typically inversion of such forward model is not an easy task.

To be able to tackle more challenging scientific problems, it is necessary to research methods for constructing more elaborate models and elicitation of the prior knowledge from the expert of the applied research area. Complex models may have a large number of unknown parameters, for example, thousands in brain signal analysis, which will cause difficulties for computational methods in Bayesian integration. Bayesian methodology group supports applied Bayesian research in the laboratory by providing expertise in model construction and computation.

For example, methods developed in the group were used in concrete quality prediction problem in collaboration with concrete expert Dr.Tech Hanna Järvenpää (Lohja Rudus Oy). The model assessment methods had important part in describing the reliability of the predictions. Using Bayesian modeling in this challenging problem produced excellent results. By using the models and conclusions based on them made by the concrete expert, it is possible to achieve 5-15% savings in concrete factory. Furthermore, it is possible to reduce the proportion of natural gravel from 50–100% to 5-20% and thus help saving non-renewable natural resources.
**Predicting model performance**

Researchers: Aki Vehtari and Jouko Lampinen

Statistical and machine learning models are becoming increasingly complex, due to advances in computational methods and computer performance. This emphasizes the importance of methods for estimating the performance of the models, for comparing and choosing the model, and for predicting the usefulness of the model in the target task.

We have been developing methods for estimating and comparing complex Bayesian models, such as neural networks, and assessing (predicting) their practical performance. When dealing with complex phenomena it is reasonable to assume that all models are approximations (there is no "correct" model), in which case the only reasonable way of comparing models is to compare the consequences of using them, that is, their predictive utilities.

The ideal approach is to use external validation, where the model is used to make predictions on future data, and collected data is then compared with the predictions. Before getting new data, external validation can be approximated using the present data, with three basic approaches: analytic, asymptotic and sample re-use, all of which have been proposed decades ago, but their use in Bayesian modeling has not been widespread. Now advances in computational methods and computer performance allow more complex models and thus there is increased interest in the approaches for estimating predictive performance of the model.

Our research on model assessment is based on cross-validation (sample re-use) approximations for the predictive performance, since it has several benefits over other approaches. For example, it can be used for arbitrary likelihoods and utility functions and it does not rely on asymptotic approximations. Main contributions so far have been in theoretical and methodological advances, which provide solid framework to assess the performance of the complex models, while taking properly into account the associated uncertainties.

Important work in progress is model selection in case of large number of models and estimation of selection induced bias, which are common problems in variable selection. We assume that we have been able to construct the full model, which we think gives the best predictions given the data and our prior beliefs. Proposed method is based on Kullback-Leibler divergence from the predictive distribution of the full model to the predictive distributions of the reduced submodel. The goal is to find the simplest submodel which has a similar predictive distribution as the full model.

The results have direct applications to various industrial problems in numerous projects, with some of the models being currently in use in, for example, concrete and steel manufacturing industry.

**Dynamic State Estimation for Surveillance**

Researchers: Simo Särkkä, Aki Vehtari and Jouko Lampinen

This project is part of the Tekes project Development of Management Systems for Infrastructure Maintenance in Infra Technology Programme. The goal of the project is to develop new estimation methods for remote surveillance of tunnels and physical processes, which are indirectly observed through inaccurate sensors. The methods are applicable to detection of sensor failures and malfunction, and modeling other abnormal behavior of the sensors. This allows, for example, automatic detection and compensation of broken sensors, which opens possibility for using cheaper but less reliable sensors.
The problem is much related to multiple target tracking and for this reason the recently developed new sequential Monte Carlo (particle filtering) based methods for multiple target tracking are directly applicable:

- The methods that have been developed for clutter modeling and estimation can be also used for detection of the sensor failures, malfunction and abnormal behavior.
- The data association methods are also applicable to on-line adaptive classification. These methods would allow classification of different time-dependent events based on multiple sensors. For example, detection of human movement in buildings or sudden temperature changes in tunnels.
- The methods that have been developed to tracking an unknown number of targets can be also applied to on-line segmentation, clustering and change point detection.

Figure 1 shows the estimation result in case of unknown number of 1D signals. The Figure 2 shows the corresponding results for a 2D state estimation (tracking) problem.

Figure 1: Filtering (left) result, smoother result (middle) and the estimated number of signals (right) of 1D scenario with an unknown number of signals

Figure 2: Filtering (left) result, smoother result (middle) and the estimated number of signals (right) of 2D tracking scenario with an unknown number of targets
Recursive Bayesian Inference on Stochastic Differential Equations

Researchers: Simo Särkkä, Aki Vehtari and Jouko Lampinen

The purpose of this project was to provide new Bayesian methods for optimal continuous-discrete filtering and smoothing, that is, new algorithms for recursive estimation of states of systems, which can be modeled as discretely observed stochastic differential equations. The emphasis is in stochastic differential equations with non-linear drift terms and measurement models with non-linear and non-Gaussian components, where the classical linear Kalman filter cannot be used. These kind of non-linear continuous-discrete filtering problems have been previously solved using Taylor series expansion based approximation methods (extended Kalman filters), but other types of methods have been less developed for the continuous-discrete case. The results of the project are as follows:

• By taking the formal limit of the unscented Kalman filter and the unscented Kalman smoother when the prediction time step size goes to zero the continuous-discrete unscented Kalman filter and smoother have been derived. By taking the formal limit, when both the prediction and measurement time step sizes go to zero the unscented Kalman-Bucy filter, which is a continuous-time version of the unscented Kalman filter, have been derived.

• Novel Girsanov theorem based methods for performing continuous-discrete sequential importance resampling, that is, continuous-discrete particle filtering have been derived. Also a Rao-Blackwellized continuous-discrete particle filter have been developed.

• The new methods have been applied to target tracking, estimating the spread of a disease and to estimation of state of a physical phenomenon from indirect sensor measurements.

Figure 3 shows the results of applying discrete UKF (DUKF) and continuous-discrete UKF (CDUKF) to a simulated reentry vehicle tracking problem, and the results of applying the continuous-discrete particle filter to the classical Bombay plague data.

![Figure 3](image)

Figure 3: (left) Mean squared error (MSE) versus time step size in the reentry filtering problem. (Right) the result of applying the continuous-discrete particle filter to the classical Bombay plague data.

The results of the reentry filtering problem are from 200 Monte Carlo runs per time step with the continuous-discrete UKF (CDUKF) and discrete UKF (DUKF). The higher errors of DUKF with longer time step sizes are caused by numerical problems on the prediction step.
Bombay plague data consists of the number of deaths occurred weekly during the period December 1905 to July 1906. These filtered estimates are conditional to the previously observed measurements only. The estimate on week $t$ is the estimate that could be actually computed on week $t$ without any knowledge of the future observations.

**New analysis methods for healthcare process management**

Researchers: Elina Parviainen, Jaakko Riihimäki, Markus Siivola, Aki Vehtari and Jouko Lampinen

The project focuses on healthcare data analyzing systems. The goal is to create tools to aid healthcare agents (e.g. doctors and administration) to produce and evaluate regional healthcare key figures, and anticipate the expected cost effect of a treatment for a single patient or a treatment process. The project is a part of Tekes FinnWell - Healthcare technology programme.

In our part of the project we develop methods for analysis of large scale patient data, in which time dependent phenomena and various hierarchical levels (a single patient, regional, hospital, healthcare region) can be taken into account. Methods are based on Bayesian hierarchical and temporal models. The pilot projects are in institutionalization of the elderly (city of Vantaa), hip fracture (Finland) and orthopedics (city of Espoo).

The purpose in the Vantaa pilot is to study the reasons why the elderly become institutionalized. The aim is to recognize groups with different patterns of behavior, and find out which kind of events precede the final placement in a care institution. Bayesian hierarchical methods make it possible to combine group-level and individual-level information in a flexible way.

The treatment chain of hip fracture patients is modelled using various types of approaches from models based on Coxian phase-type or mixture of Weibull distributions to Bayesian neural network classifiers. MCMC methods are utilized for estimating these multistate models to study, for example, the hazard functions or the prediction accuracy for the length of stays. Also inspecting the effects of explanatory variables and considering areal level indicators such as home municipality statistics are in concern. The hip fracture pilot is conducted in cooperation with National Research and Development Center for Welfare and Health (Stakes).

![Figure 4: A state transition model describing the situation of the elderly moving between different types of care.](image)

![Figure 5: The predicted expected values for the duration of rehabilitation period after the hip fracture surgery.](image)
Disease mapping tools for spatial epidemiology

Researchers: Markus Siivola, Aki Vehtari and Jouko Lampinen

Demographic data registers in Finland provide accurate coordinates for each individual. Consequently, information from several data registries can be linked to geographical locations through personal identification numbers. This can be utilized in the study of spatial epidemiology, which seeks to reveal geographical variations in health outcomes and risks to health.

In this work the aim was to create customized GIS (Geographical Information Systems) tools to estimate and visualize geographical variations in relative risk of death. The adaptive binned kernel estimation method involved the use of circular computation areas operated on a grid with a maximum resolution of 250 m x 250 m allowed by the data. Risk estimates were based on comparing area-specific expected numbers of deaths to actual death counts within an averaging moving window. An example image illustrating variations in the death risk due to cerebral vascular diseases is presented in Figure 6.

Figure 6: Estimated relative risk of death caused by cerebral vascular diseases between 1995 and 2000. The estimates were based on a standard population of 4.8 million and around 18000 deaths.

The results showed that geographical variations exist. The exploratory method featured fast and interactive creation of disease maps due to a simple algorithm and graphical interface. Its primary purpose will be to provide preliminary analysis over large scopes of data, but it does not facilitate the inclusion of explanatory variables aiding further understanding of the detected phenomena. Future implementations will feature Bayesian methods for an improved control of smoothing and statistical significances, and the flexible use of explanatory variables.
Bayesian Object Matching

Researchers: Toni Tamminen and Jouko Lampinen

The goal of the project is to develop a system that can locate and recognize objects in a natural scene. In our approach we study model based methods using full Bayesian inference. The objects in a scene are defined by prior models that are learned from example images.

We have developed a distortion tolerant feature matching method based on probability distributions of Gabor filter responses. An object is defined as a set of locations, with associated Gabor features, and a learned prior model that defines the variations of the feature locations. The appearance and shape models are combined to produce the posterior distribution of feature locations.

For exploring the posterior distribution, we have constructed efficient MCMC samplers for drawing samples from the posterior distributions of the feature locations, mainly using Gibbs and Metropolis sampling. We have also developed a sequential Monte Carlo approach which handles multimodal posterior distributions better than MCMC samplers. This is especially important when some of the object features are occluded, as is often the case in real matching situations. Currently we are extending the matching model to multiple resolutions, which would allow the matching of objects of greatly varying sizes. Figure 8 shows an example of the sequential matching process and figure 9 illustrates matching when the target objects are occluded.

Figure 8: Sequential feature matching. The black circles mark the drawn locations of the current feature, while the green circles are the previously drawn features. The shape (yellow lines) represent the mean of the shape prior.

Figure 9: Matching in the presence of occlusion. Even though the target objects are heavily occluded, the system is able to find the approximate locations of the features.
**Image segmentation by MCMC methods**

Researchers: Timo Kostiainen and Jouko Lampinen

The goal of this work is to develop computationally efficient techniques for the division of natural colour images into meaningful segments. Segmentation is an essential step in image interpretation and computer vision. The slowness of many segmentation methods has been an obstacle to their use in many computer vision applications.

Our approach is based on statistical models for the textures of the segments. We use a probabilistic Markov chain Monte Carlo (MCMC) algorithm to determine how to divide an image such as a natural photograph into segments. The MCMC approach requires the processing of a large number of different sample segmentations. The computational cost depends critically on the quality of these samples. In this work we develop efficient methods to generate good samples for the algorithm by taking advantage of many types of information contained in the images, such as edges.

![Segmentation Results](image_url)

Figure 10: Examples of segmentation results: an artificial example and four real images.
Steerability Properties of Gabor Filters

Researchers: Ilkka Kalliomäki and Jouko Lampinen

Gabor filters are information-theoretically optimal oriented bandpass filters which have been traditionally used in pattern recognition as a generic framework for the representation of visual images. Gabor-based features are widely used in face recognition, for example. Neurological studies have found Gabor-type structures on the visual cortex of mammals. This fact suggests that the Gabor representation is an efficient one in pattern recognition tasks.

We have derived analytical steering equations for Gabor filters, which enable Gabor filters to be used as approximately steerable filters, whose responses can be interpolated to arbitrary orientation. Some families of steerable filters are quite close to Gabor filters in terms of impulse responses, and the steering performance of Gabor filters can be understood via this connection.

Steerability can be used to implement rotation invariant similarity measures for feature detection. We have applied the developed methods to human face detection, alignment and recognition under plane and depth rotations.

Figure 11: Behavior of three different similarity functions with a synthetic test image (top row), with the test feature marked by a red cross. Center row: Normalized inner product similarity (not rotation invariant). Bottom row: Rotation invariant similarity with continuous estimation of best orientation.

Figure 12: Probabilistic feature matching without and with rotation invariant features (top and bottom, respectively), with matching scores on top of images. Rotation invariance makes matching harder but gives better similarity scores with large rotations.
5.1.2 Statistical Brain Signal Analysis

Researchers: Toni Auranen, Iiro P. Jääskeläinen, Jouko Lampinen, Kaisa Malkamäki, Aapo Nummenmaa, Cajus Pomren, Mikko Sams, Aki Vehtari

Statistical brain signal analysis research is a multidisciplinary project combining the expertise of both Bayesian Methodology group and Cognitive Science and Technology group, in collaboration with Massachusetts General Hospital–Harvard Medical School NMR Center (Dr. John W. Belliveau and Dr. Matti S. Härmäläinen).

