Laboratory of Computational Engineering
and
Research Centre for Computational Science and Engineering
Annual Report

Eeva Lampinen
Editor
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Engineering
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Introduction

Year 2004 marks for the Laboratory of Computational Engineering (LCE) & Research Centre for Computational Science and Engineering (CCSE) the fifth year as a national Centre of Excellence with truly international staff of about 80 members and of 10 different nationalities. The CCSE operates an affiliate research unit called Advanced Computational Science and Engineering (ACSE) in Wolfson College of Oxford University with the state of the art cluster-computing facilities and two full time researchers. For the purpose of international researcher training and collaboration ACSE provides every year 2-4 months visits for two to four visiting scholars from CCSE to interact and network with various Oxford scientists in the fields of Neurocognitive Science, Information Engineering, Materials Science, Mathematical Biology and Theoretical Physics. Over the three year period, with more than a dozen CCSE researchers visiting Oxford, ACSE activity has fulfilled its purpose excellently. The research in LCE, CCSE and ACSE is multidisciplinary in nature and has till recently been carried out in three mutually supportive fields: Computational information technology, Computational materials research, and Cognitive science and technology. In 2004 these activities have borne a lot of fruit: over 100 scientific publications of which about 60 in high impact factor journals, and five PhDs of which three women.

Over the recent years, research in general has been experiencing paradigm change such that many well-established disciplines have together generated new research disciplines. This change can be characterized as follows: i) focus of research lies on understanding the properties of living systems at several scales, ranging from the complex biological machinery inside living cells to networks of social interactions between humans, and ultimately to the whole ecosystem itself, ii) the viewpoint is becoming increasingly holistic, with focus on system-level behaviour instead of detailed characterization of the constituents, and iii) research is becoming increasingly multidisciplinary, partially because there is a direct need for combining knowledge and methods from various fields of research, but also because seemingly unrelated systems often share similar characteristics and can be treated within similar theoretical frameworks. These systems are called complex systems because complex, non-linear system-level behaviour can emerge in a non-trivial fashion from the rules which govern the individual interacting and simple elements. Hence, the systems have to be analyzed from several viewpoints and at several levels. This emphasises the role of computational approach in their study involving, on one hand, large-scale numerical simulations in combination with analytical treatment using related mathematical methodology, and, on the other hand, the analysis and interpretation of experimental data obtained from measurements.

In recognition of this paradigm shift LCE, CCSE and ACSE is adopting as its new research mission Complex Systems Research, which consists of four focus areas: 1. Models & Methods, including activities 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.

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
- Sutton Adrian Professor, FRS
- Tulkki Jukka Professor

Adjunct Professors (Docents/Visiting Professors)
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- Alexandrov Yurii 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)
- Parkkinen Jussi Prof. (University of Joensuu)
- Rissanen Jorma Prof. (IBM Research Center, Almadena, USA)
- Räähi Kari-Jouko Prof. (University of Tampere)
- Trio Henry Prof. (University of Helsinki)

Secretaries
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- Lampinen Eeva

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- Klucharev Vasily Ph.D.
- Koskela Timo Dr. Tech.
- Kuronen Antti Academy Fellow, Ph.D.
- Leppänen Teemu Dr.Tech.
- Möttönen Riikka Ph.D.
- Patra Michael Marie Curie Fellow
- Patriarca Marco Ph.D.
- Rodriguez Mirta Ph.D.
- Róg Tomasz Ph.D.
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<td>Vehtari Aki</td>
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**Researchers**

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Pihlström Kim
Saira Olli-Pentti
Sandholm Niina
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 2004

- S-114.100 Computational science (3 cr) L
- S-114.101 Cognitive neuroscience (3 cr)
- S-114.155 Business game (2 cr)
- S-114.200 Special course in computational engineering (4 cr) L
- S-114.202 Advanced topics in Bayesian modeling (2-5 cr) LV
- S-114.204 Modelling of perception (3 cr) L
- S-114.210 Individual project in computational engineering (2 cr)
- S-114.220 Research Seminar on Computational Science (2 cr) L
  Topic: Spatial Modeling
  Topic: Research-oriented graduate seminar on Complex systems
- S-114.220 Research-oriented graduate seminar on Complex systems (3 cr) L
- S-114.240 Seminar on computational engineering (2 cr) V
  Topic: Computational methods in understanding nature
- S-114.245 Laboratory seminar on computational engineering (1-2 cr) LV
- S-114.250 Special topics in computational science (4 cr) L
- S-114.310 Introduction to modelling and information theory (2 cr)
- S-114.325 Physics III (S) (2 cr)
- S-114.326 Physics IV (S) (3 cr)
- S-114.425 Physics III (Sf) (4 cr)
- S-114.426 Physics IV (Sf) (4 cr)
- S-114.500 Basics for biosystems of the cell (3 cr) L
- S-114.501 Introduction to Bioinformation Technology (2 cr)
- S-114.510 Computational systems biology (3 cr)
- S-114.601 Introduction to Bayesian Modeling (3 cr) L
- S-114.710 Perception and production of speech (4 cr)
- S-114.720 Research Seminar on Communication and Cognition (2 cr) LV
  Topic: Multimodal speech perception and production
- S-114.740 Design and statistical analysis of functional MRI studies (2 cr) LV
- S-114.750 Systemic Psychophysiology
- S-114.760 Emotions and communication (4 cr)
- S-114.772 Mental and other representations (3-5 cr) L (Connet)
- S-114.780 Perception and Action (4 cr) L
- S-114.811 Computational neuroscience 3 cr L
- S-114.V Biomimetic robot navigation project course (2-4 cr) LV

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 Technology / Philosophy**
- Laura Juvonen *Monte Carlo simulations in the study of semiconductor surfaces*
- Teemu Leppänen *Computational Studies of Pattern Formation in Turing Systems*
- Ville Mustonen *Wetting, filling and interface dynamics*, University of Oxford.
- Riikka Möttönen *Cortical Mechanisms of Seeing and Hearing Speech*
- Maria Sammalkorpi *Molecular Dynamics Simulations of Strained and Defective Carbon Nanotubes*

**Licentiate of Technology**
- Paula Litkey *Neural Network Models for Predicting Steel Hardenability*

**M.Sc. - Diplomas**
- Mikko Berg *Emergent political concepts in explorative interface visualization*
- Timo Jyrinki *Pienen laitteen värinän havaitseminen - testiympäristön pystyttäminen ja tutkiminen*
- Juho Kannala *Measuring the Shape of Sewer Pipes from Video*
- Marko Knuutila *The usability of configuration management software in mobile network management systems*
- Tomas Linden *Indoor positioning systems: A case study of location-driven health care process monitoring*
- Markus Miettinen *From molten globule to swollen coil*
- Sami Savio *Network Selection Algorithm for Stream Services*
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 $10^{22}$ 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. On the system level statistical approach, only probability distributions of the individual elements are considered, and 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.

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, 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, Jarno Vanhatalo

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). Other 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**

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 this project is to examine the probabilistic roots of the Kalman filtering theory and find ways to go beyond the classical methods by combining the advantages of the classical and modern methodology. The results of the project have applications, for example, in the following fields:

- One way of combining the modern and classic methods the Rao-Blackwellized particle filtering. It has applications in several fields, for example, in multiple target tracking (see Section Sequential Monte Carlo Methods in Multiple Target Tracking).

- Cross-validation is very powerful method for estimation of parameters and maximizing the generalization (i.e. prediction) ability of the Kalman filtering and Kalman smoothing problems. Using this methodology 1 we won the first prize in the CATS time series prediction competition, which was organized as a special session of the IJCNN 2004 conference.

- The on-line adaptation of model parameters (e.g. noise variances) in state estimation problems can be also formulated in terms of Bayesian state estimation problem, which opens the possibility of applying the modern computational methods for their estimation. This is useful in applications where a large number of cheap sensors is used and the sensor drifts, temperature dependencies of noise variances and other such characteristics become significant.

- The theory of stochastic differential equations, diffusion processes and the numerical estimation methods is also classical, but has interesting relationship to Bayesian non-parametric modeling, modern machine learning and neural network modeling. In the project we have investigated the connections between Kalman filtering, Kalman smoothing, non-parametric modeling and stochastic differential equations.

- The theory of stochastic differential equations also allows modeling of non-linear continuous-time dynamic processes. This kind of processes typically result in noisy physical processes, where the geometry of the problem is made easier coordinate transformations or when the physical boundary conditions are non-linear.

Figure 1 shows example results from the Kalman smoother prediction of the CATS benchmark time series. Figure 2 is a very simplified example of estimation of time-varying noise variance (or standard deviation) in Gaussian signal. The noise process was modeled as logarithm of Brownian process with approximately known parameters.

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Figure 1: The Kalman smoother prediction of the CATS Time Series Prediction Competition data. The results are shown for the last two gaps at 3981 – 4000 (left) and 4981 – 5000 (right). The gray line is the true signal, the dashed line is the long term prediction result, and the black line is the combined long and short term prediction result.

Figure 2: Example of estimation of time-varying noise. The signal and the estimated quantiles of noise (left) and the true and the estimated standard deviation as function of time (right).

**Sequential Monte Carlo Methods in Multiple Target Tracking**

Researchers: Simo Särkkä, Aki Vehtari and Jouko Lampinen

The goal of the project was to develop multiple tracking methods for tracking an unknown number of targets or signals in cluttered and noisy multi-sensor environment. The idea of multiple target tracking is to optimally fuse information from sensor measurements and modeled target dynamics to form the best possible estimates of states of multiple targets (e.g., positions, velocities and attributes) and their uncertainties. The models and methods used in this project were based on Bayesian filtering theory.