Localising the neural currents indicating brain activity based on noninvasive magnetoencephalographic (MEG) and electroencephalographic (EEG) measurements (i.e., solving the electromagnetic inverse problem) is most naturally formulated in probabilistic terms and thus becomes a problem of statistical inference. Because of the ill-posedness of the inverse problem, reliable inference cannot be made relying on the data only. Some additional a priori information must be provided in order to obtain sensible results, motivating a Bayesian treatment of the problem.

The overall aim of this project is to apply the methods of Bayesian data-analysis to the study of cognitive brain functions as revealed by MEG, EEG, and functional Magnetic Resonance Imaging (fMRI). We employ a variety of state-of-the-art estimation techniques from Markov chain Monte Carlo (MCMC) to Variational Bayesian (VB) methods. These models are evaluated by using both empirical MEG datasets and simulated data.

The hierarchical Bayesian approach offers a novel methodology for estimating distributed MEG sources. This method generalises Minimum-Norm Estimate (MNE) by assuming zero-mean Gaussian priors with individual precisions (inverse variances) for the currents at each location of the discretised brain. Previously, such a model was introduced and estimated using the VB approximation. We analysed the model further by using simulated data and MCMC methods, with a comparison to the VB approach. Subsequently, we applied the hierarchical VB-methodology to a well-described audiovisual MEG dataset (see Fig. 13, left).

Figure 13: Left: Neural source locations and amplitude timecourses estimated for MEG responses to simultaneous short auditory tones and visual checkerboard stimuli with the hierarchical VB-approach. The locations and timecourses are found to be anatomically and physiologically consistent. Right: Illustration of a correct and erroneous MEG-MRI coordinate alignment.

However, some of the most sophisticated methods can be relatively sensitive to how well the researcher is able to align the MEG sensor coordinate frame with the structural MRI coordinate frame based on anatomical landmarks (see Fig. 13, right). We began studying the effect of erroneous coregistrations of the MEG-MRI coordinates. For this, we have imple-
mented also a Bayesian spatiotemporal MEG inverse model based on unknown number of dipolar sources.

**Computational Neuroscience**

Researchers: Harri Valpola, Harm Aarts, Heikki Joensuu, Ville Mannari, Iina Tarnanen

The project studies the system-level organization of the brain. In the brain, there are several interacting subsystems which work in concert and each contribute to the generation and adaptation of behavior. In order to understand the brain, we build computational models of these subsystems and study the complex, emergent behavior and learning of an agent which interacts with its environment. This is called embedded computational neuroscience and it requires a body and environment to interact with. To this end, we have used Webots simulator platform (simulated robots) but in the future we also aim at verifying the results with real robotic platforms. So far, the two main topics of our research have been:

1. Self-supervised motor learning
2. Development of invariant representations

Self-supervised motor learning makes use of simple reflexes and a learning scheme akin to classical conditioning. As an example, we have implemented a simple robot which balances itself much like a unicyclist. In conventional reinforcement learning, one would define reward function which would signal the success of the robot. Learning would then proceed by trial and error and gradually the successful perception-action patterns would be strengthened. Learning in this approach takes a very long time and instead, we have used simple reflexes to provide training signals. The reflexes are not able to keep the robot up at first but they activate corrective movements which help the robot stay up slightly longer. Learning aims at predicting these corrective movements and initiating them before the hand-coded reflexes do. After trial-and-error learning, the robot learns to stay up as shown in Fig. 14. Since the reflexes give more information than reward signals, learning is much faster than in reinforcement learning.

![Figure 14: Simple reflexes and trial-and-error learning have taught the robot to restore its position and balance from a tilted position (a) to central upright position.](image)

The motor control model can use sensory information to predict reflexes and hence control movements. This makes it possible to evaluate the performance of perceptual systems. For
instance, the balancing robot might ride on an uneven terrain and therefore have a behavioural need for depth vision. We are investigating how motor signals can bias the development of perceptual systems such that perception will be optimized for the behavioural needs of motor control.

**The On-line Adaptive Brain-Computer Interface**

Researchers: Jukka Heikkonen, Pasi Jylänki, Laura Kauhanen, Janne Lehtonen, Tommi Nykopp and Mikko Sams

Brain Computer Interfaces (BCIs) enable motor disabled and healthy persons to operate electrical devices and computers directly with their brain activity. Our BCI recognizes and classifies different brain activation patterns associated with real movements and movement attempts made by tetraplegic persons. Our goal is to examine whether subjects with no previous experience of BCIs could achieve satisfactory performance after a short training period.

It would be important to understand the signals used in BCI applications. We have concentrated on motor cortex activity. Like most other BCI groups, we measure the electric activity of the brain using electroencephalography (EEG). We have also examined the feasibility of magnetoencephalography, MEG, for BCI use.

We have developed an online EEG-based BCI system which uses MATLAB in data analysis. In our first online experiments healthy persons performed real finger movements. The subjects’ task was to move a circle from the centre of the screen to a target on either side of the screen. Four subjects were able to control the BCI with a mean classification rate of 73.5%.

To make the learning process faster, we have started to train the classifier online. During training periods, the classifier is adapted to the user’s brain activity after each trial in a supervised manner, i.e. information about correct class is used. Thus, subjects can start using BCI from the beginning of the experiment without a separate training session. The method was tested with 10 healthy subjects and 6 tetraplegics. Figure 15 shows one tetraplegic person using our BCI.

The healthy subjects controlled the BCI with a mean accuracy of 74.4%. The performance of the best subject was 95%. Three out of six of the tetraplegic subjects learned to control the BCI above chance level. Note that they did not move their hands but attempted to move them. Our current classification method works better with healthy people performing real hand movements than with motor-disabled persons attempting hand movements.

One of our present interests is to examine if classification could be done more often than every 2 s. We also aim to find out more robust signals and analysis methods so that most tetraplegics would learn the use of BCIs relatively quickly.

Our research is funded by European Union (MAIA project), the Academy of Finland, the Finnish Graduate School in Electronics, Telecommunications and Automation, and the Finnish Cultural Foundation.
Hierarchical Bayesian model for feedbacks in simple visual perception

Researchers: Juho Kettunen and Jouko Lampinen

The goal of this project is to generate a hierarchical Bayesian model that could be used to model simple visual perception in the primary visual cortex. Created hierarchy consists of four layers for different kinds of processes. The layers are presented in Figure 16. The bottom layer is called the feature layer and it represents all the sensory measurements from the surrounding world. It is created by filtering a grayscale image with a set of Gabor-filters, which detect phenomena like edges and lines. The second layer represents also Gabor-responses of the image, but in addition to sensory inputs it receives feedback from the higher parts of the hierarchy. The third layer is called the line-process layer and it represents the distribution of edges and lines in the image. Its activation is a combination of the edge responses from the previous layer and the outline information from the top layer’s objects. The object layer contains prior information about the structure of the world, which in this case means a model for the rectangle-shaped objects. The system works in an iterative manner in which all the layers receive bottom-up information from the feature layer and at same time top-down priors from the object layer. This feedforward-feedback iteration finally creates a full interpretation of the scene, throughout the whole hierarchy. The algorithm used for this communication between layers is called nonparametric belief propagation. With this algorithm the distributions of layers can be presented and computed efficiently. The tests done with simple examples show promising results that encourage for further development of the model. For example due to feedbacks the effects of illusory contours can be seen in the lower layers of the hierarchy. The perception of this illusion is presented in Figure 16.

Figure 16: A hierarchical Bayesian model of a simple visual perception (left) and the perception of this illusion (right)
5.2 Computational Materials Research

In LCE and CCSE the computational materials research has been focused on the study of physical properties, processing methods and functional properties of selected new materials. During 2005 a transformation toward computational complex systems research, a new Center of Excellence Programme to be started from the beginning of 2006 at LCE, has become evident as the weight of the research has moved toward nano-bio materials and systems. In our research, we combine multiphysics and multiscale research methods with a system engineering approach to identify technologically relevant material structures, processes and phenomena. The research is organized into three research groups: Biophysics and Statistical Mechanics, Modelling of Structure and growth of Materials and Engineered nanosystems for electronic, photonic, and biosensing applications.

5.2.1 Atomic Level Modelling of Structure and Growth of Materials

This research has been concerned with the study of structural and growth properties of solid materials. These studies rely on microscopic modeling, in which the inter-atomic interactions are described by pairwise or more often to many-body semiempirical model potentials specifically in case of semiconductors. In some other cases like carbon nanotubes more accurate tight-binding approach has been used as a complementary method to describe inter-atomic interactions. In this research there are two main focuses, to look (i) at the structure and energetics of grain boundaries in silicon, and (ii) at the mechanical properties of carbon nanotubes and related to that the distribution of particles on curved surfaces. In addition, since the used computational methods, like Molecular Dynamics (MD) and Monte Carlo (MC) simulations, are large scale, their execution have been done using mostly our in-house parallel cluster computers. This has entailed the development of efficient parallel programming and for visualisation graphical user interfaces.
Structure and energetics of grain boundaries in silicon

Researchers: Sebastian von Alftan, Adrian Sutton, and Kimmo Kaski

Grain boundaries are formed when two crystalline slabs are put into contact with each other, so that the crystals are rotated with respect to each other. These are formed in polycrystalline silicon, which is used widely for solar cells and thin-film transistors. In pure twist grain boundaries the axis around which the crystals are rotated, is perpendicular to the interface. After the two crystals have been put into contact the atoms at the interface will self-organize into their minimum energy configuration. The atomistic structure of the interface is still considered controversial. The main question is the degree to which various twist grain boundaries are either ordered or disordered.

In this work we are using computational methods to study the atomistic structure of twist grain boundaries of different rotation angles. We are interested in knowing if the interface of all grain boundaries is comprised of a thin amorphous layer, or if there are certain angles for which the interface is crystalline.

Using molecular dynamics methods we have found crystalline structures for several twist grain boundaries in silicon. We have found that some boundaries are formed out of the same basic building blocks which are called structural units. The main degree of freedom that has to be taken into account, in order to find these boundaries, is the number of atoms at the interface. These results are supported by experimental evidence since these grain boundaries have been measured to have a low grain boundary energy. We have also validated the model by calculating the energy for some of the structures using ab initio methods. These results contradict some previous computational studies which suggested that all grain boundaries are amorphous. These structures have never before to this authors knowledge been presented previously, and as such are of great interest.

Figure 17: A twist grain boundary, Σ25, with a misorientation angle of 16° is plotted from three directions, a plan view and two side views. When ΔN=47 atoms have been removed from the ideal Σ25 twist grain boundary a new ordered low energy state is formed comprising structural units. The two structural units are highlighted by a light gray background.

Figure 18: Four twist grain boundaries with a misorientation angle of 23° are plotted in a plan view. By altering the density of atoms at the interface (ΔN) we find that structural units can form a variety of different low energy structures.
Mechanical Properties of Carbon Nanotubes

Researchers: Maria Sammallorpi, Kaisa Kauto, Antti Kuronen, and Kimmo Kaski

Carbon nanotubes are cylindrical all-carbon molecules composed of concentric graphitic shells with extremely strong covalent bonding of atoms within the shells but very weak van der Waals type interaction between them. Due to the unique atomic structure nanotubes have exceptional electronic and mechanical properties which imply a broad range of possible applications as constituents of nanometer-scale devices and novel composite materials.

The properties of a carbon nanotube depend on the local atomic configuration and defects. For composite and device development it is essential to understand how structural changes affect the properties and our work strives after shedding some more light on the occurring phenomena. Current projects concentrate on evaluating irradiation and irradiation induced defects as a means to improve carbon nanotube strength, load transfer and inter-shell friction. The tools employed are both classical molecular dynamics and dynamical tight binding methods. Fig. 19 shows an example of a defect typical to irradiation and how such defects can link tubes which efficiently prevents tube-tube slippage.

Figure 19: Left: A defect typical to irradiation, a vacancy. Right: Example of a nanotube bundle in which the nanotubes are linked together by the presence of vacancies.
Theoretical Particle Distributions on Curved Surfaces

Researchers: Kaisa Kautto, Maria Sammalkorpi, Adrian Sutton, and Kimmo Kaski

This work has been motivated by the general lack of knowledge concerning the analytic influence of surface curvature on the distribution of particles on the surface. This is relevant for understanding many optimal packing related problems of materials science, for example, biomolecular packings, changes in the vicinity of dislocations and, as in here, nanostructures of carbon. The long term aim of the work is to be able to model deformed carbon nanotubes. This involves understanding uniform distributions of points on curved surfaces and the connection between these distributions and atomic structures. The simplest curved surface is the sphere and therefore we started the analysis by considering the spherical fullerene C60. This carbon structure also known as the buckminsterfullerene corresponds to the uniform distribution of 32 points on a sphere. Studies have also been extended to ellipsoidal surfaces and to the analysis of uniform point distributions of other than 32 points.