The main topic of the project was tracking of an unknown number of targets, which is substantially harder task than tracking a known number of targets. Because the number of visible targets changes in time, the estimation has to be done on-line and the estimation procedure cannot be simply separated into subtasks of estimation of number and estimation of states of the targets. The developed estimation method forms joint hybrid Gaussian/MC estimate of the states of unknown number of targets by Rao-Blackwellized particle filter.
The multiple target tracking methods have also applications in other fields:

- The methods that have been developed for clutter modeling and estimation can be also used for detection of sensor failures, malfunction and modeling abnormal behavior of sensors. This allows, for example, automatic detection and compensation of broken sensors, which opens possibility for using cheaper but less reliable sensors.

- 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 3 shows the estimation result in case of unknown number of 1D signals. The Figure 4 shows the corresponding results for a 2D state estimation (tracking) problem.

Figure 3: Filtering (left) result, smoother result (middle) and the estimated number of signals (right) of 1D scenario with an unknown number of signals

Figure 4: Filtering (left) result, smoother result (middle) and the estimated number of signals (right) of 2D tracking scenario with an unknown number of targets
New analysis methods for healthcare process management

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

The project is part of FinnWell - Healthcare technology programme.

Focus of the project is to develop healthcare data analyzing systems. 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.

In our part of the project, we develop a method 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. Method will be based on hierarchical temporal models. The pilot projects will be in orthopaedics and special services for the elderly.

We also develop a theme map software for representing regional healthcare key figures (e.g. mortality, diagnoses). Key figures are shown in standardized form using color codes and variation in time is shown as sequential images or movies.
Monitoring the Condition of Sewer Network

Researchers: Juho Kannala, Jukka Laurila, Sami Brandt, Aki Vehtari and Jouko Lampinen

The project’s goal was to develop methods for the analysis of video sequences that are scanned by a robot moving in the sewer. The project was done in co-operation with the VTT Building and Transport and was funded by Tekes.

The work was divided into two parts: 1) Automatic detection of pipe surface defects and pipe joints. 2) Automatic reconstruction of the 3D shape of the pipe. Displaced joints and surface cracks are among the most common types of defects in a sewer pipe. Detecting the cracks is challenging because of the large variation in surface texture. We tested several line detection algorithms for crack detection in the pipe surface and joints between pipe sections. Figure 5 shows an example of pipe segment and crack candidates and joints. Post-processing included thresholding with hysteresis and by feature size and naïve Bayes classification to combine information from the location and surrounding texture. Approach was compared to crack detection made by an expert. Results showed that approach based on edge line detectors could detect obvious cracks and results were improved to previous line detector based method. However, expert could also detect faint cracks based on additional information, like trail left by water dripping through crack and crack continuation on the other side of pipe. Implementation of similar expert knowledge and more holistic approach is not however trivial.

![Figure 5: Crack detection results. (a) Original image of ’unwrapped’ pipe surface. (b) Detected cracks and joints.](image)

The information on the shape of the sewer pipe is important, because the bendings and compressions may indicate upcoming failure. In order to obtain 3D information from the video the imaging geometry of the fish-eye lens camera must be determined. We developed an accurate and easy-to-use method for the calibration of fish-eye lenses. The calibration is possible by using only one view of a planar calibration object as Figure 6 illustrates. After solving the problem of calibration, we were able to use known multiple view techniques to track points through the image sequence and to make 3D reconstruction of the sewer pipe.

![Figure 6: Fish-eye lens calibration using only one view. (a) Original image. (b) The image corrected to follow the pinhole model. Straight lines are straight as they should be.](image)
**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 7 shows an example of the sequential matching process and figure 8 illustrates matching when the target objects are occluded.

![Figure 7: 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.](image)

![Figure 8: 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)
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. The results can be applied to further processing of the image, for example object recognition.

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 a given image 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 samples for the algorithm by taking advantage of many types of relevant image information such as edges and homogeneous areas.

Advantages of this model-based, probabilistic approach are numerous. The model allows the inclusion of different texture models as well as new methods for producing proposal samples. The model provides a flexible framework for scene analysis, since it gives a probabilistic explanation to each part of the image.

We have applied the results to a robot navigation problem, where a vision system is used for real-time path planning. We are also extending the work to take into account properties of specific types of objects.

Figure 9: Examples of segmentation results.
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.

Steerable filters are another variety of 2D oriented filters. While non-optimal in terms of joint space-frequency uncertainty principle, steerable filters have other desirable properties as oriented feature detectors. The most notable of these is the ability to compute filter responses in arbitrary orientation by weighting the responses of a fixed filter bank with a handful of different orientations.

We have derived analytical steering equations for Gabor filters, which enable Gabor filters to be used as steerable filters. 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.

Steerable filters provide a computationally efficient way to implement rotation invariant feature detection. With suitable parameters, Gabor filters offer approximative steerability while having also good feature localization capability and angular resolution. The design of a filter bank for feature detection is, in general, a compromise between feature specificity and genericity, but the properties of the filters and their spatial arrangement have a large effect on detection performance.

![Figure 10: Feature similarity functions in spatial and orientation dimensions obtained using three different filter banks. Left: Original images, with the matching local maxima marked with ed crosses. Right, top row: a) Inner product similarity using regular Gabor filters. b) Similarity using nearest neighbor rotation invariance with the same filters. The feature loses specificity and localization becomes worse. c) Same filters and rotation invariance method using a different spatial arrangement of the filters. Localization is greatly improved. Bottom row: Corresponding similarities in the orientation dimension evaluated at the spatial local maxima of the similarity functions.](image-url)
Statistical Brain Signal Analysis

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

Statistical brain signal analysis project is multidisciplinary project combining the expertise of both Bayesian Methodology group and Cognitive Science and Technology group.

Localizing the neural currents indicating brain activity based on noninvasive MEG and 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 based on the data only. Some additional a priori information must be provided to obtain sensible results, necessitating a Bayesian treatment of the problem.

Our aim is to apply the methods of Bayesian data-analysis to the study of cognitive brain functions as revealed by MEG, EEG and fMRI. Our focus is especially on the computationally more intensive methods such as Markov chain Monte Carlo (MCMC). By using a state-of-the-art data simulation model, we have studied generalizations of previously proposed MEG/EEG data-analysis methods in collaboration with Massachusetts General Hospital–Harvard Medical School NMR Center (Dr. John W. Belliveau and Dr. Matti S. Hämäläinen).

We performed a Bayesian analysis to the MEG inverse problem with $\ell^p$-norm priors. Our model contains as special cases the minimum-norm estimate (MNE; $\ell^2$) and minimum-current estimate (MCE; $\ell^1$), which are both widely used in practice. With our method, the joint posterior distribution of all the model parameters can be obtained, making it possible to investigate the uncertainties of almost equally probable solution estimates rather than only a maximum a posteriori (MAP) estimate. Furthermore, the arbitrary choice between the $\ell^1$- and $\ell^2$-norm priors is inferred from the data by introducing a continuous parameter $\beta$ between the limiting cases of MCE and MNE. The method is automatic, yet mathematically very straightforward enabling the addition of almost any kind of feasible prior information to improve the source localization. The results with real somatomotor MEG data look promising (Fig. 11).

![Figure 11](image.png)

Figure 11: a) Measured data plotted on the MEG helmet sensor locations with red color denoting positive and blue color negative values. b) The solution estimate (red line) is plotted against the original data (blue dots) with one sigma error bars. c) Right index finger lifting produces activation contralaterally on the left hemisphere somatomotor hand areas (plotted on inflated brain surface). d) Posterior distribution of parameter $\beta$ defining the $\ell^p$-norm order.

We also proposed an alternative hierarchical extension of the model corresponding to the minimum norm estimate. Instead of assuming a single Gaussian prior for the neural currents, we built a hierarchical structure to the model by imposing individual Gaussian priors with a common hyperprior distribution. This method is applicable to full spatiotemporal datasets without significant increase in computational burden. We have made tentative comparisons of the approach with a recently proposed similar variational Bayesian method.
Statistical Methods in Vision Geometry

Researchers: Sami Brandt

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 seen as a most natural approach.

Our aim has thus been approaching geometric problems from a pure statistical viewpoint. As our recent research activities on this area, we have introduced the probabilistic epipolar constraint (Fig. 12) and developed affine structure-from-motion algorithms by revisiting the problems of affine reconstruction and affine autocalibration. Some of the results have been successfully applied in the image alignment problem in electron tomography.

Figure 12: Illustration of the probabilistic epipolar constraint. (Left) Five points selected on the left image. (Right) One thousand independent samples drawn from each epipolar pdfs which are the probabilistic form of the epipolar lines. The colour indicates the distribution of the probability mass.
Brain Computer Interfaces (BCIs) enable motor disabled and healthy persons to operate electrical devices and computers directly with their brain activity. Our approach bases on an artificial neural network that recognizes and classifies different brain activation patterns associated with real and attempted movements. We pursue to develop a robust classifier with short classification time and a low misclassification rate. Figure 13 demonstrates our BCI in use.

We are especially interested in the neurophysiological basis of BCIs. Before the signals can be classified they need to be understood. We concentrate on activity of the motor cortex.

Like most other BCI groups, we measure the electric activity of the brain using electroencephalography (EEG). In addition, we measure the magnetic activity of the brain with magnetoencephalography (MEG, Fig. 14). MEG signals are more local than EEG signals. This facilitates, e.g., the separation of activities generated in the left and right sensorimotor cortices.

We have been working on an online EEG-based BCI. EEG signal related to finger movements are used as input to the classifier. The exact timing of the movements is measured with light ports. An LED provides a cue to move. We are testing the system now with healthy subjects and will modify it to be used also by paralyzed users.

Our research is funded by EU (MAIA project), the Academy of Finland, the Graduate School in Electronics, Telecommunications and Automation and the Finnish Cultural Foundation.

One of the highlights of 2004 was that Laura Kauhanen won the first prize in the poster competition in BCI 2004 Workshop and Training Course in Graz, Austria.
5.2 Computational Materials Research

In LCE and CCSE the computational materials research is focused on the study of physical properties, processing methods and functional properties of selected new materials which we expect to have great potential in the emerging information technologies, future systems biology applications and complex engineering systems in general. 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 Nanotechnology and Coherent Quantum Systems.