Figure 20: A structure (on the left) that is closely related to the atomic configuration of the fullerene C_{60} is obtained as the dual, or Voronoi diagram, of the uniform distribution of 32 points on a sphere (on the right).
Computational modelling and analysis of DNA’s elastic behaviour

Researchers: Riku Linna, Julia Yeomans*, and Kimmo Kaski
*Rudolf Peierls Centre for Theoretical Physics, Oxford University, UK

Polymer deformations in a solvent under perturbations is a fundamental problem. The elastic behaviour of DNA is of crucial importance in understanding complex biological processes such as polymer folding. Computational modelling seems the only feasible option in attempting to explain the sometimes contradicting experimental results on DNA stretching. The approach taken is one of finding the underlying generic features and mechanisms by implementing and using a computational model based on coarse-grained description of the solvent, so called Stochastic Rotation Dynamics (SRD), and using and comparing different general polymer models. SRD is one of the very few computational methods that take hydrodynamic interactions correctly into account.

The elastic characterisation and analysis of the generic model polymers under two mechanical forcing schemes, constant-force and constant-extension stretching, and under Poisseuelle flow were performed. The results show that DNA extension under these different schemes can be described in unified and very general framework omitting the details of the DNA structure. For example the experimental scaling of DNA with the length $L$ under flow was obtained for the first time computationally with excellent precision, see Fig 21.

![Figure 21](image)

Figure 21: (a) The ratio of the projected length $z$ and the contour length $L$ as a function of $v \times L^{0.59}$, where $v$ is the flow velocity. Contour lengths (number of beads) are 50 (+), 100 (x), and 200 (*). The coefficients $k$ for the lines $v = k \Delta p$ are 6, 6.6, and 7.2.
Transition from driven diffusion to ballistic flow in 2D nanofluid


*Rudolf Peierls Centre for Theoretical Physics, Oxford University, UK

Microfluidics has recently become a subject of great interest, as recent experimental successes in controlling the flow of µLitre sized droplets of fluid has generated the anticipation of a wide range of industrial applications. We are investigating the transfer of fluid nanodroplets across i.e. chemically patterned surfaces. The computational method implemented and used is the so called N-Fold Monte Carlo method which performs well for processes at relatively low temperatures.

A transition from diffusion of individual lattice gas particles to a ballistic motion of the whole droplet across step edges has been found. The control parameter for the transition was found to be the step potential, and a finite-size scaling approach is being applied for the analysis. The droplet assumes varying shapes at different control parameter values when crossing the step edge, Fig 22.

Figure 22: A droplet originally located in the lower half of the substrate crossing the step edge down the step potential to the upper half.
5.2.2 Research in Biophysics, Soft Materials and Pattern Formation

The soft matter and biophysics group started at LCE in September 2000. In general, the research is geared towards the interface between condensed matter physics, biology and material science. The great diversity of these systems, ranging, for instance, from complexes of DNA and cationic liposomes used in gene transfer to unexpected morphological evolution of polymers under shear flow and to pattern formation in biological processes, provides new challenges in both fundamental and applied research.

Typically, biological processes take place under non-equilibrium conditions. Modeling these processes provides many theoretical challenges since eventually the validity of equilibrium concepts, such as universality and scaling laws, breaks down. It is important to study their range of validity, and how the emergence of new time and length scales, and possibly a steady state, is manifested in dynamical systems. A good example of that is the shear flow behavior of complex fluids where the dynamics of order-disorder transition depends intimately on the application of shear. As vast number of industrial processes involve complex fluids and polymer mixtures under shear flow conditions, it is clear that a better theoretical understanding of these processes has immediate practical applications.

Another challenge arises from the interdisciplinary nature of these problems. A strong interaction between theory, computation, and experiments is essential in order to get insight into the physical mechanisms producing these complex, often collective, phenomena. A clear example of this is the study of lipoplexes, i.e., the formation and behavior of DNA-cationic liposome complexes. There exists a large amount of experimental data, and in vivo experiments have shown that clinical application of lipoplexes is effective and safe. However, the processes and physical mechanisms, e.g., those involving interactions of electrostatic origin, that control the formation of these complex structures are not well established. Theoretical studies and, in particular, simulational studies, have the potential of helping to characterize better these complex processes.

The studies introduced below briefly describe our efforts in soft matter and biophysics. For details and up-to-date information, please see the corresponding project home page as given in connection of each project.

The group has been very active during its young life and at the end 2003 the Biological Physics Team consisting of our group together with Dr. Ilpo Vattulainen’s group at the Laboratory of Physics was selected as a Helsinki University of Technology Young Center of Excellence for 2004-2005 (in Finnish: tutkimuksen kärkiryhmä).
It is difficult to overestimate the importance of transmembrane proteins in the biological membranes. Membrane bound proteins control many aspects of cell life: signalling, structural integrity of the cytoskeleton, enzymes and to form channels and facilitate the passage of molecular species into and out of the cell. These studies investigate the behaviour of these nanopores, focusing on phenomena such as anaesthesia and biosensing.

Molecular dynamics simulations of lipid bilayers exposed to an anaesthetic gas are the first step towards the justification of the hypothesis that the key to the mechanism of some anaesthetics lies not in their interaction with binding sites, but in the effect that they have on the cell membrane and on integral proteins embedded within a model membrane. These channels are able to modify the efficiency of ion diffusion through the bilayer. Which in turn such affects may control the potential across the membrane. This voltage across the bilayer is essential for nerve impulses to be conducted along a neuron. Hence, modifications in the lipid bilayer can be directly related to anaesthetic effects.

In the present simulations, the effect of anaesthetic gas is quantified by measurable quantities such as the geometric conformation of parts of the system, order parameters, the area per lipid and radial distribution functions. These properties can help in the formation of a description of the local environment of a protein in a cell membrane under various conditions.

![Simulation snapshot illustrating the accommodation of xenon gas in the cell membrane](image-url)
Dielectric responses of graded materials

Researchers: Lei Dong, Mikko Karttunen, and K. W. Yu *
*Physics Department, The Chinese University of Hong Kong, Hong Kong

Project home page: http://www.softsimu.org

Analysis and manipulation of cell populations and submicrometer particles are essential in many practical applications spanning from identification of cancerous cells to chemical analysis of environmental pollutants. Dielectric properties of particles depend on the nature of their surface, e.g., size, shape, and charge density. This is why these methods are important in, e.g., diagnostics. For example, since the composition and shape of cancer cells differ from those of healthy cells, these differences are reflected in their dielectric characteristics which can be exploited in identifying them. We generalize the Bergman-Milton spectral representation, to extract the spectral density function for the effective dielectric constant of a graded composite. Moreover, we apply our theory to a special case, multilayer material, which is more convenient to fabricate in the experiments. After the data analysis (figure below), we obtained that there are always \( N \) sharp peaks for \( N \) layers, and one smooth curve with \( N \to \infty \).

![Spectral density function of various multilayer film.](image)

Figure 24: Spectral density function of various multilayer film.
5.2.3 Research on engineered nanosystems for electronic, photonic, and biosensing applications

Project homepage: http://www.lce.hut.fi/research/eas/nanosystems/

The research of micro- and nanoelectronic materials and devices is getting a wider interface with problems of molecular and cell biology and medicine. This offers a manifold of new challenges for multidisciplinary theoretical research and computational science. Accordingly we are extending our research to biosensing systems and other fields combining information and communication technologies and systems biology. At micro- and nanoscale the interaction of semiconductor, polymer and metallic surfaces with molecular level biosystems and the modulation of this interaction with microscopic voltage probes, light or chemical agents will be subject of extending research in the next years.

Information storage and communication systems utilizing quantum and all-optical devices are areas where fundamentally new nanomaterials and their technological applications are being worked out. In these areas we have continued to work in the field of fast all-optical devices. Research on nonlinear optical materials, coherent nonlinear systems and light-induced quantum effects will be crucial in the development of future all-optical information processing. Related to optical communications, we are have introduced a new fast coherent all-optical flip-flop memory. In nonlinear materials we have studied carrier dynamics in quantum dots excited simultaneously by terahertz radiation from a free electron laser and an Ar-ion laser. The theoretical model and simulations are used to analyse recent experiments at UCSB. This work involves also collaboration with University of Tokyo.

Photonic crystals are periodic dielectric structures for which the period is of the order of the wavelength of light. Photonic crystals exhibit band gaps for light as a result of interference. Light with a frequency inside the band gap cannot exist in the photonic crystal. In this a area Ms Anu Huttunen has completed his doctoral thesis "Analysis and optimization of photonic crystal components for optical telecommunications" under supervision of prof. Päivi Törmä from University of Jyväskylä.

Recently started research of low power biomorphic neural circuits based on floating gate MOS and SET transistors has been continued. In this project neuro-MOS and neuro-SET based neural networks are developed and studied, especially for fast and power efficient signal processing. Neuro-MOS structures, including MOS capacitor based, and neuro-SET structures, are studied and optimized in deep sub-micron line width processes. Power optimisation will be studied, based on physical and architectural ideas from extremely power-efficient biological neurons. New efficient algorithms utilizing the benefits of neuro-structures are developed. Models for simulation of neuro-SET structures are developed. The applicability of floating gate structures - either MOS or SET - to higher level neural architectures, e.g. recurrent or CNN, has been studied.
The commercial integrated electronics is mainly based on silicon, while compound semiconductors (CS), e.g. gallium arsenide, are used in very special applications. For example light detectors, light emitters and very-high frequency devices are usually fabricated using CS due to the better optical and electron mobility properties of these materials. Quantum mechanical devices are a potential application for CS. For quantum mechanical operation phase coherence is crucial and it has been found difficult to obtain long phase coherence lengths in Si structures. This advantages of CS is due to both a different fabrication technique and different electronic properties. We are studying quantum effect electronics both in silicon and CS. The motivations are lower power consumption, faster operation and smaller device size.

We are developing general tools for strain analysis, band structure calculations and the modeling of photonic processes. The final aim is to model photonic and electronic devices starting from the structural properties and ending up with more macroscopic properties like the light amplification in the device. We simulate the strain field using the finite element model (FEM) and the electronic structure using the eight-band $k \cdot p$ model. The material gain of the laser device is obtained from a numerical integration scheme based on the electronic structure and Fermi distributions of the charge carriers. Hence, the optical properties rely completely on the underlying electronic bands, which in turn depend on the device geometry and crystal orientation.

In particular we have been modeling the material gain in quantum well lasers and its dependence on the polarization of the laser field. We have studied the effect of the carrier concentrations, the temperature, and the orientation of the QW etc. Figure 25(a) and (b) show the temperature dependence of the transverse magnetic (TM) and transverse electric (TE) field polarizations of the gain in a 10 nm wide, lattice-matched Ga$_{0.47}$In$_{0.53}$As/Al$_{0.48}$In$_{0.52}$As (001) QW for (a) TM and (b) TE polarizations. The insets show the definitions of the polarization with respect to the quantum well (QW) plane.

![Figure 25](image-url)
**Strain-induced quantum dots**

We have studied strain-induced quantum dots (SIQD) which are formed in InGaAs QW’s by the strain field of a InP stressor island above the QW. Figure 26(a) shows the geometry of a typical SIQD. The local strain field lowers the band edge of the QW near the island, forming a potential minimum of both electrons and holes. The stressor island induces also a strong piezo-electric potential, which considerably modifies the SIQD eigenstates and the carrier dynamics.

We have calculated the strain field and the electronic structure of these SIQD’s using the finite element method and the eight-band $k \cdot p$ technique. We have shown that the piezoelectric potential induces strong potential minima in the valence band. Figure 26(b) shows the potential profile of a SIQD. We have furthermore modeled the dynamics of the SIQD carrier population under the influence of a low-energy THz radiation. These minima play a considerable role in the carrier relaxation and recombination from the SIQD’s. Figure 27 shows schematically how the charge carrier relax through the piezo-electrically induced side minima to the actual QD.

![Figure 26](image1.png)

Figure 26: (a) Strain-induced quantum dot. The InP island is typically 15…25 nm high and 60…100 nm in diameter. The QW is typically 6.5…10 nm thick. (b) Numerical (solid) and experimental (dashed, Solid-State Electron. 40, 601 (1996)) photoluminescence of SIQD’s.

![Figure 27](image2.png)

Figure 27: Schematic recombination (green arrows) and relaxation (black arrows) model of a SIQD. The red arrows represent external laser pumping.
Modelling optical components for access networks

Researchers: Jani Oksanen and Jukka Tulkki

In the long haul network backbone where complex logical operations, like routing, are not needed, electrical components have been superseded by optical ones during the last decade. This has enabled an enormous boost in the data rates of the backbone, but left the electronic solutions in the metropolitan area and access networks outdated. However, to date there are no technologically viable solutions for replacing all the electronics by optics. This project concentrates on constructing models and ideas for new all-optical devices, with the needs of the access networks in mind.

In the project we have this far investigated 1) the differences of the quantum well and dot lasers with respect to their chirp under direct current modulation, 2) the operation of an optical amplifier linearized using gain clamping in vertical direction (also known as linear optical amplifier, or LOA), 3) the use of quantum cascade lasers in free space optical communications 4) all-optical signal regeneration using partly coherent laser networks and 5) all-optical flip-flop memories and decision circuits essentially based on coherent feedback between two laser amplifiers.

The above devices are studied using analytical and numerical models ranging from band structure calculations to stochastic rate equations.

![Figure 28: a) A schematic representation of an optical flip-flop memory realized with laser amplifiers and coherent feedback. The optical isolator in the image are used for clarity only. The complete structure comprises only of lasers, band pass filters and interferometers. b) The operation of the flip-flop. Applying an input to the set (reset) port sets (resets) the flip-flop. The advantage of the structure is that the lasers are operated above their lasing threshold and their response time is therefore enhanced.](image)
Quantum Transport in the Ballistic Conductors

Researchers: Fredrik Boxberg, Teppo Häyrynen and Jukka Tulkki

If electrons move through a conducting device without scattering the transport of electrons is ballistic. Ballistic transport is observed when the length of the channel is small compared to the mean free path of an electron. In the ballistic transport regime a device can be modeled in terms of transmission probabilities which are calculated for different combinations of source and drain eigenmodes.

We have used the mode matching (MM) method within the Landauer-Büttiker formalism to calculate the conductance of a silicon on insulator (SOI) quantum point contact (QPC).

We have calculated how the strain affects to the conductance in the QPC due to the changes in the electron eigenstates (see Fig. 29).

(a) The strain-induced potential profile of the QPC. (b) The potential for electrons in 001 minima at 7 nm above the bottom. (c) The cross-sectional potential in the middle of the QPC. (d) The cross-sectional potential at the end of the QPC.

Figure 29: The effect of oxidation-induced strain on the conductance of the QPC.
**Research on biomorphic single electron circuits**

Researchers: Teppo Häyrynen and Jukka Tulkki

Our goal is to enhance the computational power with the circuit models that imitate the systems in nature.

Although noise is always present in biological systems those can perform complex tasks robustly with low energy consumption.

Analog parallel circuits may offer fast, energy efficient and robust system for computing.

In Fig. 30 we show a voltage characteristics of a single electron A/D/A circuit which can be used for signal level restoration and noise reduction after analog computing stages.

![Figure 30: The voltage characteristics of the single electron A/D/A converter.](image)
5.2.4 Photonic Crystal Fibers

Researchers: Anu Huttunen and Päivi Törmä

Photonic crystals are periodic dielectric structures for which the period is of the order of the wavelength of light. Photonic crystals exhibit band gaps for light as a result of interference. Light with a frequency inside the band gap cannot exist in the photonic crystal. Photonic crystal fiber has a photonic crystal cladding, i.e., the cladding of the fiber is periodic in the plane that is perpendicular to the direction of propagation of light in the fiber [see Fig. 31(a)]. Many of the limits of fiber optics have been overcome with this new class of fibers.

We study photonic crystal fibers that are used as fiber amplifiers. In high-gain efficiency fiber amplifiers, the overlap between the light distribution and the doped area of the fiber is maximized, and thus they usually have small mode areas. Photonic crystal fibers with small mode areas have relatively large dispersion and nonlinearity, and these parameters also depend strongly on the wavelength. The effect of the wavelength dependence of gain, nonlinearity and dispersion in high-gain efficiency photonic crystal fiber amplifiers was investigated using the optical nonlinear Schrödinger equation. The wavelength dependence of the parameters was shown to create asymmetry to the spectrum and chirp, but to have a moderating effect on the pulse broadening.

Figure 31: (a) Cross section of a photonic crystal fiber. (b) Pulse shape after it has propagated 10 cm in the photonic crystal fiber amplifier. Blue curve represents the simulation with wavelength dependent parameters and red dashed curve with constant parameters.
5.3 Cognitive Science and Technology

Cognitive Science and Technology Group studies human neurocognitive mechanisms and develops methods for brain signal analysis (see section 5.1.2). On the basis of the results obtained we also construct system level models, which can guide future experiments and provide ideas for automatic recognition and synthesis of, for instance, audiovisual speech. Neural basis of cognition is studied using electroencephalography (EEG), magnetoencephalography (MEG) and functional Magnetic Resonance Imaging (fMRI). Psychophysical and EEG experiments are conducted in our research laboratories located in the fourth floor of the HUT’s new Magnet House, and fMRI studies using a 3-T MRI device (General Electric 3T Signa, with Excite update) in the Advanced Magnetic Imaging (AMI) Centre, located in the Magnet House at the HUT campus. MEG is recorded using the whole-head neuromagnetometers (Vectorview, Neuromag Ltd) of the HUT’s Low Temperature Laboratory and the Biomag laboratory of the Helsinki University Hospital. Our brain signal analysis methods development work aims at capitalizing on the complementary information provided by MEG, EEG, and fMRI to significantly enhance the spatiotemporal accuracy in our cognitive neuroimaging efforts. Following the principles of neuroinformatics, we are also committed to making our tools as well as data freely available to benefit the greater neuroscience community. Together with Computational Information Technology group we are developing Brain-Computer interfaces. This research is described in section 5.1.2.

We aim to develop an integrated theoretical model to predict how dynamic interactions within and between brain areas, as disclosed by data obtained using complementary non-invasive neuroimaging and psychophysical measures, give rise to emotion-motivated (goal-directed) audio-visual selective attention. In 2005, there were a number of research highlights that are briefly summarized below.
5.3.1 Neural basis of speech perception

Researchers: Iiro Jääskeläinen, Jaakko Kauramäki, Daniel Kislyuk, Virpi Lindroos, Riikka Möttönen, Ville Ojanen, Johanna Pekkola, Mikko Sams, Kaisa Tiippana

Processing of sine-wave speech in the human brain: neural mechanisms

According to previous neuroimaging studies, brain areas critical for speech perception are localized within the left posterior temporal cortex. However, since speech sounds are acoustically different from other sounds, it is possible that the assumed speech-specific activity reflected sensitivity to the complex acoustic structure of speech sounds. In our recently published study (Möttönen et al. Neuroimage 2005) we used "sine wave speech" (SWS) stimuli, which can be perceived as speech or non-speech depending on previous experience of the stimuli, to study neural speech-specificity. We scanned subjects using 3T functional MRI in two sessions, each including SWS, control stimuli, with an intervening period of speech training. In the pre-training session, subjects perceived the SWS stimuli as non-speech, and in the post-training session, the identical stimuli were perceived as speech. Activity elicited by SWS stimuli was significantly greater in the post- vs. pre-training session within left posterior superior temporal sulcus (STS), while activity elicited by the control stimuli, which were always perceived as non-speech, did not change during the whole experiment (see Fig.32). We conclude that left posterior STS subserves neural processing specific for speech perception. This study was done in collaboration with the FMRIB Centre in the University of Oxford.

Figure 32: Speech-specific activation in the left posterior STS. The left side of the figure shows the region, which was activated more in the post- than in the pre-training session for the SWS stimuli. The analysis was carried out within a left superior temporal ROI (indicated as blue). Statistical images were thresholded using clusters determined by $Z > 2.3$ and a cluster significance threshold of $P < 0.05$, corrected for multiple comparisons across the ROI. The right side of the figure depicts the mean (±SEM) BOLD signal changes in the left posterior STS for all stimulus types in the pre- and post-speech training sessions ($n = 16$). The statistical significances are indicated. Modified from Möttönen et al. (in press Neuroimage 2005).
Processing of audiovisual speech in the Broca’s area

We investigated neural mechanisms underlying processing of audiovisual phonetic information in humans using functional magnetic resonance imaging (fMRI) (Ojanen et al. Neuroimage 2005). Ten healthy volunteers were scanned with a ‘clustered volume acquisition’ paradigm at 3T during presentation of phonetically congruent and incongruent audiovisual vowels /a/, /o/, /i/ and /y/. Comparing activations to congruent and incongruent audiovisual vowels enabled us to specifically map the cerebral areas participating in the audiovisual speech processing at the phonetic level. Phonetic incongruency (e.g., visual /a/ and auditory /y/), as compared with congruency (e.g., visual and auditory /y/), significantly activated the Broca’s area, the prefrontal cortex and the superior parietal lobule in the left hemisphere (see Fig. 33). In contrast, we failed to see any enhanced activity to phonetically congruent stimulation in comparison to the incongruent stimulation. Our results highlight the role of the Broca’s area in the processing of audiovisual speech and suggest that it might provide a common representational space for auditory and visual speech.

Figure 33: Across-subjects (N=10) z-statistic maps overlaid on an anatomical template. Congruent audiovisual speech activated the auditory and the visual cortical areas, as well as the inferior frontal, the premotor and the visual-parietal areas bilaterally (upper panel). Incongruent audiovisual speech caused a similar but more extensive pattern of brain activity (middle panel). The difference reached significance in three left hemisphere areas: Broca’s area (BA44/45), superior parietal lobule (BA7) and prefrontal cortex (BA10) (lower panel). In the contrast ‘Congruent > Incongruent’ no statistically significant voxels were detected. Activation images were thresholded using clusters determined by voxel-wise Z>3.0 and a cluster significance threshold of p<0.05, corrected for multiple comparisons. (Ojanen et al. in press Neuroimage).
In a further study (Ojanen et al. submitted 2005), we investigated the neural basis of auditory and visual speech processing using a "clustered volume acquisition" functional magnetic resonance imaging (fMRI) pulse sequence at 3T (see Fig. 34). Common activation areas to presentation of auditory and visual vowels were observed in the left Insula, the Broca’s area, the lateral premotor cortex, and the inferior parietal area as well as the right superior temporal gyrus/sulcus. Significantly stronger activation for visual than auditory speech was observed in the left motor and sensory areas, inferior parietal lobule, posterior cingulate gyrus and visual sensory specific areas. Significantly stronger activation for auditory speech, in turn, was observed in the left lingual gyrus, the left insula, anterior cingulate bilaterally and auditory sensory specific areas. These results suggest that the speech motor areas, in addition to Broca’s area, provide a common representational space for auditory and visual speech.

Indeed, the ability to internally simulate other persons’ actions is important for social interaction. In monkeys, neurons in the premotor cortex are activated both when the monkey performs mouth or hand actions and when it views or listens to actions made by others. Neuronal circuits with similar “mirror-neuron” properties probably exist in the human Broca’s area and primary motor cortex. Viewing other person’s hand actions also modulates activity in the primary somatosensory cortex SI, suggesting that the SI cortex is related to the human mirror-neuron system. Viewing other person’s hand actions also modulates activity in the primary somatosensory cortex SI, suggesting that the SI cortex is related to the human mirror-neuron system. To study the selectivity of the SI activation during action viewing, we stimulated the lower lip (with tactile pulses) and the median nerves (with electric pulses) in eight subjects to activate their SI mouth and hand cortices while the subjects either rested, listened to other person’s speech, viewed her articulatory gestures, or executed mouth movements (Möttönen et al. Neuroimage 2005b). 55-ms SI MEG responses to lip stimuli were enhanced by 16% (P<0.01) in the left hemisphere during speech viewing whereas listening to speech did not modulate these responses. The 35-ms responses to median-nerve stimulation remained stable during speech viewing and listening. Own mouth movements suppressed responses to lip stimuli bilaterally by 74% (P<0.001), without any effect on responses to median-nerve stimuli. Our findings show that viewing another person’s articulatory gestures activates the left SI cortex in a somatotopic manner. The results provide further evidence for the view that SI is involved in “mirroring” of other persons’ actions.

In a psychophysical study (Möttönen et al. Cognitive Brain Research 2005), we investigated modification of auditory perception in three different conditions in twenty subjects: 1) observing other person’s discordant articulatory gestures deteriorated identification of acoustic speech stimuli and modified the auditory percept, causing a strong McGurk effect. A similar effect was found when 2) the subjects watched their own silent articulation in a mirror and acoustic stimuli were simultaneously presented to their ears. Interestingly, a smaller but significant effect was even obtained when 3) the subjects just silently articulated the syllables without visual feedback. On the other hand, observing other person’s or one’s own concordant articulation and silently articulating a concordant syllable improved identification of the acoustic stimuli. The modification of auditory percepts caused by visual observation of speech and silently articulating it are both suggested to be due to the alteration of activity in the auditory cortex. These findings support the results of our neuroimaging studies suggesting that there is a close relationship between speech perception and production.

Recent studies have yielded contradictory evidence on whether visual speech perception (watching articulatory gestures) can activate the human primary auditory cortex in addition to secondary auditory areas and the speech motor regions. To circumvent confounds due to inter-individual anatomical variation, we defined our subjects’ Heschl’s gyri and assessed blood oxygenation-dependent signal changes at 3 T within this confined region during visual
speech perception and observation of moving circles (Pekkola et al. NeuroReport 2005). Visual speech perception activated Heschl’s gyri in nine subjects, with activation in seven of them extending to the area of primary auditory cortex (see Fig. 34). Activation was significantly stronger during visual speech perception than during observation of the moving circles. Further, a significant hemisphere by stimulus interaction occurred, suggesting left Heschl’s gyrus specialization for visual speech processing.