5.2.1 Atomic Level Modelling of Structure and Growth of Materials

This research is concerned with the study of structural properties of and growth phenomena in solid materials. All studies rely on microscopic modeling, in which the inter-atomic interactions are described through pairwise and many-body model potentials. In generic studies we have used Lennard-Jones potentials, while in more specific cases the Tersoff, Stillinger-Weber and Valence Force Field potentials as regards to the study of semiconductors and Effective Medium and the Embedded Atom model potentials as regards to studies of metals have been used. Because these semiempirical potential models have their drawbacks and limitations when attempting to describe bonding in certain materials (especially carbon in tubular form) the more accurate tight-binding approach has been used as a complementary method to describe inter-atomic interactions.

The main topics of investigation in the case of semiconductor materials have been structure and mechanical properties of surfaces, interfaces and various nanostructures – e.g. thin films, quantum dots, clusters and carbon nanotubes. In addition to crystalline materials recrystallization of amorphous silicon has been studied by computational methods. As regards to metals, the focus has been on detailed microscopic structure and dynamics of dislocations.

Large scale Molecular Dynamics (MD) and Monte Carlo (MC) simulations have been the standard tools employed in all these studies and their execution have been done using mostly our in-house parallel cluster computers. This has entailed program development especially for parallel computing purposes. In connection with the MD simulations, development of the graphical user interface for the simulation programs has been continued. In addition interactive simulation programs have been developed and used to study dislocation dynamics and strain relaxation in two and three-dimensional heteroepitaxial systems and mechanical and structural properties of carbon nanotubes. A more general development of scientific visualization has also been done using the open-source program package OpenDX.
Hetero-structures

Researchers: Marco Patriarca, Antti Kuronen, and Kimmo Kaski

The study of nucleation and dynamics of dislocations in lattice-mismatched heterostructures has a special interest, due to its technological importance for potential applications. In this type of systems, dislocations may arise from instabilities appearing already during the formation of the hetero-structure, e.g., during the growth of the overlayer, due to different origins. In the present work we analyze, in particular, thermodynamical instabilities – whose main characteristics are only related to the properties of the two materials.

We employ a numerical molecular dynamics approach to the problem, in order to fully take into account the atomic nature of the scale of the problem. To this aim the misfit \( m \) is then slowly modified, by changing some parameters of the interaction potential, starting from the initial value, \( m = 0 \), until the critical misfit \( m = m^*(h) \), corresponding to the given height \( h \), is reached and one or more dislocations are nucleated in the overlayer. The transformation is carried out slowly enough (adiabatically) and under some suitable controls, in order to be reversible and such that the system is always almost in thermal equilibrium at a given temperature \( T_0 \). This procedure should be compared with (the simulation of) a real growth process, in which the misfit \( m \) is fixed, while it is the (average) height \( h \) which increases.

Fig. 15 shows a sample with sizes \( 15 \times 20 \times 100 \) lattice constants. A step was created around the over-layer in order to give it the structure of a dot. Atoms of type \( A_1 \) in the lower part are supposed to represent a very large substrate, on which a dot of atoms of type \( A_2 \) is present. When the misfit reached the critical threshold \( m^* = -0.9 \), one can observe a sudden release of kinetic energy, with visible oscillations and misfit dislocation nucleation.

For a review see M. Patriarca and A. Kuronen, Atomistic modeling of hetero-structures, to be published in Handbook of Theoretical and Computational Nanotechnology Michael Rieth and Wolfram Schommers Editors, ASP, in press.

Figure 15: Left: For a misfit close to the critical value \( m = -0.9 \) there are no dislocations yet, but a cut of the sample along the interface shows a zone with regularly shaped zones under high strain induced by the mismatch. Right: The dislocations have appeared and the stacking fault left by a nucleated misfit dislocation appears as a step on the surface of the system. Atoms are colored according to a potential energy mapping.
Interactive graphical tool for numerical experiment

Researchers: Marco Patriarca, Antti Kuronen, and Kimmo Kaski

Numerical simulations represent an invaluable contribution to the current description of the behavior of matter. They are particularly helpful in describing the processes in solid state systems in which employ many-body potential models are to be used. Interactive numerical simulations, based on the association of a visualization tool, such as a graphical user interface (GUI), with a numerical simulation code, present specific advantages. First of all the amount of memory storage required can be greatly reduced. Furthermore, the possibility of a real time variation of the simulation parameters, such as temperature and applied fields, and the analysis of the corresponding feedback made possible by the graphical environment offer the possibility to perform a fine tuning in the regions of parameter space for a better monitoring of the evolution of a process, similarly to what is done in a real experiment. This is best done with a program which can effectively visualize the system, e.g. by a selective visualization of only a part of the atoms, according to some criterion defined by parameters which can be changed in real time. For instance, one can choose those atoms with single-particle potential energy in a suitable energy window. Finally, numerical experiments allow one to vary parameters which are normally fixed, thus exploring the behavior of a system along dimensions not directly accessible to experiment, e.g. by varying the atomic interaction potential or the particles mass. This also allows a straightforward verification of the consistency of specific predictions of theoretical models, for which it would be difficult to set up a real experiment. The program developed at LCE can study N-particle systems, in which particles interact with each other either via a pair-wise or a many-body potential. While the MD code performs the standard computations and evolves the system in time, the GUI visualizes the system, at the same time allowing the user to modify the system parameters and chose an optimal visualization mode for the atoms. The program has been written in C and developed for an X11 Window System platform, all graphics being based on the MOTIF library, used by many UNIX workstations.

![Graphic User Interface](image)

Figure 16: Left: Graphical user interface.
Modeling of thin semiconductor films

Researchers: Laura Juvonen, Francesca Tavazza*, David P. Landau*, Antti Kuronen, and Kimmo Kaski

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Understanding the growth of thin semiconductor films is crucial for developing new types of nanoelectronic devices. We are studying the structure and properties of heteroepitaxial Ge/Si(001) systems which are estimated to be one of the most promising materials for novel electronic and optoelectronic components.

Semiconductor surfaces are often difficult to study because these systems are strongly influenced by the strain-related effects and long-range elastic interactions which requires using large-scale simulation methods. Conventional algorithms can easily get trapped into metastable states, which prohibits the simulation from reaching the correct equilibrium structure.

In order to overcome these problems, we have developed advanced Monte Carlo algorithms which can be applied to problems where substantial configurational rearrangement is required. In the dimer-jump algorithm, trial MC moves consist of long displacements of atom pairs followed by a local relaxation using Molecular Dynamics.

Figure 17 shows a snapshot of a Si(001) surface on which small Si islands are forming. All surface atoms (shown red) are mobile.

Figure 17: Formation of small Si islands on Si(001) using the dimer-jump algorithm. All red atoms are mobile (atom pairs are moved as a unit). The color coding of the atoms in the underlying layers reflects their energy (green is higher and blue lower in energy).
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. In Figure 1 one can see an example of how a twist grain boundary is formed. After the two crystals have been put into contact the atoms at the interface will self-organize into their minimum energy configuration. One cannot experimentally see the atomistic structure of twist grain boundaries, only the grain boundary energy can be measured. Therefore the atomistic structure of the interface is still considered controversial.

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. We are also interested in the grain boundary energy, since it can be compared to experimental results.

Using a combination of molecular dynamics and atomistic Monte Carlo methods we have found crystalline structures for many of the grain boundaries. These results are supported by experimental evidence since these grain boundaries have been measured to have a lower grain boundary energy. These are very important results since previous computational studies 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.
Dislocations in FCC Metals: Interaction of Moving Dislocation with Defects

Researchers: Péter Szelestey, Marco Patriarca, and Kimmo Kaski

$\frac{1}{2}[110]$ type of dislocations, the most common in face-centered-cubic materials, generally dissociate into two partials connected by a stacking-fault region. These dislocations have been the object of much research in recent years especially from their mobility point of view because of its importance in plasticity of materials. The interaction of the moving dislocation with defects is one mechanism obstructing dislocation motion, and the computational approach to study this problem has become an increasingly interesting topic in the past years. We used atomic level, Molecular Dynamics simulations, with the aid of the previously developed Embedded Atom potentials and visualization and tracking methods, in order to investigate the detailed interaction processes.

Our study concentrated on the interaction process of a $\frac{1}{2}[110]$ screw dislocation with a perfect, vacancy-type stacking-fault tetrahedron (SFT). The detailed reaction turned out to depend on several factors, such as the size and the orientation of the defect and the internal structure, the separation distance of partials, of the moving dislocation. When the glide plane of the moving dislocation is the same as one of the planes that bound the SFT, the interaction process includes dislocation reactions, jog line formation and significant bending of the dislocation line. As an important quantity, the critical stress required to move the dislocation through the defect was measured.

Our study has importance in understanding the pinning process of a moving dislocation due to SFT, and the stability and destruction mechanisms of SFT. From the practical point of view our research has special relevance in nuclear materials, which are required to have exceptional mechanical properties while having a typically high concentration of SFTs induced by irradiation.

Figure 20: Snapshots of a stacking-fault tetrahedron (pyramid shaped object) intersected by a dissociated screw dislocation corresponding different defect orientations. The two partials can be identified by the blue lines. Only atoms in the dislocation core and the edges of SFT are shown.
Mechanical Properties of Carbon Nanotubes

Researchers: Maria Sammalkorpi, Kaisa Kauutto, 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. 21 shows an example of a defect typical to irradiation and how such defects can link tubes which efficiently prevents tube-tube slippage.