Figure 34: Watching speech activates primary auditory cortex. Significant (Z>2.3, p<0.01, corrected), activations during visual speech perception within Heschl’s gyri (HG) are shown, overlaid on axial MR images. The yellow line outlines HG, the medial parts of which accommodate primary auditory cortex. The statistical parametric maps and the HG outline are collapsed into a 2D plane. The middle column displays coronal, axial, and left sagittal high-resolution MR images of subject 6 with overlaid activations.
Perception of matching and conflicting audiovisual speech in dyslexia as assessed using functional MRI

As a clinical research application of our audiovisual speech research, we presented phonetically matching and conflicting audiovisual vowels to ten dyslexic and ten fluent-reading young adults during "clustered volume acquisition" functional magnetic resonance imaging (fMRI) at 3 Tesla (Pekkola et al. in press Neuroimage 2005). We further assessed co-variation between the dyslexic readers' phonological processing abilities, as indexed by neuropsychological test scores, and BOLD signal changes within visual cortex, auditory cortex, and Broca’s area. Both dyslexic and fluent readers showed increased activation during observation of phonetically conflicting compared to matching vowels within the classical motor speech regions (Broca’s area and the left premotor cortex), this activation difference being more extensive and bilateral in the dyslexic group. The between-groups activation difference in the conflicting > matching contrast reached significance in the motor speech regions and in the left inferior parietal lobule, with dyslexic readers exhibiting stronger activation compared to fluent readers (see Fig. 35). The dyslexic readers’ BOLD signal change co-varied with their phonological processing abilities within the visual cortex and Broca’s area, and to a lesser extent within the auditory cortex. We suggest the findings to reflect dyslexic readers’ greater use of motor-articulatory and visual strategies during phonetic processing of audiovisual speech, possibly in order to compensate for their difficulties in auditory speech perception.

Figure 35: Significant activation differences between dyslexic and fluent readers during matching and conflicting stimulation, with dyslexic readers showing stronger activation during both conditions. Dyslexic readers’ stronger activation within basal ganglia, cerebellar vermis, and ventral visual cortex is situated in deeper brain structures and thus not shown in these surface reconstructions. SMA = supplementary motor area, AC = anterior cingulate cortex.
5.3.2 Neural basis of selective attention

Researchers: Jyrki Ahveninen, Marja Balk, Iiro Jääskeläinen, Jaakko Kauramäki, Mikko Sams

We studied the effects of sound presentation rate and attention on supratemporal cortex (STC) activation with 3-Tesla functional magnetic resonance imaging (fMRI) in 12 healthy adults (Rinne et al. Human Brain Mapping 2005). The sounds were presented at steady rates of 0.5, 1, 1.7, 2, or 4 Hz while subjects either had to focus their attention to the sounds or were to ignore the sounds and attend to visual stimuli presented with a mean rate of 1 Hz in all conditions. Consistently with previous results obtained in separate studies, we found that both increase in the stimulation rate and attention to sounds enhanced activity in bilateral STC. Further, we observed larger attention effects with higher stimulation rates (see Fig. 36). Our results separate the rate-dependent and attention related modulation of STC activation and indicate that both factors should be controlled in fMRI studies on auditory processing.

Figure 36: LEFT: sounds activated STC bilaterally. Contrasts between all rates of both conditions vs. baseline are shown. RIGHT: Mean ±SEM percent changes of activation across conditions within the ROI shown on the left disclose a significant attention vs. rate interaction.

Observing a speaker’s articulatory gestures can contribute considerably to auditory speech perception. At the level of neural events, seen articulatory gestures can modify auditory cortex responses to speech sounds and modulate auditory cortex activity also in the absence of heard speech. Possible effects of neural events on this modulation have, however, remained unclear. To investigate the effect of attention on visual speech-induced auditory cortex activity, we scanned ten healthy volunteers with functional magnetic resonance imaging (fMRI) at 3 Tesla during simultaneous presentation of visual speech gestures and moving geometrical forms, with the instruction to either focus upon or ignore the seen articulations (Pekkola et al. in press Human Brain Mapping 2005). Secondary auditory cortex areas in the bilateral posterior superior temporal gyrus and planum temporale were active both when the articulatory gestures were ignored and when they were attended to. Attention to visual speech gestures, however, enhanced activity in the left planum temporale compared to the situation when the subjects saw identical stimuli but engaged in a non-speech motion discrimination task. These findings suggest that attention to visually perceived speech gestures modulates auditory cortex function, and that this modulation takes place at a hierarchically relatively early processing level.

In our ongoing collaboration with Massachusetts General Hospital / Harvard Medical School NMR Center, we aim at elucidating and modelling the neural mechanisms underlying processing of and selectively attending object and spatial location information. In these studies, we have found that neural ensembles occupying regions posterior to the human primary auditory cortex are specifically tuned to 3-D sound location cues, while processing of
acoustic features of phonemes takes place in areas anterior to HG. Further, we observed that selective attention to sound location features selectively "sharpened" the 3-D location tuning of the underlying neurons (Ahveninen et al. submitted 2005). These studies were conducted at our collaborative laboratory, the Massachusetts General Hospital - Harvard Medical School - Massachusetts Institute of Technology Athinoula A. Martinos Center for Biomedical Imaging in collaboration with Drs. Jyrki Ahveninen, Tommi Raij, Sari Levänen, Matti Hämäläinen and John W. Belliveau.

During 2005 we also explored and modelled audiovisual illusions induced by rapid flashes and beeps; spatially and temporally coincident auditory and visual information is often bound together to multi-sensory percepts. Shams et al. (2000) have reported an audiovisual fission illusion where a single flash is perceived as two when two rapid tone beeps are presented concurrently. We have extended their findings, and modelled the illusion for the first time. Using an experimental set-up very similar to that of Shams et al, we have shown the existence both fusion and fission illusions. The latter is a novel finding where two flashes are perceived as one when accompanied by one beep. Furthermore, by instructing subjects to count beeps rather than flashes and decreasing the sound intensity to near threshold, we have also discovered a corresponding visually induced auditory illusion. We have modelled these phenomena with Maximum Likelihood Integration (MLI). MLI models are theoretically attractive because the goals and assumptions of sensory information processing are explicitly stated in such optimal models. When subjects perceive stimuli categorically, as opposed to on a continuous scale, MLI can occur before or after categorization, i.e., early or late. We have shown that early MLI is a categorization early or late. We have shown that early MLI is a better fitting and more parsimonious model than late MLI, suggesting that integration occurs before categorization. Finally, we have also shown that, unlike many other multisensory phenomena, this illusion is insensitive to the relative locations of auditory and visual stimuli.
5.3.3 Emotion perception and processing

Researchers: Marja Balk, Michael Frydrych, Jari Kätsyri, Mikko Sams, Mikko Viinikainen

In our research we have studied how people recognize and process emotions both from facial expressions and other emotional stimuli.

We have recorded a collection of posed emotional facial expressions containing video sequences of six basic emotions (anger, disgust, fear, happiness, sadness and surprise) from six Finnish actors. We conducted an evaluation study with 16 subjects to evaluate how well the basic emotions were recognized from our collection and from pictures selected from a standard facial affect collection.

Figure 37: The results show that disgusted emotions were recognized more accurately and fearful emotions less accurately from our (TKK) collection than from the standard (Ekman-Friesen) collection.

In another study with our collection, we compared the effect of controlled degrading (low-pass filtering) and motion on the recognition of basic emotions by subjects with Asperger Syndrome (AS) and neurotypical subjects. Our preliminary results suggest that the AS subjects recognized emotions slightly worse for the most degraded stimuli than the neurotypical subjects but only with still pictures.

We have also initiated dimensional studies with emotion-related pictorial stimuli, using 3T fMRI. Different emotional qualities are processed on specific brain regions.

Figure 38: Emotional intensity of pictures shows significant positive correlations with ventro- and dorsomedial prefrontal cortex (VMPFC, DMPFC) and posterior cingulate cortex (PCC) and negative correlation with right dorsolateral prefrontal cortex (DLPFC). Group, Bonferroni corrected p < 0.05.
5.4 Complex Systems and Networks

In the recent years we have seen much progress in the analysis, modelling, and theoretical studies of complex systems, with the result that seemingly very different systems share similar characteristics. Typically, these natural, social, and man-made systems comprise highly interconnected parts on many scales. Examples include financial markets, biological regulatory networks, and the Internet to mention a few. In such systems, the interaction patterns and topology can be highly intricate. Together with stochasticity, these often result in emergent system-level behavior, such as self-organisation and pattern formation. The interactions between the constituent elements can also result in highly non-trivial structural properties of the system, such as the scale-freeness of the connectivity distribution discovered in several kinds of network systems.

Complex systems are typically analyzed in an interdisciplinary way from several viewpoints, combining methods and frameworks from e.g. statistical physics, theoretical biology, information theory, game theory and social sciences. Further, computational modelling and large-scale computer simulations are often required. Our research on complex systems focuses on empirical and theoretical studies of the characteristics of complex networks, as well as dynamic phenomena taking place on such networks. We also approach complex systems from an agent-based modelling perspective, e.g. in modelling economic systems and evolutionary games. Studied systems include social networks, networks of disease spreading, and biological systems.
Software Tools for Complex Networks Research

Researchers: Jörkki Hyvönen, Ville Mäkinen

The study of complex networks requires advanced tools for simulations, analysis and visualization. We have developed two software packages, Himmeli for visualizing complex networks, and a c++-software library for fast, memory-efficient analysis and simulations.

-Himmeli A general graph constitutes a multi-dimensional object so to draw it on a flat surface involves a coarse simplification of its nature. In any case, a visualization of an interesting network gives a researcher a glimpse to the abstract mathematical world of complex graphs. Himmeli is designed for the most difficult cases of weighted and densely connected graphs were no regularities can be exploited. The core algorithm is a mix of simulated annealing and molecular dynamics and employs a cell grid memory structure to reduce unnecessary computing. Himmeli can be downloaded at http://www.artemis.kll.helsinki.fi/himmeli/.

-The c++ library. From the computational point of view, network simulations can be extremely demanding. The common methodology calls for computation of ensemble averages over many realizations of networks comprising millions of nodes and edges. In addition, data sets on experimentally observed networks of a similar order of magnitude have recently become available. In order to cope with these challenges, a software library extremely efficient in terms of memory footprint and computational performance has been implemented. In its development, special emphasis has lied on ease of usage. The expressive power of the language has been utilized for e.g. side effects, that is, transparent updating of the data structures taking place when the networks are manipulated. The library is expected to be released to the public under an open-source licence during 2006-2007.

Figure 39: The strongest 4% links in the network of international trade relationships between the world’s countries during year 2000, visualized using Himmeli.
Discovering the structural and dynamical properties of social networks is an inspiring topic of complex networks research that has received much attention in recent years. Our group has had an excellent opportunity to study a very large data set of the network of people communicating over mobile phones. This has brought insight into the structure of social networks and inspired new methods to analyze it. A prominent characteristic of social networks is that they are organized into communities, with dense connections within communities and weaker links between them. Based on these findings, we have developed a network model with similar structure. This model provides a realistic platform for studying sociodynamic phenomena, such as propagation of information and opinion formation.
**Weighted Complex Networks**

Researchers: Jukka-Pekka Onnela, Jari Saramäki, Kimmo Kaski, Gergely Tibély*,
János Kertész*

* Budapest University of Technology and Economics

Complex networks provide a very general framework for studying systems with large numbers of interacting elements. The nodes of the network represent the elements and the links correspond to interactions between them. Studies of network characteristics have produced many unexpected findings, e.g. the ubiquity of scale freeness and the small-world phenomenon. Currently, there is a growing interest in extending the complex networks framework to *weighted* networks, where the edge weights depict the strengths of interactions. This provides researchers with improved tools for understanding the functionality of the complex systems in question.

![Weighted metabolic network of Escherichia coli](image)

**Figure 41**: The weighted metabolic network of Escherichia coli. The nodes correspond to chemicals (metabolites) and they are linked if connected by a metabolic reaction. The weight of the link is associated with the net reaction fluxes between the connected chemicals. We have characterized this network by studying the intensity and coherence of its subgraphs, including paths and cycles. Our results show that inclusion of weights in these types of motif ensemble studies may considerably modify the conclusions drawn from them. The network was visualized using the Himmeli software package.

We have developed generalized weighted measures related to appearance frequency of subgraphs, so-called *motifs*, and the networks’ clustering properties. We have defined two novel characteristics, motif *intensity* and *coherence*, and studied empirical and theoretical networks using these measures. Our research has also focused on percolation methods, where edges are successively removed in order of weight, and the connectivity properties of the remaining network are studied, as well as generalizing current theories on the spectral properties of matrices representing networks. All of the above methods yield information on correlations.

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between the networks’ topology and weights, which can be related to network functionality. So far, these methods have been applied in studies of social networks, market interactions, and biological systems.

**Dynamic Processes on Complex Networks**

Researchers: Jari Saramäki, Jukka-Pekka Onnela, Jörkki Hyvönen, Jussi Kumpula, Tapio Heimo, Antti Niinikoski, Kimmo Kaski

Systems well suited for studies in the complex networks framework are ubiquitous – neural networks, social networks, the Internet, networks of epidemic spreading. The main strength of this approach is its ability to capture the salient features of the systems in question with simple building blocks and then derive system-level properties from their relationships. The most surprising result has been that the systems often share similar properties, such as the common short average vertex-to-vertex distances (the small-world property), scale-free connectivity distributions, and high clustering. The interest in these common properties is twofold: i) network structure carries traces of the evolutionary processes shaping the networks, and ii) dynamics of processes taking place on networks are heavily affected by the structure. Recently, there has been wide interest in dynamic phenomena on networks. Examples include models of opinion formation and the dynamics of spreading via contact processes, such as the propagation of information in social networks and epidemic spreading of disease. During 2005, we have studied several variants of spreading processes. One example is modelling the spreading of influenza-like disease on dynamically changing small-world contact networks (see Fig.42, which has also been extended to a “country model”, where spreading is simulated in individual cities, connected via a traffic network. We have also investigated the case of several simultaneous spreading processes, where e.g. adoption of competing products takes place via word-of-mouth marketing in a social network. In the context of social networks, we study dynamics of searches along the network’s links with noisy information, and the relationship of dynamics of information spreading to the network topology and edge weights.

![Figure 42](image_url)

**Figure 42:** The dynamics of two influenza A epidemics, a) in the US during winter 2001-2002, and b) in the UK during winter 2003-2004. The solid circles indicate laboratory-confirmed weekly cases, and the solid and dashed lines theoretical curves produced by fitting our model to the data. For the dashed lines, only a small number of data points in the beginning of each epidemic were used.
Networks in Econophysics

Researchers: Jukka-Pekka Onnela, Jari Saramäki, Kimmo Kaski, Gergely Tibély*, János Kertész*

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Network theory provides an approach to complex systems with many interacting units, where the details of the interactions are of lesser importance. In the financial market companies interact with one another, creating an evolving complex system. These complicated interactions are reflected in temporal correlations of e.g. stock prices and flows of capital. The goal of our work is to improve our understanding of interdependencies, clustering and dynamics of the financial market.

We have approached the market from a complex networks perspective. The time series of stock returns have been utilized to calculate correlation matrices for set time windows; selecting the strongest correlations yields a weighted “interaction” network depicting interactions during each window. This network can be approached using tools from the complex networks theory. The networks display clear clusters corresponding to industry sectors, and the effect of the 1989 Black Monday is reflected as a shrinking of the overall network topology. Weighted network measures such as cluster intensities and coherences indicate that in most cases intra-cluster interactions are considerably stronger and more coherent than the market as a whole. In addition, the spectral properties of the underlying correlation matrices carry traces of the cluster structure.

Figure 43: Relative intensities of clusters corresponding to industry sectors as function of time. For all cases except Basic Materials the intra-cluster interactions are considerably stronger than those of the whole market. Inset: absolute cluster intensity of the whole market used for normalisation
5.5 Computational Systems Biology

Computational systems biology (CSB) is a rapidly developing field of research with focus to understand structure and processes of biological systems at molecular, cellular, tissue and organ level, through computational modelling and novel information theoretic data- and image analysis methods. With the breakthrough in deciphering the human genome using the most up-to-date computational approaches and modern experimental biotechnology, it has become possible to understand the structure and function of biomolecules, information stored in DNA (bioinformatics) and its expression to proteins, protein structures (proteomics), metabolic pathways and networks, intra- and inter-cell signalling, and the physico-chemical mechanisms involved in them (biophysics). Using the computational information theoretic analysis and modelling methodologies to experimental genotype and phenotype data obtained with for example microarray techniques, gel-based techniques and mass-spectroscopy of proteins, molecular and cell imaging and microscopy, etc., it is possible to understand the structure and function of biosystems. Generally speaking, CSB focuses either on information processing of biological data or on modelling physical and chemical processes of bio-systems. Through this type of quantitative systems approach CSB can play a central role in predicting diseases, preventive medicine, gene technology, pharmaceuticals, and in other biotechnology fields. Because of this potential, the CSB has also been added to the educational curriculum of the Laboratory of Computational Engineering. The aim of this curriculum is to train all-around computational biology experts for research, development, design, consulting, and services in public as well as private sector.

In the Laboratory of Computational Engineering the main focus areas of Computational Systems Biology research are Bioimaging with emphasis on studying e.g. CryoEM of biomolecular assemblies, 3D electron and optical tomography, Gene interaction Networks, and development of new information theoretic imaging methods; Biospectroscopy with emphasis on studying e.g. NMR spectroscopy of lipoproteins and plasma from the biophysics and biomedical perspectives, Clinical diagnostics and molecular aspects of acute coronary syndrome, and development of their analysis methods; Biomolecular modelling with emphasis on studying e.g. biomembranes and biomolecular systems with computational multiscale methods such as Molecular dynamics, Dissipative particle dynamics and Lattice Boltzmann modelling (These are presented above in the section of Computational Materials Research).
Researchers: Sami Brandt, Danai Laksameethanasan, Markos Mevorah, Vibhor Kumar, Ville Lilja, Peter Engelhardt, Jukka Heikkonen, and Kimmo Kaski

The AUTOMATION consortium, financially supported by the Sixth Framework Programme of the European Union, develops a novel imaging system aiming at high-content high-throughput multi-dimensional analysis of microscopic biological structure inside non-adherent living cells. To study structural relationships among bio-molecules, three-dimensional imaging used with a cell-manipulator technology, which smoothly rotates individual, non-adherent living cells in suspension. The three-dimensional imaging techniques are developed to provide multi-dimensional reconstruction of the microstructure inside the cells. The project is coordinated by Dr. Spencer Shorte, Institut Pasteur, France.

Our research group studies two image processing problems involved in the micro-rotation imaging system. First, the 3D motion of a living cell has to be automatically estimated from light microscopic image-series. This problem is related to the discipline of computer vision as the motion, pose, and deformation of the object is to be determined from the image series. Second, the living cell has to be reconstructed from the microscopic, micro-rotation image series. The second part of the research work is closely related to inverse problems especially from the viewpoint of statistical inversion theory and tomography. A long-term aim is to develop motion estimation and reconstruction methods for dynamically deforming, individual living cells.

Figure 44: A stereo view from the reconstruction of prophase chromosomes in a cell mitosis.
Statistical Methods in Vision Geometry

Researchers: Sami Brandt, Kimmo Palander, Jukka Heikkonen

The field of computer vision is aimed at the development of intelligent artificial vision systems, and research on image understanding, image analysis and related areas. The geometric branch of computer vision has been focusing on geometry related problems such as autonomous motion detection, motion estimation, imaging geometry estimation, and 3D reconstruction of the scene. Since the solutions must deal with data corrupted by both measurement noise and outliers, statistical approach can be seen as a most natural approach.

As our recent research activities in geometric vision we have developed affine structure-from-motion algorithms by revisiting the problems of affine reconstruction and affine autocalibration from a statistical viewpoint. Robust estimation is also a related topic that has been considered. Some of the obtained results have been successfully applied in the image alignment problem in electron tomography. In addition, we have considered a novel approach for the dense reconstruction problem from a stereo view pair of a scene.

Figure 45: Reconstructions from the Hotel sequence. (a) An example image, the dataset is from the CMU VASC Image Database. (b) Front-view of the points reconstructed where the affine autocalibration was computed by bundle-adjustment; (c) Top-view of the points.
Image Alignment in Electron Tomography

Researchers: Sami Brandt, Ville Lilja, Vibhor Kumar, Peter Engelhardt, and Jukka Heikkonen

In structural biology, electron tomography is used in reconstructing three-dimensional objects such as macromolecules, viruses, and cellular organelles to learn their three-dimensional structures and properties. The reconstruction is made from a set of transmission electron microscope (TEM) images which may be obtained by tilting the specimen stage by small angular increments (single axis tilting). In order to successfully perform the 3D reconstruction in electron tomography, transmission electron microscope images have to be accurately aligned or registered. The alignment problem can be posed as a motion estimation problem that can be solved by using geometric computer vision methods.

We have developed automatic image alignment methods for electron tomography over six years, and currently we are able to align conventional critical-point-dried samples with similar accuracy level that was previously obtained only by using fiducial gold markers. Our state-of-the-art marker-less, feature-based alignment method (c.f. Fig. 46) is based on tracking certain interest points on the intensity surface of the images by utilising the geometric constraints between views. The development of the alignment algorithms is still going on for wider applicability and to take computational aspects into consideration.

Figure 46: Fig. 1 (3). IET (Immuno Electron Tomography) reconstruction of pretreated chicken fibroblast cells with a brief detergent TX-100 and blocking solution treatment (1-2 min) showing the difference of immuno-labeling with prefixation. With this method intracytoplasmic staining is very prominent. The cells were immunogold-labelled for cytoplasmic structural proteins: vinculin with 3.5 nm and FAP52 (seen as red bigger particles) and with 1.4-nm gold conjugates (seen as red smaller particles) and post-fixed. Vinculin appears widely distributed but also small delicate clusters of 1.4-nm FAP52 labels are clearly distinguished.
Type 1 diabetes and kidney disease: A computational approach to complex data sets

Researchers: Ville-Petteri Mäkinen, Carol Forsblom, Maija Wessman, Kimmo Kaski and Per-Henrik Groop

Type 1 diabetes is the autoimmune variant among disorders in glucose metabolism and has a peak incidence at adolescence. The rapid and exhaustive loss of pancreatic insulin production leads to a life-long dependence on exogeneous insulin to maintain the supply of glucose from blood to tissues. Although the treatment is life-preserving, it cannot entirely match the intricacy of the intact biological system. As a side effect, the body is exposed to various harmful processes, most notably the destruction of kidney cells (diabetic nephropathy) in some patients.

The FinnDiane study, headed by Doc. Per-Henrik Groop from the Folkhälsan Research Centre, aims for the identification and early detection of diabetic complications. As more and more clinical and genetic data is collected on the nearly 5000 patients that are currently participating in the study, the role multi-factorial statistics becomes crucial.

From a genetic point of view, the selection of patients for expensive genotyping studies is of vital importance. For this reason, a new pedigree visualisation software was developed to ease the task of selecting the most informative families. Launched already in 2003, the CraneFoot software, published this year in the European Journal of Human Genetics, has turned out to be a useful tool in data management for numerous researches in Finland and abroad.

Figure 47: A FinnDiane pedigree (left) and a random pedigree (right) with integrated clinical and genetic information.

H NMR Metabonomics for Disease Risk Assessment - Molecular Aspects of Atherothrombosis

Researchers: Jukka Heikkonen, Kimmo Kaski, Niko Lankinen, Ville-Petteri Mäkinen, Aino Salminen, Jari Saramäki, Teemu Suna, Pasi Soininen, Reino Laatikainen, Károly Héberger, Matti Jauhiainen, Petri Ingman, Sanna Mäkelä, Antti Nissinen, Minna Hannuksela, Markku Savolainen, Marja-Riitta Taskinen, Per-Henrik Groop, Mika Ala-Korpela

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Corresponding author

The genomics, transcriptomics and proteomics represent the genome-oriented main discipline in life sciences. Physiology constitutes the triggering of specific functional pathways by environmental signals and thereby, the phenotype of a biological system is largely reflected by its metabolite composition and their interactions. An essential and complementary ‘omics’-approach in understanding of biomolecular function is therefore metabonomics - the quantitative measurement of the time-related multiparametric metabolic responses of multicellular systems to pathophysiological stimuli or genetic modification.

Measuring metabolites is not new. For decades, clinicians have charted chemistries in blood, urine, and other body fluids - e.g., using glucose to track diabetes and cholesterol to monitor heart disease. What is new in the metabonomics approach is that we are now casting a wider net, attempting to gather an unbiased sample of metabolites that can serve as a snapshot of an organism’s physiology. We could also talk about ‘global biochemistry’. The ultimate goal of metabonomics is to be able to distinguish between an individual who is healthy and someone who has (diagnosis) - or might develop (risk assessment) - a disease. In the field of metabonomics, mass and NMR spectroscopy have become the two key technologies. An appealing feature of NMR spectroscopy for metabonomic applications is its specific yet non-selective nature. Particularly, 1H NMR has the advantage of efficiently obtaining information on large numbers of metabolites in biofluids in vitro as well as in various tissues ex vivo and in vivo.

Our biomedical focus is understanding atherothrombosis - the various complex life long processes of harmful lipoprotein particle elevation and their modifications leading to lipid accumulation and potentially to a thrombus formation and a subsequent heart attack. Applications of 1H NMR metabonomics to study human serum are experimentally rather fast and straightforward. Measuring lipoprotein subclass profiles by 1H NMR therefore contrasts favourably to other lipoprotein measurement protocols and is currently receiving wide academic and commercial interest. The independent role of lipoprotein subclasses for the risk assessment and development of atherothrombosis is currently well recognised. We have indeed recently illustrated the inherent suitability of 1H NMR metabonomics for automated studies of lipoprotein subclass related metabolic interactions in a clinically relevant context and demonstrated the power of self-organising map (SOM) analysis in an extensive and representative case of 1H NMR metabonomics (see Fig. 48).
Atherosclerosis is a diffuse systemic disease that is characterised by the local build-up of lipid-rich plaques within the walls of large arteries. The atherothrombotic processes are multi-genetic, being influenced also by dietary and environmental components, and are apparent as early as the second decade in life with an increased incidence in the elderly. Atherothrombosis involves inflammatory processes with an array of metabolic, molecular and cellular manifestations in tissues, e.g., those depicted within the arterial wall in the Figure. A varying degree of these intimal processes are reflected by the biochemistry of body fluids, such as serum. The biological heterogeneity as well as the slow development and progression of pathological conditions make the borderline between 'health' and 'disease' indistinct. One option to approach the problem, as previously presented by us, is 1H NMR metabonomics of serum equipped with a chemometric classifier, e.g., a SOM. On the left in the Figure a hypothetical SOM is shown together with four overlapping clusters that are thought to represent the metabolic changes in the arterial intima. While definite classification as 'healthy' and 'diseased' may not be available by nature, the metabonomics approach with a holistic look at the multidimensional metabolic changes may prove useful in the assessment and follow up of an individual 'health path' (represented by the light green line within the SOM) alongside the interplay between metabolic pathways and their consequences.