Figure 21: 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 $C_{60}$. 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 22: 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).](image)
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 of 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).
Sterol Interaction with Membrane Lipids

Researchers: Tomasz Róg, Ilpo Vattulainen and Mikko Karttunen
Laboratory of Physics and Helsinki Institute of Physics, HUT

Cholesterol (Chol) is an important constituent of eukaryotic cell membranes where it accounts for up to 50 mol% of the membrane lipids. The biological roles of Chol involve maintenance of proper fluidity, formation of glyco-sphingolipid-Chol-enriched raft domains, reduction of passive permeability, and increasing the mechanical strength of the membrane. The Chol molecule consists of a planar tetracyclic ring system with the 3\(\beta\) -hydroxyl group and a short 8-carbon atom chain. The planar tetracyclic ring system of Chol is not symmetric about the ring plane. The sterol ring has a flat side with no substituents (\(\alpha\)-face) and a rough side with two methyl substituents (\(\beta\)-face). In natural and model membranes, Chol effectively increases the order of saturated alkyl chains of phospholipids (ordering effect) and the membrane surface density (condensing effect). Chol analogues, whose molecular structures often differ little from that of Chol, affect membrane ordering and condensation much less. Thus, the molecular structure of Chol seems to be optimal for its biological membrane functions.

The main goal of these studies has been to elucidate the relationship between the Chol structure and its effect on the bilayer made of saturated and unsaturated PC molecules. In this aim six model of lipid bilayers were constructed - three composed of DPPC (dipalmitoylphosphatidylcholine), and three of DOPC (dioleoylphosphatidylcholine). To the pure PC bilayer cholesterol and modified cholesterol were added. 100 ns of the molecular dynamics simulation of these systems were performed using GROMACS software. In the modified cholesterol molecules both methyl substituents were removed from the \(\alpha\)-face, so the molecule has two flat faces. Analyses of obtained trajectories will provide information about the role of \(\alpha\) and \(\beta\)-faces of cholesterol as well as help as understand the evolutionary pathway of sterol family on which we observed removal of methyl group.
Molecular dynamics simulations of fully hydrated 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. Such simulations allow an understanding of the structural and dynamic modifications that are necessary to accommodate the anaesthetic molecules within the bilayer. This information may then be used to impose similar environmental influences on integral proteins embedded within a model membrane. These changes to the nanopores or channels in the membrane have a number of repercussions such as to modify the efficiency of ion diffusion through the bilayer. 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.

At present the simulations involved in this work are conducted using GROMACS software. The systems under investigation involve 128 lipid molecules in a bilayer surrounded by solvent water molecules. The lipid bilayers being investigated are dipalmitoylphosphatidylcholine, dioleoylphosphatidylcholine and combinations of each of those with cholesterol. For each bilayer a number of different simulations with different concentrations of anaesthetic gas are considered and the effect on the membrane is quantified by measurable quantities such as the geometric conformation of parts of the system, the lateral pressure profile, 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.

Figure 23: Simulation snapshot illustrating the accommodation of xenon gas in the cell membrane
Computer Simulations of a Polymer Chain under Shear Flow

Researchers: Markus Miettinen, Mikko Karttunen, Michael Patra and Ilpo Vattulainen*

*Laboratory of Physics and Helsinki Institute of Physics, HUT

Project home page: http://www.lce.hut.fi/research/polymer/

The effect of shear flow on rheological properties of polymer mixtures is of great interest because the nonequilibrium nature of the problem makes it theoretically and computationally difficult. On the other hand, looking from the practical point of view, industrial processes often involve polymer mixtures under shear flow. A better theoretical knowledge of how to, e.g., control viscosity and phase separation would have immediate consequences in developing more efficient processes.

Dissolved polymer chains are known to undergo a globule to open coil transition as the solvent quality changes from poor to good. Likewise, it has been found out that an individual polymer chain undergoes a collapsing – stretching behaviour when the solute is exposed to shear. In this study, we look into the combined effect of shear flow and solvent properties to the conformational changes of the polymer chain.

The first part of the study has concentrated on the effect of solvent quality, i.e., studying the properties of a freely floating chain as a function of solubility. This offers a sturdy reference for the second part, which will introduce applying shear to the system. The chain properties will be measured as a function of both the shear strength and the solvent quality.

The solvent is modeled explicitly by monomers interacting with each other through a Lennard-Jones -type (LJ) potential. The polymer model is made up of a few dozen LJ-monomers freely jointed together by nonlinear FENE-springs. The first part of the study will be performed by carrying out Molecular Dynamics (MD) simulations in three dimensions, changing the solvent properties by modifying the interaction coefficients of the LJ-potential. The second part shall consist of Nonequilibrium Molecular Dynamics (NEMD) simulations using the SLLOD algorithm with Lees-Edwards boundary conditions for implementing the shear.

Figure 24: Stretching and collapsing of a single molecule under shear flow.
Dissipative Particle Dynamics Studies of Coarse-grained Polymer Systems

Researchers: Petri Nikunen, Mikko Karttunen, and Ilpo Vattulainen *

*Laboratory of Physics and Helsinki Institute of Physics, HUT

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

The physics of polymeric liquids has been a problem of considerable interest in recent years. From a modeling point of view, these systems are problematic due to the fact that numerous phenomena take place at mesoscopic time and length scales, which are not accessible by detailed simulation techniques such as molecular dynamics. To overcome this problem, a number of “coarse-grained” approaches have been suggested and developed to simplify the underlying microscopic model without changing the essential physics.

One candidate to work with is the dissipative particle dynamics method. It is a particle-based simulation technique which suits particularly well for studies of soft condensed matter systems. Due to this, it has been applied to various systems, including the structure of lipid bilayers, self-assembly, and the formation of polymer-surfactant complexes. In our project, we concentrate on methodological aspects of this method, and apply it e.g. to vesicle formation (figure below).

![Figure 25: Formation of a vesicle. Time goes from left to right, top row illustrating the vesicle from outside and bottom row from inside.](image-url)
5.2.3 Research on Semiconductor Quantum Structures, Bioelectronics and Physics of New Information Technologies

Project home page: http://www.lce.hut.fi/research/nanotech/.

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.

The ever-decreasing size of the basic components of information processing will give quantum effects an important role in future technologies. Recent developments such as quantum cryptography and the idea of a quantum computer have shown that, rather than being only harmful, these effects can probably be utilized to a great extent. In communications technologies, optical transmission is setting the trend in the development of the networks. The full harnessing of the huge bandwidth provided by light still requires for replacing the switching, routing and processing electronics by all-optical components. Research on nonlinear optical materials and light-induced quantum effects will be crucial in the development of future all-optical processing technologies. Related to optical communications technology, we are studying all-optical switching and processing using nonlinear materials, combined with novel material structures such as photonic crystals.

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, will be studied.

Modelling of nanoscale semiconductor devices

Researchers: Fredrik Boxberg, Roman Terechonkov and Jukka Tulkki

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 and the electronic structure using the eight-band \( \mathbf{k} \cdot \mathbf{p} \) 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 modelling 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 26(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 \( \text{Ga}_{0.47} \text{In}_{0.53} \text{As}/\text{Al}_{0.48}\text{In}_{0.52}\text{As} \) (001).

Our model could in future work be extended to dynamic photon and electron processes or many-particle simulations. These kind of simulations would be very valuable for the understanding and development of quantum information processes and related devices.

![Figure 26: Material gain in a lattice-matched \( \text{Ga}_{0.47} \text{In}_{0.53} \text{As}/\text{Al}_{0.48}\text{In}_{0.52}\text{As} \) (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.](image)

**Electron structure calculations of quantum wire superlattices**

The electronic and optical properties of semiconductor quantum structures are governed by the band structure. The band structure can be used to calculate the transition matrix elements, for example, which then can be used to predict the intensity of photoemission as a function of the wave length and excitation (injection) intensity.

The accurate band structure calculations are computationally very intensive. The smart band structure model, discretization and code parallelization are needed for effective electronic structure calculations. The electronic structure of the semiconductor quantum structures we calculate using the eight-band \( \mathbf{k} \cdot \mathbf{p} \) method. In the confinement potential we account for the band edge discontinuity, strain induced deformation potential and piezoelectric potential.

It was observed that for some semiconductor structures the 8-band \( \mathbf{k} \cdot \mathbf{p} \) method gives spurious non-physical eigenstates in addition to the real physical. On the basis of numerical
experiments we found that the origin of the non-physical solutions is in the use of 8-band $k \cdot p$ Hamiltonian which is valid close to the $\Gamma$-point only. A consistent generic solution of this problem would be to start from a full band $k \cdot p$ model and to use it as the starting point of the envelope wave function method but this requires much more computational resources. We found that it is possible to find tune the material parameters in such a way that the bulk dispersion fits the experiment very and at the same time the spurious states are excluded. This method makes the problem to be computationally feasible.

Fig. 27(a) shows the schematic drawing of the corrugated $In_{0.2}Ga_{0.8}As$ quantum well embedded in $Al_{0.2}Ga_{0.8}As$. We used the PARPACK library to diagonalize the Hamiltonian matrix discribing this structure. Fig. 27(b) shows the electron probability density functions calculated for the ground conduction (CB) and valence (VB) band states with confinement energies 0.164 eV and 0.122 eV, correspondingly. Fig. 28 shows the conduction and valence energy bands for the corrugated quantum well structure 27(a). We observed that the spin twice degenerate states at $\Gamma$-point are splitted in $k_x$ and $k_y$ directions. This spin-splitting related to the lack of the structure inversion symmetry.

Figure 27: (a) Schematic drawing of the corrugated $In_{0.2}Ga_{0.8}As$ quantum well embedded in $Al_{0.2}Ga_{0.8}As$. The shaded region between the corrugated surfaces is the quantum well. $P_{QW}$ is the period of the corrugation, $T_{QW}$ is the thickness of the quantum well and $\theta$ is the disorientation angle of the vicinal (111) substrate. (b) The electron and hole probability densities of the conduction and valence band ground states for two periods of the periodical structure 27(a).

**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 slightly 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 and 4) all-optical signal regeneration using partly coherent laser networks. At the moment we are focusing our attention on an all-optical memory element, that could operate faster than the previous bistable systems composed of one or two lasers (See fig. 5.2.3).