It is our main aim to perform extensive metabonomic NMR studies in various clinically relevant sets of serum samples and to develop as well as to apply data analysis approaches capable of detecting differences in the biomolecular status of the individuals in relation to disease risk assessment and diagnosis. We have started our clinically oriented NMR metabonomic applications within two projects: i) alcohol related anti-atherogenic processes and diseases and type 1 diabetes and the risk of diabetic nephropathy and vascular complications. The studies involve systematic linking of various biochemical and biophysical methodologies to study atherothrombosis and lipoprotein related phenomena. This coalition integrates currently approximately 25 scientists, from 8 different institutions, working in close collaboration. Within these studies we will put particular effort toward a comprehensive systems biology approach in which we will be integrating complementary metabolic data from NMR spectroscopy with all available other data of clinical significance (including various clinically utilised biochemical markers, diagnostic data, other spectroscopic data and genetic information).
Our preliminary results in both of the abovementioned application areas have shown that the new 1H NMR metabonomics approach, combined with newly developed multi-factorial statistical analysis methods, is capable of finding clear metabolite alterations in the serum samples of various patient groups. The spectra contain an unforeseen wealth of information on serum metabolites, for example, in relation to type 1 diabetes and diabetic nephropathy. These data provide a systems biology view on metabolism, an aspect that cannot be captured by a handful of conventional clinical variables. It is our intention to develop NMR metabonomics towards increased biomolecular understanding and thereby to improve individual disease risk assessment and to develop more specific molecular markers for the detection and follow-up of atherothrombosis.
Network approaches in sociological data analysis - mediated relationships

Researchers: Jukka Heikkonen, Kimmo Kaski, Jari Saramäki, Teemu Suna, Riitta Toivonen, Jouni Huhtinen, Michael Hardey, Mika Ala-Korpela

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Hull / York Medical School, Social Informatics Research Unit, University of York, UK
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Internet and computerised production and use of information have by now created one of the largest societies of over 970 million associates. Within this context online relationships and dating have existed for roughly ten years. In this network world, with increasing emphasis on careers and economic success, a growing proportion of single households are arising. For example, 40 per cent of American adults are single, and half of them - more than 40 million Americans - are currently using online dating services, and, generating multi-million dollar market along the way. The recent rise and popularity of Internet dating services is an indication that online dating has gone mainstream, i.e., online dating attracts "ordinary" people, or at least ordinary people who use the Internet. In fact, it has recently been indicated that online daters are sociable and self-confident thereby thrusting away the late 90’s allegory of online daters being as social isolates lacking social skills.

Everyday activities including shopping, arranging holidays and the exchange of correspondence represent the way everyday activities have increasingly moved online. As Hardey suggests, Internet dating sites are only one example of Internet resources that reflect and shape users’ offline lifestyles. Indeed many of the new resources that have developed for the Internet have been designed to address offline needs. Therefore, in contrast to visions of another ‘life-world’ occupied by users with multiple identities, the Internet, for many, is just a different space where they meet others and make use of a vast number of services and resources. The anonymity of individuals that characterises the online dating rarely seems to facilitate the construction of fantasy selves, but acts as a foundation for the building of trust and establishing real world relationships. Users of Internet dating sites are seeking to identify a stranger and form an online interaction that may move to a successful offline relationship. Indeed, the emphasis on communication, negotiation, equality, reciprocity and trust in contemporary relationships is reflected in the mediated and text based nature of Internet dating.

Rather than forming a distant cyberspace culture, the Internet is opening up new opportunities to shape the existing line and contents of social life. The vision of a logical, disembodied late modern intimacy, based on talk rather than passion, negotiation rather than commitment, and the advancement of the self rather than the development of the couple, suggest that the Internet is uniquely placed to facilitate such relationships. Indeed, recent studies have clearly shown a strong truthful connection sought by majority of online daters between the disembodied anonymous online selves and the real, offline selves. However, this does not mean that the rules governing how people construct and negotiate virtual identities and relationships online would match the rules governing formation of romantic relationships offline. In fact, little is known about the mating rituals in the digital domain.

Since the online dating seems to have taken its place in our repertoire of romantic relationship formation, it would be important to gain understanding of how people find the mutual trust online that leads to meetings offline. It would also be essential to be able to link what kind of people use the Internet dating services and how their characteristics affect their behaviour both online and offline. In addition, keeping in mind the risen business in the area of online dating, the dating services can truly exemplify the issues associated with information disclosure intended for marketing use. It is well known that people are, in general, particu-
larly reluctant to provide any personal information over the Internet. However, as the most popular Internet dating sites reveal, if information is meant for love and matchmaking aiming to find a potentially optimal mate, this reluctance partly disappears. This is also our experience for "intelligent" dating and political matchmaking services in the Internet in Finland. Although dating services are relatively unique as a service point of view, the actual use of customer data is not so unique. The user data obtained from online daters can thus be utilised for management of customer relationships in general.

Figure 49: Illustration of a SOM in sociological data analysis. The SOM transforms the individual and multidimensional data into a two dimensional plane. Each node in the SOM is described by a feature vector representing the original multidimensional parameter space, i.e., the input data. The feature vectors form, via the self-organising process, from the parameter vectors of all individuals. Thus, the feature vectors characterise average individuals using exactly the same multidimensional parameter space as originally utilised for the individuals. The SOM shown in this figure is for 3321 men and labelled for the cultural age parameter.

In our work we have focused on the capabilities of self-organising maps (SOMs) in sociological data analysis. While SOM is increasingly used in biological and other fields its application in social science is rare. We have recently described an application of SOM methodology to an extensive data acquired via an online dating service, consisting of answers for an extensive Internet questionnaire from 3321 men and from 1655 women. Such an extensive data set is exceptional in the area of social networks where data is traditionally obtained through painstaking interviews. Our results indicate that SOM analysis provides a good way of 'sorting people' out from complex data. The resulting visual maps and the defined 'model individuals' demonstrate the ability of SOMs to reveal interrelated parameters and to represent complex social situations. Through this analysis of the information about the characteristics of individual users, as well as those of the partner they desire from the e-dating site, we have identified what we refer to as a 'cultural age', as opposed to user's stated age, as being central to the selection of potential partners. This suggests that, one parameter such as the age stated by users, must be situated within a more nuanced characterisation of individuals’ profiles and desires in order to understand the role of e-dating in searching for new relationships. We have also indicated that SOM analyses are capable of revealing information that would be hard to capture by other methodological techniques. Overall, our results suggest that the SOM approach offers a proven methodology that can be easily applied also to complex sociological data sets.
Molecular Structure of Lipoprotein Particles

Researchers: Peter Engelhardt, Jukka Heikkonen, Kimmo Kaski, Vibhor Kumar, Jussi Kumpula, Linda Kumpula, Niko Lankinen, Riku Linna, Pasi Soininen, Reino Laatikainen, Matti Jauhiainen, Petri Ingman, Katarina Lähdesmäki, Katarina Öörni, Petri T. Kovanen, Sanna Mäkelä, Minna Hannukela, Markku Savolainen, Sarah Butcher, Mika Ala-Korpela

aDepartment of Chemistry, University of Kuopio; bDepartment of Molecular Medicine, National Public Health Institute; cDepartment of Chemistry, Instrument Centre, University of Turku; dWihuri Research Institute, Helsinki; eDepartment of Internal Medicine, University of Oulu; fInstitute of Biotechnology, Electron Microscopy Unit, University of Helsinki

Lipids are carried in the circulation in water(blood)-soluble lipoprotein particles that consist of a hydrophobic core consisting mainly of esterified cholesterol and triglycerides, and a hydrophilic surface of mainly unesterified cholesterol, phospholipids and apolipoproteins. Apolipoproteins (i.e., the protein molecules in various lipoprotein particles) maintain the structural integrity of lipoprotein particles and direct their metabolic interactions with cell-surface receptors, hydrolytic enzymes, and lipid transport proteins. The low density lipoprotein (LDL) particles are the major cholesterol carriers in circulation and their physiological function is to carry cholesterol to the cells. In the process of atherogenesis these particles are modified and they accumulate in the arterial wall. Although the composition and overall structure of the LDL particles is well known, the fundamental molecular interactions and their impact on the structure of LDL particles are still not well understood. The HDL particles are the key cholesterol carriers in the reverse cholesterol transport, i.e., transfer of accumulated cholesterol molecules from the arterial intima to liver for excretion. HDL particles have several documented functions, although the precise mechanism by which they prevent atherosclerosis still remains uncertain.

We have earlier brought together existing pieces of structural information on LDL particles and also combined computer models of the individual molecular components to give a detailed structural model and visualisation of the particles. We have presented strong evidence in favor of such molecular interactions between LDL lipid constituents that result in specific domain formation in the particles. We termed these local environments as nanodomains. It is becoming evident that the molecular structures of individual lipid molecules initiate interaction phenomena that intrinsically control the complex lipoprotein cascades in our bloodstream as well as in the intimal areas, the site of atherosclerotic LDL cholesterol and lipid accumulation. The very same lipid molecules also form HDL particles making the nanodomain approach also relevant to molecular studies of reverse cholesterol transport.

Recent findings suggest that small alterations in the chemical structure of lipoprotein lipids may also relate to the effects of alcohol and alcoholism on reverse cholesterol transport; it is known that alcohol does have beneficial effects on lipoprotein metabolism in general and that small amounts of "abnormal" lipids, e.g., phosphatidylethanol, are formed in the presence of ethanol and are associated with lipoproteins in plasma. Ethanol and ethanol-induced modifications of lipids are likely to modulate the effects of lipoproteins on the cells in the arterial wall. The molecular mechanisms involved in these processes are complex, requiring further study to better understand the specific effects of ethanol in the pathogenesis of atherosclerosis.

Using proton NMR we have recently been able to identify and quantify lysophosphatidyl-
choline (lysoPC) (in addition to PC and sphingomyelin) in LDL particles. This finding is particularly important concerning studies of LDL particle modifications in various pH conditions. Recent evidence suggest that atherosclerotic plaques and plaque vulnerability are related to acidic pH and recent results have also pointed out remarkable differences in the LDL particle modifications at different pH after enzymatic modifications. LysoPC may also induce various cell related phenomena in the intima since it is known to have some functions in cell signalling.

Recently we have also been developing a computationally optimised, general structural model for spherical lipoprotein particles. Our preliminary modelling, based on extensive biochemical data on the molecular compositions of different lipoprotein particles, indicates new aspects in relation to the distribution of hydrophobic lipid molecules, such as triglycerides and cholesterol esters, in the particles. The obtained molecular distributions seem to be a characteristic of each metabolic lipoprotein category revealing a molecular rationale for the lipoprotein metabolism.

In the current multidisciplinary collaboration we will study the molecular structures of lipoprotein particles, focusing on HDL particles in relation to reverse cholesterol transport as well as on native and modified LDL particles in relation to early atherosclerotic lesion formation. To reach the general goal - detailed molecular understanding of lipoprotein structure and dynamics - we will be applying and combining various experimental and computational approaches.

Figure 50: A schematic molecular model of a reconstituted spherical HDL particle: the depicted particle has a diameter of 9.5 nm, including a surface monolayer of 2 nm (light yellowish background), and a composition of 3 apoA-I molecules, approximately 100 phosphatidylcholine, 5 sphingomyelin, 5 cholesterol, 5 triglyceride and 70 cholesterol ester molecules. The colour coding for the molecules is: dark blue - phosphatidylcholine, light blue - sphingomyelin, dark yellow - cholesterol ester, red - cholesterol, green - triglyceride, and grey - apolipoprotein A-I. The molecular shapes and scales are derived from molecular dynamics simulations.
5.6 Wolfson College, Oxford: Advanced Computational Science and Engineering

Since the beginning of 2002 Research Centre for Computational Science and Engineering (CCSE) has operated an affiliate research unit called Advanced Computational Science and Engineering (ACSE) in Wolfson College of Oxford University with its own computing facilities, one part-time director and two full-time researchers. During this time it has also run Wolfson College visiting scholar programme for CCSE researchers to interact with various Oxford scientists in the fields of Theoretical Physics, Information Engineering, Neurocognitive Science, Materials Science, and Mathematical Biology. So far more than a dozen of CCSE researchers have visited Oxford thus fulfilling for it the role of international research training. Since our new Centre of Excellence (CoE) for 2006-2011 will be focusing on Computational Complex Systems Research (CCSR), it has been agreed with Wolfson College of Oxford University that the affiliate unit will continue its operation also for 2006-2011 with similar goals, with strengthened staff, and with better facilities than the former ACSE. In line with the goals of CCSR and in collaboration with the Oxford University Research Cluster of Complex Agent-Based Dynamic Networks (CABDyN) our Wolfson College affiliate unit will from now on concentrate on Computational Complex Systems and Network Research (CCSNR).