The above devices are studied using analytical and numerical models ranging from band structure calculations to stochastic rate equations. The obtained information can be used in improving the existing devices and possibly in creating new ones as well.

Figure 28: The band diagram of the corrugated quantum wire superlattice Fig. 27(a). The band energy is given with respect to the unstrained valence band edge of bulk Al\textsubscript{x}Ga\textsubscript{1-x}As.

Figure 29: a) A schematic representation of a 2R regenerator structure, whose operation is based on partly coherent signals. The structure composes of lasers, optical isolators and band pass filters. b) The simulation results show how the input signal is modified while passing through the device. The picture shows both the regeneration ability and the potential for fast operation.
Quantum Transport in the Ballistic and Coulomb Blockade Regimes

Researchers: 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 in selected two- and three-dimensional channels (See fig. 30). Furthermore we calculated the conductance of a silicon on insulator (SOI) quantum point contact (QPC) by using the MM method at small temperatures where the step like behavior of conductance was observed. The calculated result agrees qualitatively with the measured conductance [M. Prunnila et al., Silicon quantum point contact with aluminum gate, Mat. Sci. Eng. B, 74(1-3):193-196,2000]. Currently we are modeling how the strain affects to the conductance in the QPC and in the quantum wire (QWR) structures due to the changes in the electron eigenstates.

Figure 30: Calculated conductance of the QPC at $T = 0 K$ and $T = 1.5K$. 
5.2.4 Photonic Crystals

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.

We study waveguides in thin slabs of two-dimensional photonic crystals. Conventionally, waveguides in two-dimensional photonic crystals are made by introducing a line defect (see Fig. 31(a)). We have shown that the material on top/below the slab changes the band gap of the photonic crystal slab and we suggest to use this phenomenon to make a new type of waveguide by patterning the photonic crystal slab (see Fig. 31(b) and (c)).

![Figure 31](image)

Figure 31: (a) Conventional defect waveguide. (b) and (c) New type of waveguide: photonic crystal slab with no defects is patterned with a material that changes the band gap of the photonic crystal.

We also study photonic crystal fibers, which have a periodic cladding. We found that when there is a defect ring in the cladding, the fiber has extremely high dispersion, but still a large mode area (see Fig. 32). This type of fiber can be used for dispersion compensation of high power pulses.

![Figure 32](image)

Figure 32: Geometry and dispersion parameter (D) as a function of the core refractive index ($n_{core}$) of the photonic crystal dispersion compensating fiber.
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). 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, e.g., audiovisual speech. Neurophysiological mechanisms of communication are studied by electroencephalography (EEG), magnetoencephalography (MEG) and functional Magnetic Resonance Imaging (fMRI). Psychophysical and EEG experiments are made in our research laboratories located in the fourth floor of the HUT’s new Magnet House. fMRI measurements are made using a new 3-T MRI device (General Electric 3T Signa) in the Advanced Magnetic Imaging (AMI) Centre, located in the Magnet House at the HUT campus. MEG recording are made 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.

5.3.1  Neurocognitive mechanisms of multisensory perception

Researcher: Tobias Andersen, Toni Auranen, Iiro Jääskeläinen, Vasily Klucharev, Riikka Möttönen, Ville Ojanen, Johanna Pekkola, Mikko Sams, Kaisa Tiippana

Effect of preceding audiovisual context on auditory perception

We studied the representations underlying audiovisual integration using a priming paradigm. Audiovisual primes, preceding auditory targets, were either incongruent (auditory /ba/ & visual /va/) or congruent (auditory /va/ & visual /va/, auditory /ba/ & visual /ba/). The targets were /ba/ or /va/. The intensity of the prime’s auditory component was either 50 dB or 60 dB. Identification speed of the target /ba/ was strongly affected by the nature of the prime. The effect of the incongruent audiovisual prime depended on the intensity of its acoustic component. Our results can be explained by assuming that some properties of the visual representation were mapped into the auditory representation.

Processing of sine-wave speech in the human brain

Neural mechanisms for speech perception are localized in left posterior temporal cortex according to previous neuroimaging studies. However, since speech sounds are acoustically different from other sounds, it is possible that the assumed speech-specific activity reflects sensitivity to the complex acoustic structure of speech sounds. “Sine wave speech” (SWS) provides a tool to study neural speech-specificity using identical acoustic stimuli which can be perceived as speech or non-speech, depending on previous experience of the stimuli. 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) (see figure 33). Importantly, activity elicited by the control stimuli, which were always perceived as non-speech, did not change.
during the whole experiment (see figure 33). 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 33: Speech-specific activation in the left posterior STS.](image)

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. 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. 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.

**Modulation of auditory cortex activation by sound presentation rate and attention**

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. 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. 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.

**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) (See figure 34). 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 lobe in the left hemisphere. 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.

**Auditory and visual speech perception activate the speech motor regions** 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 figure 35). 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 lobe, 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. Our results suggest that the speech motor areas provide a common representational space for auditory and visual speech.

**Effects of lip-reading in the auditory cortex** How auditory cortex works is generally less well understood than e.g. functions of the visual cortex. Only recently, evidence has emerged about active information processing and possible multisensory engagement in the auditory areas. For example, lip-reading is known to activate secondary auditory areas, and, in deaf people, even simple visual stimuli (like moving dots) have been shown to activate "auditory" temporal lobe areas.

Using fMRI (functional magnetic resonance imaging), we studied which areas of the auditory cortex would be activated by silent lip-reading, specially focusing to the primary auditory cortex (See figure 36). During fMRI scanning the subjects were intermittently shown a face either silently uttering vowels or a still image of the same face.

We found secondary auditory cortex activation by visual speech in all subjects and primary auditory cortex activation in seven out of ten subjects. This suggests, that primary auditory cortex could actually receive visual input, or possibly modulation of its function by attentional mechanisms (where visual speech cues would "sensitize" the auditory cortex to listening).

In a related study, we utilized 306-channel magnetoencephalography (MEG) in 8 healthy volunteers to test whether seeing speech modulates the responsiveness of auditory-cortex neu-
Figure 34: 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)

rons tuned on phonetic stimuli. Specifically, we hypothesized that seeing a visual articulation causes adaptation of auditory cortex MEG responses to a subsequently presented phonetic sound. Auditory 'test' stimuli (Finnish vowels /ä/ and /ö/) were preceded (500-ms lag) by auditory (/ä/, /ö/), and the F2-midpoint between /ä/ and /ö/) or visual articulatory (/ä/ and /ö/) ‘adaptor’ stimuli. As a separate control, the auditory /ä/ and /ö/ stimuli were presented without the adaptors. The subjects’ task was to behaviorally discriminate between the /ä/ and /ö/ test stimuli. The amplitude of the left-hemisphere N1m response to test stimuli was significantly suppressed with auditory (P<0.001) and visual (P<0.05) adaptors, this effect being significantly greater with the auditory adaptors (P<0.01) (see Fig.37). These findings suggest that seeing the articulatory gestures of a speaker influences auditory speech perception via modulation of the responsiveness of auditory cortex feature-detector neurons tuned on phonetic sounds features. This may relate to recent animal studies suggesting that tuning properties of auditory cortex neurons are modulated by the attentional/motivational state of the organism. The fact that adaptation was significantly greater when auditory as compared to visual adaptors preceded the test stimuli can be explained by additional adaptation to acoustic stimulus features.
We also investigated integration of audiovisual speech (i.e., speech sounds and seen articulatory gestures) and non-speech (i.e., simple tones and seen expanding ellipsoids) objects in the human auditory cortex using EEG. We found out that the auditory N100 response was suppressed when both acoustic and visual components of an object were speech. However, when either acoustic or visual component (or both) was non-speech, the N100 response was not suppressed. The results suggest that the human auditory cortex is involved in integration of speech-specific features of audiovisual speech objects.
5.3.2 Auditory cortex “what” and “where” processing streams

Researcher: Iiro Jääskeläinen, Jyrki Ahveninen

Recent studies have provided evidence for the existence of segregated pathways within the auditory cortex for processing of auditory object/content and location features. These processing pathways have been termed as the “what” and “where” processing streams, analogously to the visual system. The “what” processing stream has been suggested to progress anteriorly/laterally from the koniocortex as a function of increasing complexity of auditory stimulation from simple sinusoids to more complex auditory patterns, such as phonetic sounds. Conversely, increased specificity for “where” information has been observed in areas posterior to the koniocortex. Supporting evidence has been detected by cellular-level measurements in non-human primates, human non-invasive imaging studies, as well as by abnormalities of spatial hearing in patients with lesions in posterior auditory cortex. This segregation of the processing streams is also reflected in areas outside of the temporal lobe; the posterior “where” processing stream was observed to involve parietal cortex and superior aspects of prefrontal cortex, whereas the “what” processing stream was noted to involve activation of the inferior frontal gyrus. Also, in monkey tracer studies the “what” and “where” processing streams were connected anatomically to different areas of the prefrontal and parietal cortices.

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 object and spatial location information. In our recent study (Jääskeläinen et al. NeuroReport 2004)
et al. PNAS 2004), electromagnetic activity was localized using our fMRI/MEG/EEG analysis techniques to areas corresponding with those implicated in previous work to underlie the “what” and “where” processing streams. We observed differential frequency-tuning in the posterior and anterior auditory-cortex areas that could reflect the “what” and “where” processing streams, the neurons in the posterior “where” pathway being more broadly tuned on sound frequency than neurons in the anterior “what” pathway involved in fine discrimination of object features. Further, we observed a close relationship between the suppression of the posterior auditory-cortex N1 activity and reduced behavioral distractibility, implicating that the “where” pathway conducts a relatively fast and coarse stimulus novelty analysis, which could be intimately linked to behavioral “flight-or-fight” responding. Conversely, the anterior N1 activity is presumably generated in areas processing the “what” information. This is also suggested by our preliminary results showing that the anterior N1 activity corresponds to the mismatch response, which in turn predicts attentional discrimination of minute differences in sound frequency, a hallmark of the “what” processing.

In our further studies, we have tentatively confirmed that neural ensembles occupying regions posterior to the human primary auditory cortex are specifically tuned to 3-D sound location cues. Further, we observed that selective attention to sound location features selectively "sharpened" the 3-D location tuning of the underlying neurons (see Fig.38). 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 Häimiläinen and John W. Belliveau.

Figure 38: Grand-average ECD amplitude waveforms for the posterior (Top) and anterior (Bottom) N1m sources in the right hemisphere of 5 subjects. The subjects were here attending to the sound location. Note that the amplitude of the posterior N1m to the second sound (Top) was clearly larger when the sound location changed in relation to the first sound.
5.3.3 Artificial Person

Researchers: Martin Dobšík, Michael Frydrych, Jari Kätsyri, Mikko Sams

Speech is both heard and seen. Visible articulatory movements significantly improve speech perception, especially when the acoustic speech is degraded because of, e.g., hearing impairment or environmental noise. There is an evidence that the speech perception improves significantly also with computer animated audio-visual speech synthesizers, talking heads.

We have developed a toolkit for real-time computer animation of Finnish-speaking talking head, "Artificial Person". We have paid special attention in improving the quality of audio-visual speech. Synchronized auditory and visual speech are automatically produced from input text, which can be enriched by user definable commands to perform specific gestures, as for example facial expressions (Fig. 39). The Artificial Person is able to express six basic emotions (anger, disgust, fear, happiness, sadness and surprise) and their combinations.

![Artificial Person](image)

Figure 39: Artificial Person. Expressions from left: neutral, sad and surprised.

5.3.4 Modeling Emotion

Researchers: Michael Frydrych, Vasily Klucharev, Jari Kätsyri, Mikko Sams

Face plays an important role in social interaction. It conveys information of, e.g., person’s identity, gender, attractiveness, health, emotional expressions, gaze (attention) direction, cultural group and social status. Facial movements may accentuate spoken information, convey additional information or regulate conversation between several speakers. Understanding how people process, recognize, and interpret each other’s faces and facial motion is a challenging task that has attracted hundreds of scientists in both the social science, computer vision and psychology communities.

We started creation of the first Finnish digital collection of natural emotional facial expressions. The database contains recordings of six basic facial expressions (anger, disgust, fear, happiness, sadness, and surprise) acted by 8 human subjects. We studied identification and naturalness of basic emotional expressions with both natural and synthetic stimuli. The expressions were presented as static (pictures) and dynamic (movie sequences). We also studied the effect of distortion on facial expression identification (Fig. 40).

We have also developed a toolkit for real-time computer animation of Finnish-speaking talking head. Current version produces synchronized auditory and visual speech from input text, and displays facial expressions.
Figure 40: The identification scores for dynamic presentation decrease less with increased distortion.

Using fMRI we investigated what brain areas are activated when observing static vs. dynamic (naturally moving) facial expressions of happiness and disgust. Dynamic facial expressions invoked stronger activations in comparison to still pictures in areas MT, STS, and FFA (Fig. 41). The results suggest that STS is activated more by natural motion from neutral to emotional face than by picture of the same emotional face alone and that moving emotional facial expressions elicit stronger activation in certain emotion-specific areas.

Figure 41: Difference in brain activations for dyn_hap>sta_hap. From left to right: Medial temporal area (MT/V5), superior temporal sulcus (STS), fusiform face area (FFA) and globus pallidum (PLD).
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 theoretical and numerical 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.
During the recent years, the network approach to complex systems has turned out to be extremely fruitful. In this approach, diverse systems are viewed as networks, so that the interacting elements are described by network vertices and their interactions and/or relationships by edges connecting the said vertices. Systems well suited for studies in this framework are ubiquitous in Nature – neural networks, social networks, the Internet, networks of epidemic spreading, metabolic networks in cells. Perhaps the main strength of this approach is its ability to capture the salient features of the systems in question with simple building blocks - the edges and vertices - 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) and the ubiquitous scale-free connectivity distributions.

In addition to the structural properties of these systems, there has been wide interest in dynamic phenomena taking place on such networks. Examples include models of opinion formation and the dynamics of spreading via contact processes, such as the propagation of rumours and information in social networks and epidemic spreading of disease. Related to the latter, one example of our research is a model of the spreading of influenza-like disease on dynamically changing small-world contact networks; this framework yields readily to an analytical treatment in addition to numerical simulations. Although the model is rather minimal and the structure of the contact network is simple, the spreading dynamics produced by the model matches real-world data with very good accuracy (see Fig. 42).

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.
Weighted Complex Networks

Researchers: Jukka-Pekka Onnela, Jari Saramäki, Kimmo Kaski, Janos Kertesz*

* Budapest University of Technology and Economics

Complex networks provide a very general framework, based on the concepts of statistical physics, for studying systems with large numbers of interacting agents. The nodes of the network represent the agents and the links correspond to interactions between them. The network approach to complex systems, ranging from the WWW to the metabolism of cells, has turned out to be extremely fruitful during the last few years. Studies of network characteristics have produced unexpected findings, e.g. the ubiquity of scale freeness and the small-world phenomenon. The local structure of unweighted networks can be characterized by the appearance of small subgraphs, so-called motifs, and the networks’ clustering properties, which have been related to network functionality. We have generalized these approaches by providing a set of theoretical and practical tools for analyzing weighted complex networks, an effort motivated by the community’s growing need in this direction. We have studied these concepts for both empirical networks and theoretical network models. We have also studied the formation and self-organization of weighted complex networks starting from local microscopic mechanisms and transmission of information on weighted networks.

Figure 43: 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 Himmeli software package by Ville Mäkinen.
Multiagent models for complex adaptive systems

Researchers: Marko Sysi-Aho, Jari Saramäki, Kimmo Kaski, Janos Kertesz*
* Budapest University of Technology and Economics

The self-organization of a population of agents with limited capabilities for scarce resources is an interesting problem and has potential applications in biology, economics and social sciences. For instance, predators that choose their turfs for hunting prays, and data routing in mobile network fit into this framework. The minority game (MG) is a simple agent-based model reminiscent of these systems. The game consists of $N$ (odd) agents who decide between two alternatives, A and B. Those who belong to the minority, win. The agents have access to a global history, a historical record of the past $M$ winning sides, and they are endowed with $S$ strategies that assign a choice for each possible history. Regardless of the individual agents’ self-interested pursuit, the population of agents shows coordinated behaviour. Previous studies indicate that in case the agents are allowed to evolve, they tend to evolve such that the population as a whole performs the best. To allow evolution, we have applied genetic algorithms to the MG. Our results show that natural selection and genetic algorithms are efficient methods to boost the performance of the population as well as individual agents in this toy world.

Figure 44: Coordination among agents in minority games: lower values mean good coordination. Application of genetic algorithms lead to a considerable improvement in coordination compared to the basic game.
Multi-agent models of economy systems

Researchers: Marco Patriarca, Anirban Chakraborti, and Kimmo Kaski

The importance of studying economy models is related to the fact that there are well known regularities in the structure of real systems. For instance the century old Pareto law in Economics states that the higher end of the distribution of income \( f(x) \) follows a power-law, \( f(x) \propto x^{-1-\alpha} \), where \( x \) is the income (money) and the exponent \( \alpha \) has a value in the interval 1 to 2. We study a simple statistical model of closed economy, in which \( N \) agents can exchange money in pairs between themselves, which can be solved either numerically or analytically, in order to investigate the relation between its internal dynamics and the corresponding final equilibrium distribution. All the agents are initially assigned the same money amount. Agents are then let to interact. At every “time step”, a pair \( (i,j) \) is randomly chosen and the transaction carried out. During the transaction, a fraction \( (1 - \lambda) \) of the agent money \( x_i \) and \( x_j \) is randomly reassigned between the two agents. The exchange law is such that the money is conserved during the transaction, i.e. \( x_i + x_j = x_i' + x_j' \),

\[
x_i' = \lambda x_i + \epsilon (1 - \lambda)(x_i + x_j),
\]

\[
x_j' = \lambda x_j + (1 - \epsilon)(1 - \lambda)(x_i + x_j).
\]

where \( \epsilon \) is a random number and \( \lambda \) the saving propensity (0 < \( \lambda \) < 1). Money distributions for arbitrary \( \lambda \)'s are well fitted by the function

\[
f_n(x) = a_n x^{n-1} \exp(-a_n x) ,
\]

\[
n(\lambda) = 1 + 3\lambda/(1 - \lambda).
\]

where \( \Gamma(n) \) is the Gamma function and \( a_n = \Gamma(n)^{-1} (n < x >)^n \) is a normalization factor. This particular form of \( n(\lambda) \) was suggested by a mechanical analogy between the closed economy model with \( N \) agents and the dynamics of a gas of \( N \) interacting particles. In fact this is just the Maxwell-Boltzmann distribution for the kinetic energy of a gas in \( D - 2n \) dimensions and at a temperature \( T \sim < x > / nk_B \). The fitting curves for the distribution (continuous curves) are compared with the numerical data in the figure [for details see M. Patriarca, A. Chakraborti, and K. Kaski, Physica A 340(2004)334 and Phys. Rev. E 70(2004) 016104].

![Figure 45: Money distributions and interpolating functions (linear and log scale in the y axis).](image)

52
Simple models for language evolution and diffusion

Researchers: Marco Patriarca, Teemu Leppänen

History and distribution of languages still represent open problems. Recently, a master equation based model was successfully used for describing the high rate at which world’s languages are disappearing [D. M. Abrams and S. H. Strogatz, Nature 424 (2003) 900]. In this model languages are treated similarly to competing species, – i.e. as non-evolving entities – despite their evolution is probably described more realistically from an evolutionary point of view [Christian Schulze and Dietrich Stauffer, cond-mat/0411162]. The model however provides a satisfactory quantitative description of their interactions and predicts that, in a situation of homogeneity and close interaction between all the speakers, only one language survives. We suggest a generalization by introducing a space-dependence in terms of a reaction-diffusion equation. The model can take into account more special situations, in which, due to geographical constraints, a language can actually survive, despite the presence of a more influential language, as in the example shown in the figure [for details see M. Patriarca and T. Leppänen, Physica A 338(2004)296].