Figure 51: Panoramic view of Wolfson College, Oxford.
6 Research Activities

6.1 Visits to the Laboratory

- Douglas Abraham, Prof. Theoretical Physics, University of Oxford, UK.
- Yuri Alexandrov, Prof., Russian Academy of Science, Russia.
- Michael Allen, Prof. Dept. of Physics, University of Warwick, UK.
- Agnès Alsius, M.Sc., Departament de Psicologia Bàsica, Universitat de Barcelona
- Mike Ashworth, Dr., CCLRC Daresbury Laboratory, UK.
- Rafael Barrio, Prof. Autonomous University of Mexico, UNAM, Mexico.
- Gemma Calver, Dr., Oxford Centre for Functional Brain Imaging, University of Oxford, UK.
- Marcelo del Castillo Mussot, Dr., Dept.of Physics, Autonomous University of Mexico, Mexico.
- Tim Cootes, Dr., Division of Imaging Science and Biomedical Engineering, University of Manchester, UK.
- Chris Davis, Dr., School of Behavioural Sciences, University of Melbourne, Australia.
- Victor Eguíluz, Dr., University of Mallorca, Spain.
- Michale Hardey, Prof., Dept. of Criminology and Sociological Studies, University of Hull, UK.
- Ortwin Hess, Prof., Dept. of Physics, University of Surrey, UK.
- Janos Kertész, Prof., Institute of Physics, Budapest University of Technology and Economics, Hungary.
- David Landau, Prof., University of Georgia, USA.
- Kourosh Madani, Prof. Université Paris XII, France.
- Subhrangshu Sekhar Manna, Dr., Satyendra Nath Bose National Centre for Basic Sciences, Kolkata, India.
- Maxi San Miguel, Prof., Instituto Mediterraneo de Estudios Avanzados, Universitat Illes Balears, Mallorca, Spain.
- Ole Mouritsen, Prof. MEMPHYS, University of Southern Denmark, DK.
- Krzysztof Murzyń, Dr., Dept. Biophysics, Jagiellonian University, Poland.
- Galina Paramei, Doc., Hanse-Wissenschaftskolleg, Delmenhorst, Germany.
- Marta Pasenkiewicz-Gierula, Prof. Dr. Hab., Dept. Biophysics, Jagiellonian University, Poland.
- Josef P. Rauschecker, Prof., Dept.of Physiology and Biophysics, Georgetown Institute for Cognitive and Computational Sciences, USA.
- Jorma Rissanen, Prof. Emer., IBM Research Center, Almaden, USA.
- Jean-Luc Schwartz, Dr., Institut de la Communication Parlée, CNRS, France.
- Paul Sherwood, Dr., CCLRC Daresbury Laboratory, UK.
- Sitabhra Sinha, Dr., Theoretical Physics group, Institute of Mathematical Sciences, Chennai, India.
- Adrian Sutton, Prof, FRS, Dept. of Physics, Imperial College, UK.
- Gergely Tibély, Institute of Physics, Budapest University of Technology and Economics, Hungary.
- Kin Wah Yu, Prof., the Chinese University of Hong Kong, China.
- Adrian Wander, Dr., CCLRC Daresbury Laboratory, UK.
6.2 Visits by Laboratory Personnel

Mika Ala-Korpela
- European Commission’s Joint Reserach Centere, 23.-25.2.2005, Ispra, Italy
  - Invited talk: Metabonomics by 1H NMR: Current Situation, Plasma Lipoprotein Sub-class Quantification, and Potential Applications on CHD Diagnosis.

Sami Brandt

Lei Dong
- The Chinese University of Hong Kong, Physics Department, Hong Kong, 1.1.-30.6.2005

Mikko Karttunen
- Princeton University, Dept. of Mechanical Engineering, USA.
- University of Western Ontario, Dept. of Applied Mathematics, Canada
- University of Ottawa, Dept. of Physics, Canada
- McGill University, Dept. of Physics, Canada, February 2005
- University of Hokkaido, Japan, September-October, 2005
- The Chinese University of Hong Kong, October, 2005

Kimmo Kaski
- Universidad Nacional Autónoma de Mexico, Instituto de Fisica, Mexico City, Mexico, 26.8.-1.9.2005.
- Universitat Illes Balears, IMEDEA, Palma de Mallorca, Spain, 26.10.-3.11.2005.

Markus Miettinen
- McGill University, Montreal, Quebec, Canada, 31.1.-2.3.2005.

Jari Saramäki
- Budapest University of Technology and Economics, Theoretical Physics Department, 9.-19.5.2005
  - Talk: The role of weak links in a huge social network.
- Budapest University of Technology and Economics, Theoretical Physics Department, 9.-14.10.2005.

Lorna Stimson
- Department of Chemistry, University of Durham, UK.

Harri Valpola

6.3 Participation in Conferences and Seminars

Mika Ala-Korpela
- Finnish Atherosclerosis Club Meeting, 11.-12.3.2005, Helsinki, Finland
  - Invited plenary lecture: Applications of Modern NMR Methodology in Cardiovascular Research
- 27th Finnish NMR Symposium, June 8-10, Iso-Syöte (Oulu), Finland
  - Talk: 1H NMR Metabonomics and Atherothrombosis
  - Invited talk: Chemometrics in 1H NMR Metabonomics of Plasma and Lipoprotein Quantification

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• Abstracts

Sebastian von Alfthan
  • Physics Days, Otaniemi, Finlands
    - Talk: Structure and energetics of twist grain boundaries
  • Computational Chemistry and Materials Science (CCMS) Summer Institute at Lawrence Livermore National Lab (LLNL), 7.6.-18.8.2005

Sami Brandt
  • 14th Scandinavian Conference on Image Analysis (SCIA 2005), Joensuu, Finland, June
    - Poster: A Bayesian Approach for Affine Auto-Calibration

Ilkka Kalliomäki
  • 14th Scandinavian Conference on Image Analysis, June 19-22, 2005, Joensuu, Finland.
  • GETA Winer Course: Signal Processing Challenges for Software Defined Radios.

Mikko Karttunen
  • Summer School: Modeling of Biomolecular Systems, May 30-June 1, 2005
    - Co-organizer with Dr. I. Vattulainen and Prof. K. Laasonen
  • Invited talks in
    - Summer School of Regroupement Quebecois des Materiaux de Pointe (www.rqmp.ca/en_index.html), July 1-3, 2005, Sherbrooke, Canada
    - Mathematical Workshop Mathematical Issues in Molecular Dynamics, June 4-9, 2005, Banff, Canada
    - XXXIV Winter Meeting on Statistical Physics, January 6-9, 2005, Taxco, Mexico.

Kimmo Kaski
  • AAAS Annual Meeting, February 16-22, 2005, Washington, USA
  • Second Annual Meeting. Cost Action P10, Physics of Risk, April, 23-26,2005, Toledo Spain
  • Econohysics Colloquium, Australian National University, November 12-19, 2005, Canberra, Australia.
    - Talk: Network Perspective to Financial Market

Markus Miettinen
    - Poster: M. Miettinen, C. Dias, M. Grant, I. Vattulainen, T. Ala-Nissila and M. Karttunen: Pulling out a globule

Ville Ojanen
  • International Multisensory Research Forum Annual Meeting, June 5-8, 2005, Rovereto, Italy
Mikko Sams
- 6th International Multisensory Research Forum Annual Meeting, June 5-8, 2005, Trento, Italy
  - Talk: Visual influences on auditory processing of speech
- Biology of Cognition, April 8-9, 2005, University of Helsinki, Finland.
  - Talk: Neurocognitive research in the Laboratory of Computational Engineering: Complex neurocognitive systems?
- SCIL-CICERO Colloquium, October, 13-14, 2005, Stanford, USA
  - Organizer of the colloquium
  - Organizer of a session: Brain and Learning
  - Talk: Neurocognition of multisensory perception
- Abstracts:
  - Tiippana, K. and Sams, M. Does stimulus location influence a visual illusion induced by sound. 6th Multisensory Research Forum, June 5-8. 2005, Trento, Italy

Lorna Stimson
- Research Seminar: Using molecular dynamics simulations to investigate the possibility of a membrane-mediated mechanism for general anaesthesia, June 9, 2005. Department of Physics and Centre for Scientific Computing, University of Warwick, UK.
- Invited talk at Modelling of biomolecular systems international summer school, May 30, 2005, Helsinki, Finland.
- Contributed talk at 11th Amphiphiles and their aggregates meeting, May 17-20, 2005, Wroclaw, Poland.
- Contributed talk at Lipid Forum, Biomedicum, University of Helsinki, April 1, 2005, Finland.
- Contributed talk and poster at Finnish Physics Society Meeting: Physics Days, March 17, 2005, Helsinki University of Technology, Finland.
- Contributed talk at Biomembranes Workshop, April 4-6, 2005, CECAM, Lyon, France.

Kaisa Tiippana
- International Multisensory Research Forum Annual Meeting, June 5-8, 2005, Rovereto, Italy
  - Poster: Tiippana K., Sams, M.: Does stimulus location influence a visual illusion induced by sound?
6.4 Memberships in scientific societies

Sami Brandt:
- Member of the Institute of Electrical and Electronics Engineers (IEEE)
- Member of the Computer Society of the IEEE
- Member of the International Association for Pattern Recognition (IAPR)
- Member of the Pattern Recognition Society of Finland
- Member of the Finnish Inverse Problems Society

Ilkka Kalliomäki:
- Member of HATUTUS, Pattern Recognition Society of Finland
- Member of the International Association for Pattern Recognition (IAPR)

Mikko Karttunen:
- National representative and a member of the steering committee of the European Science Foundation initiative Functional Dynamics in Complex Chemical and Biological Systems (FUNCDYN)
- Member of European Science Foundation network SIMU - Challenges in Molecular Simulation and its successor MOLSIMU
- Member of the American Physical Society, USA
- Member of the Biophysical Society, USA
- Member of the Finnish Physical Society

Kimmo Kaski:
- Fellow by invitation of the American Physical Society, USA
- Member of Association for Computing Machinery
- Fellow by invitation of the Finnish Academies of Technology
- Fellow and Chartered Physicist by invitation of the Institute of Physics, UK
- Fellow by invitation, Academica Europaea
- Member of American Association for the Advancement of Science (AAAS), USA
- Fellow by invitation of the Finnish Academy of Science and Letters
- Fellow of the Royal Statistical Society
- Supernumerary Fellow, Wolfson College, University of Oxford, UK

Jouko Lampinen:
- Board member of Brain Research Society of Finland (BRSF)
- Member of International Neural Network Society (INNS)
- Member of Pattern Recognition Society of Finland, HATUTUS (member of IAPR)

Harri Valpola:
- Board member of Finnish Artificial Intelligence Society
- Member of Pattern Recognition Society of Finland, HATUTUS (member of IAPR)

Aki Vehtari:
- Board member of Pattern Recognition Society of Finland, member-society of IAPR (International Association for Pattern Recognition)
- Fellow of the Royal Statistical Society
- Member of the International Society for Bayesian Analysis
- Member of the European Network for Business and Industrial Statistics
6.5 Other Activities

Mika Ala-Korpela has acted as
- Reviewer in journals
  - Biochemistry
  - Chemistry and Physics of Lipids
- Member of the management group of a Tekes project for Neste Oil Ltd in relation to oil product development

Sami Brandt has acted as
- Reviewer in journals:
  - IEEE Transactions on Systems, Man and Cybernetics
  - IEEE Transactions on Image Processing
- Reviewer in conferences:
  - 14th Scandinavian Conference on Image Analysis (SCIA 2005)

Mikko Karttunen has acted as
- Member of the Editorial Board in
  - Biointerphases
- Reviewer in
  - European Journal of Pharmaceutics
  - Chemical Physics Letters
  - Chemistry and Physics of Lipids
  - Biophysical Journal
  - Physica A
  - Physical Review Letters
  - Europhysics Letters
  - Langmuir
  - Nature Materials
  - Journal of Chemical Physics
  - Surface Science
  - Physica E
  - IEEE Transactions on Nanotechnology
  - Biochim. Biophys. Acta
- Appointments
  - Docent in Computational Science and Biological Systems in Helsinki University of Technology, Finland.
  - Assistant Professor, Dept. of Applied Mathematics, University of Western Ontario, London, Canada.
  - Cross-appointment as an Assistant Professor in the Dept. of Physics, University of Western Ontario, London, Canada.

Kimmo Kaski has acted as
- Member of the Editorial Board in
  - International Journal of Modern Physics C
- Reviewer for
  - European Science Foundation - Review of Self-organized nanosystems (SONS) programme
  - Science Foundation Ireland - Programme Review
  - Belgian Science Policy Office: Interuniversity Attraction Poles network review
- Reviewer in Journals:
Jouko Lampinen has acted as
- Organizing committee member in international conferences:
  - European Symposium on Artificial Neural Networks, ESANN 2005
  - NORDSTAT2006 - 21st Nordic Conference on Mathematical Statistics
- Reviewer in Journals:
  - IEEE Trans. on Neural Networks
  - Neural Networks
  - Neurocomputing
  - Journal of Human Evolution

Mikko Sams has acted as
- Official reviewer of doctoral thesis:
  - University of Kuopio, Dept. of Clinical Neurophysiology
- Member of Editorial Board in
  - Tiede (Finnish popular science magazine)
  - Polysteekki

Harri Valpola has acted as
- Opponent of doctoral thesis:
  - DTU, Dept. of
- Member of Editorial Board:
  - Neurocomputing
- Reviewer in journals and book series:
  - Journal of Machine Learning Research
  - IEEE Transactions on Signal Processing
  - Neurocomputing
  - International Journal of Neural Systems
  - Synthesis Lectures on Signal Processing
- Reviewer in international conferences:
  - The Fourth International Conference on Development and Learning
  - The 6th International Conference on Independent Component Analysis and Blind Source Separation

Aki Vehtari has acted as
- Opponent of doctoral thesis:
  - University of Turku, Dept. of Information Technology
- Official reviewer of doctoral thesis:
  - Helsinki University of Technology, Dept. of Computer Science and Engineering
- Member of
  - the board in Pattern Recognition Society of Finland, Hatutus
- Reviewer in journals
  - IEEE Transactions on Neural Networks
7 Publications