Figure 46: Population densities of language A (lower row) and B (upper row). From left to right: initial, intermediate, and final stationary configuration. A and B zones are explicitly shown only in the initial state.
Internet and computerized production and use of information have by now created one of the largest societies of over 800 million associates. Within this context online relationships and dating have existed for roughly ten years. In the Western world a growing proportion of the population is composed of singles and career and time pressures are increasing. 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 regular people, or at least regular 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.

Hardey has recently emphasized that Internet dating sites are only one example of a growing number of virtual places that have developed to bear a potential impact on 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 characterizes 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. Thus, 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 behavior 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, particularly 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 utilized for management of customer relationships in general.

In our work we are focusing on the capabilities of self-organizing maps (SOMs) in sociological data analysis and on the small-world aspects in social networks. Currently we are analyzing a data set, 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. Using this data, we aim to illustrate the power of SOM in profiling and visualization of complex sociological data, to analyze and discuss the importance of various individual properties on online and offline relationships, and, to analyze and understand principles of online interaction and social networks.

Figure 47: Illustration of a SOM in a 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-organizing process, from the parameter vectors of all individuals. Thus, the feature vectors characterize average individuals using exactly the same multidimensional parameter space as originally utilized for the individuals. The SOM shown in this figure is for 3321 men and labeled for the age-parameter.
5.5 Computational Systems Biology

Computational systems biology is a new and rapidly developing field of research with focus to understand structure and processes of biological systems at molecular, cellular, tissue and organ level, through computational modeling and novel information theoretic data- and image analysis methods. With the break-through 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 functions of bio-molecules, information stored in DNA (bioinformatics), its expression to proteins, protein structures (proteomics), metabolic pathways and networks, intra- and inter-cell signaling, and the physico-chemical mechanisms involved in them (biophysics).

Using the computational information theoretic and modelling methodologies to experimental geno- and pheno-type 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, Computational Systems Biology focuses either on information processing of biological data or on modeling physical and chemical processes of bio-systems. Through this type of quantitative systems approach Computational Systems Biology can play central role in predicting diseases and preventive medicine, in gene technology and pharmaceuticals, and in other biotechnology fields.

For these reasons the Computational Systems Biology has been added to the educational curriculum of the Laboratory of Computational Engineering. The aim is to train all-around bio-computing experts for research, development, design, consulting, and services in public as well as private sectors.
Researchers: Jukka Heikkonen

Spectrometries, e.g. infrared or mass, are one of the best ways to analyze either liquid or gaseous samples. Traditionally in spectroscopy analysis the composition of the mixture spectra is solved using a library of reference spectra. The simplest and most common way to perform the mixture analysis of measured spectra based on linear multicomponent spectrum model is via the traditional least square (LS) technique, in which the compounds of the measured spectra to be solved are explicitly stated and assumed to be known before estimating their concentrations. In many cases, however, the measured spectra may contain unknown compound(s) that hence are not explicitly stated in the model to be solved, and the traditional methods will fail.

The goal of this project was to develop robust and efficient methods for spectroscopy based compound sample analysis. The leading idea behind our approach was to model the effect of the unknown compounds on the residual of the linear multicomponent spectrum model. The experimental results have demonstrated that when the residual model defined is combined with the Maximum Likelihood approach, the proposed new method ($ML(P_1)$) can separate the complex multicomponent mass spectra into their individual constituents more robustly compared to the traditional LS and M-estimator ($ML(P_{ME})$) solutions, as can be seen in Fig. 48.

In addition, one of the goals of the project is the development of new mathematical methods for deconvolution of identity and quantity of individual compounds present in environmental/industrial samples on the basis of simultaneously measured mixture spectra of both mass (MS) and FTIR spectroscopy techniques. When the analysis errors of the MS and FTIR methods do not correlate their combination will give more accurate solution for the concentration of the compounds.

![Figure 48: Sum squared errors of the three compound sample analysis methods for the 36 estimation cases with possible unknown compound(s) in the measured spectrum.](image-url)
**Image Alignment in Electron Tomography**

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

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 solved by using geometric computer vision methods.

During the five previous years, we have been developing automatic methods to solve the image alignment problem. The first method was designed to automatically pick fiducial gold particles from the preparation. For cases where it is not possible to use gold particles, we have proposed an alternative approach based on tracking high curvature points of the intensity surface of the images. The most previous development of these markerless alignment methods has shown to give the state-of-the-art accuracy level that have previously achieved only by using fiducial markers. The development of the alignment algorithms is still going on for wider applicability and to take computational aspects into consideration.

![Figure 49: Superimposed point tracks before (left) and after (right) image alignment. The colour indicates the track length](image)

58
Predicting Protein interactions partners and the details of interaction

Researchers: Vibhor Kumar, Jukka Heikkonen, and Peter Engelhardt

Protein interaction has been studied by two approaches, experimental approach and computational approach. Experimental approach uses techniques like mammalian two hybrid, immuno gold labeling and localizations. This experiments involve lot of time and resources, so computational approach to find interaction partners so computational approach is required to reduce the search space for interacting proteins. The computational approach uses some well known methods like studying network topology of interacting proteins and evolution, co-expression of genes and structural docking. Even after a interacting partner of a protein is known, the challenge still remains for finding the exact mode of interaction and finding the forces involved among amino acids leading to the interaction.

Figure 50: Our approach is to find interaction partners computationally and get the result validated in collaborated laboratories. We found the interaction mode of N proteins of Hanta virus, explaining the role of each and every amino acids in interactions. Presently we are involved in finding interaction partners of some of the Cell-junction proteins, in order to decipher the undiscovered cell signaling pathways. Our approach is not only using network topology and docking but also the sequence patterns of proteins. Our work progresses together with wet lab experiments, so that there is no chance of having wrong hypothetical conclusions. We also make 3D models of interaction junctions and forces among amino acids at the junction.
Gene regulatory networks
Researchers: Jukka Heikkonen, Vibhor Kumar, Aatu Kaapro

Gene regulatory networks govern which genes are expressed in a cell at any given time, how much product is made from each one, and the cell’s responses to diverse environmental cues and intracellular signals. A popular model of regulation is to represent networks of genes as if they directly affect each other. Such networks do not explicitly represent the proteins and metabolites that actually mediate cell interactions. Understanding, describing and modelling such gene regulation networks is one of the most challenging problems in functional genomics.

Technological advances have enabled us to collect different types of data at a genome-wide scale, such as gene and protein expression measurements, protein-protein and protein-DNA interaction data and DNA sequences. This flood of large scale data can be used for mining gene-to-gene interactions. Methods that have been applied to gene regulatory network inference include among others, boolean networks, bayesian networks and recurrent neural networks. There are known effects, for example time lags, that the current models do no take into account.

At the moment Bayesian network models are probably the most popular approach for inferring gene interaction networks. However, using a single type of data has proven not to be sufficient. Information from different sources needs to be combined to further enhance the performance of current inference algorithms. Bayesian methods provide an elegant framework for combining these different sources of information. We intend to further develop these algorithms and investigate their possibilities for example in experiment design.
Promoter-recognition-in silico

Researchers: Udyant Kumar, Jukka Heikkonen, Kimmo Kaski

In biological systems the flow of genetic information follows central dogma principle i.e DNA-> RNA-> Protein. The processing of DNA to RNA is called transcription and from RNA to Protein is called translation. Transcription and translation follow several steps and are controlled by several other factors which is called gene expression control. Examples of transcriptional control are DNA packing, DNA methylation, chromosome puffs and roles of promoter and enhancer regions and translational control is RNA processing, lifetime of mRNA, masked messengers, polypeptide cleaving etc. Promoters are region of DNA immediately upstream of transcription site to which multiple transcription factors bind at specific sequence boxes to promote initiation of transcription. Other DNA region upstream of transcription site which are required for promoter activation are called enhancers. Since promoters act as CPU(central processing units) of gene transcription, its proper identification in genomic sequence will give a clear picture of gene regulatory network and will lead to proper recognition of the cause of several genetic diseases. The promoter detection is carried out both experimentally and computationally. But experimental methods are often time-consuming hence it needs the help of computational methods also. But it is not easy to predict promoters and other transcription factor binding sites in a genomic sequence due to complex network of DNA-TF. The available softwares provide good solutions with limited accuracy. Hence there is a great need to provide a novel idea to predict promoters accurately which must be based on sequential structure of DNA and the physicochemical properties involved in DNA-protein interaction network.

The current project is related with the development of a novel idea for promoter recognition-in silico and its application on diabetes data.

Figure 51: Eukaryotic promoter recognition.
Automated allele calling method for capillary array electrophoresis genotyping

Researchers: Jukka Heikkonen, Janne Ojanen, Timo Miettinen *
* Finnish Genome Center, University of Helsinki

The project is done in co-operation with Finnish Genome Center.

Capillary array electrophoresis instruments provide a platform for high-throughput genotyping, on which more than 10 000 genotypes can be generated per day. However, the capacity of available genotyping software for analyzing the data does not meet the throughput of the electrophoresis instruments. In order to ensure high quality of the genotypes, most of the software require substantial manual editing following an initial semi-automated allele calling process. Therefore the current allele calling methods have become a serious bottleneck for the entire genotyping pipeline.

Our aim is to develop fully automated method to minimize user interaction. In addition we have implemented a number of quality measures to remove ambiguous results in order to avoid miscalls. Quality scores are calculated for each processing step separately to provide information on the quality of the signal and the reliability of the decision making processes of the program.

The portion of alleles that the new method was able to read correlated 100% to the number of alleles called manually. Also, the allele sizes corresponded with the sizes determined with the software provided by the manufacturer of the instrument. Thus, the new method provides a tool for fully automated, high accuracy genotyping. The automated genotyping software based on the proposed method will be made available free of charge under the GNU General Public License (GPL).

Figure 52: Capillary array electrophoresis genotyping workflow.
Proteinuria is a common medical symptom often found in association with infectious, inflammatory or immunological diseases. However, the most important cause is the progressive kidney damage due to diabetes. Kidney complications constitute more than 15% of total health-care costs in most Western countries, mainly due to increasing prevalence of diabetes-associated kidney disease.

The ADDNET consortium, funded by the Sixth Framework Programme of the European Union and headed by Prof. Harry Holthöfer at the University of Helsinki, is focused on creating a paradigm shift from kidney biopsies to advanced molecular diagnostics from patient urine. Our contribution to the project is the gene expression analysis of microarray data produced from human single gene disease CNF patient samples as well as its transgenic animal model samples.

Microarray technologies provide a way of measuring simultaneous transcriptional activities of thousands of genes. However, even though the expression levels of a multitude of genes can be determined at one time, usually the number of independent samples remains very low due to experimental costs and small amount of available tissue samples for RNA extraction. This makes the attempts of recovering biologically relevant information through means of statistical data analysis highly challenging. The ultimate aim of the gene expression analysis in ADDNET project is to discover candidate genes which could be associated in the pathogenesis of proteinuric renal disease and thus act as an input for further bioinformatic and wet-lab analysis.

Figure 53: Typical microarray experiment setting: statistical inference has to be performed with only few high-dimensional samples. (Individual genes on the horizontal axis, arrays on the vertical axis.)
Modeling of Bacterial Metabolism

Researchers: Mika Toivanen, Maija Vanhatalo, Antti Nyyssölä*, Matti Leisola* and Kimmo Kaski

Laboratory of Bioprocess Engineering, TKK

The interest in computational methods in biological applications has recently been increasing greatly. At LCE we have been active in kinetic modeling of bacterial metabolism. Specifically we have been constructing a model of glucose and xylose metabolism in a lactic acid bacterium *Lactococcus lactis*. The model is based on mechanistic rate equations or power-law kinetics. These methods will be benchmarked in terms of computation speed and rate of convergence in parameter estimation. Furthermore, we wish to use our model to study a mutant strain with a xylose reductase gene from yeast *Pichia stipitis*. The mutated strain is able to produce xylitol from xylose.

Recently, the model was transferred from Matlab to Fortran for the sake of performance. At the same time we gave up the possibility of using *in vitro* parameters in the model and turned towards parameter estimation methods. These methods are stochastic in nature and require a fast evaluation of the objective function. Transfer to Fortran has increased the performance of the model approximately 20-fold.

In November 2004 we made a set of cultivation experiments in collaboration with the Laboratory of Bioprocess Engineering and MediCel ltd. We have studied the metabolism of the native and mutated strains by measuring the concentration of internal and external metabolites during the 8 hour batch cultivation. The data was used to estimate the parameters of the model which we hope to exploit in predicting the changes in fermentation characteristics in response to genetic engineering. The goal is to propose mutations that maximize the efficiency in xylitol production.

Figure 54: The challenge we have taken is to integrate a large variety of information sources into a single model. Copyrights by M. Rousseau (INRA), INRA 2001 and Protist Information Server 1995-2005.
Genetic and Environmental Background of Kidney Disease in Type 1 Diabetes

Researchers: Ville-Petteri Mäkinen, Per-Henrik Groop*, Maija Wessman*, Carol Forsblom*

* Folkhälsan Research Center, Biomedicum Helsinki

Diabetes is turning into an epidemic in the developed world. In Finland alone, there are over 200,000 patients, of which over 30,000 have the type 1 diabetes (T1DM) that is characterised by young age of onset and total dependence on external insulin. The immediate cause of T1DM is the autoimmune reaction against the insulin-producing cells in the pancreas, but the triggering mechanism is still unknown. Although the patients can survive, the lack of natural insulin response has adverse long-term effects on the body.

After 20 years of T1D, a third of the patients have or are in the process of developing diabetic kidney disease, usually accompanied by damage to the blood vessels and heart. The gradual degradation of health is the most dangerous aspect of diabetes, since the changes are often irreversible and very costly in every sense of the word. Furthermore, at present day, there is no reliable method that would allow the detection of high-risk patients and effective early treatment.

The FinnDiane study, headed by Doc. Per-Henrik Groop from the Folkhälsan Research Center, aims for the identification and prediction of diabetic complications. Currently, the research group has accumulated clinical information of roughly 5000 type 1 diabetic patients and 1500 relatives in Finland – the largest such collection in the world. In addition, the genetic research consists of a genome wide scan of 120 selected families and association studies of candidate genes that have a biological role in the kidneys and related tissues.

Finding regularities in the patient data requires advanced statistical modelling and computational techniques. Classical methods are often built on a null hypothesis that is rejected if the data is not random. With a large number of different types of variables this approach is not applicable, and more advanced non-linear or algorithmic models must be used. Here the expertise of LCE in the field will be of critical importance.

Figure 55: Pedigree with diabetes and kidney complications from the FinnDiane database (produced by CraneFoot, see www.lce.hut.fi/~vmakine2/cranefoot/ for further details).
Structure of Lipoprotein Particles


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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 and/or bile acid formation. 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 favour of such molecular interactions between LDL lipid constituents that result in specific domain formation in the particles. We termed these local environments 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 lipid chemical structure may also relate to the effects of alcohol and alcoholism on reverse cholesterol transport; it is known that alcohol does have beneficial effects on lipid 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 unpublished 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.

In the current multidisciplinary collaboration we are focusing to study the molecular structures of both discoidal and spherical HDL particles as well as native and modified LDL particles. To reach the general goal - detailed molecular understanding of lipoprotein structure and dynamics - we will be applying, experimentally, proton and carbon-13 nuclear magnetic resonance spectroscopy, cryo-electron microscopy, microcalorimetry, surface plasmon resonance, circular dichroism spectroscopy and LC mass spectrometry, and, computationally, molecular dynamics, Monte Carlo -methods and dissipative particle dynamics.

Figure 56: 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.
The multitude of different sex determination and reproduction mechanisms found in nature is not easily approached by conventional methods. First of all, this diversity is an evolutionary paradox: Darwinian natural selection should favor and spread a good solution for a function as important as reproduction, not scatter it. Secondly, the biological concept of sex determination is based on terms like maleness and femaleness. The scientific exactness of these attributes is far from good and a more formal understanding of the origin of this dichotomous phenomenon is to be hoped for. Thirdly, the role played by the germ cells is often neglected in sex determination studies. This lack of interest is most surprising because individuals with no functioning germ cells immediately become evolutionary dead ends. Further complications are added by the observations that germ cell sex determination does not necessarily follow the same sex determination program that establishes all other sexual characteristics of an individual.

In order to explore this important area of biology we have started a systems approach that is to provide a conceptual framework in terms of which to analyze experimental results. We want to create a formal model that allows effective use of computational and mathematical modeling methods because the amount of experimental data is increasing enormously fast. It is also important that the model is presentable in a way that allows co-evolution of theory and experiment.

The preliminary results of our theoretical analysis of germ cell biology involved many different phyla and showed a novel way to link sexual reproduction and multicellular development. This is important because the persistence of sexual reproduction especially in the more complex diploid organisms has been considered to be a major problem in evolutionary theory. Further more, our work sheds light on the relationship between somatic and germ line development. This is important for both reproductive biology and stem cell research.
5.6 Wolfson College, Oxford: Advanced Computational Science and Engineering

As an extension to the Centre of Excellence activities a joint affiliate centre between CCSE and Wolfson College of Oxford University was set up in Oxford with the state of the art cluster-computing facilities and with two full time researcher concentrating on Advanced Computational Science and Engineering (ACSE). The affiliate centre hosts every year 2-3 visiting scholars from CCSE to interact with Oxford scientist for further researcher training.

The research of ACSE is collaborative effort with scientists in Theoretical Physics (Professors Sir Roger Elliott, Douglas Abraham and Robin Stinchcombe) of the Department of Physics, in Information Engineering (Professor Mike Brady) of the Department of Engineering Sciences, in Materials Science Department (Professor: Adrian Sutton), and in Mathematical Biology (Professor Philip Maini) of Mathematics Institute of the University of Oxford.

Robust segmentation of textured images

Researcher: Veit Schenk$^{1,2}$

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The aim of this project is to robustly segment, classify and quantify images of underwater scenes. The objects of interest are coral which are photographed at regular intervals. This allows to monitor the change of the coral over time, thus providing information of how environmental factors affect the growth of coral. The difficulty with performing this task manually is that the number of individual corals is large and the measuring process consequently firstly very time consuming and secondly difficult to perform accurately and repeatedly. We propose the following system to (semi-)automate the process: The first step involves distinguishing coral from other objects such as sand, rock, algae etc. To achieve this, we use a boosting-approach to positively identify individuals of each species of coral of interest. This not only removes any objects which are not coral (or at least not of the species we are interested in), but also provides a starting point for the second stage, the quantification: we fit a deformable model of the species of interest to the individual candidates. Since the data is rather noisy, as illustrated in Fig. 57 and hence difficult to segment using plain edge-detectors, we use textons to jointly segment and classify individual regions of each individual coral. Fig.58 illustrates one particular species.

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Figure 57: Section of a coral-colony. This illustrates the difficult nature of the images: the illumination is non-uniform, they are relatively noisy (in terms of image content) meaning that traditional edge-detectors would not work very well at identifying individual corals.

Figure 58: Closeup of a coral (*Diploastrea heliopora*). The centre is a very different texture compared to the ‘outside’ which spreads radially out. The outside is the same texture all around, but varies in orientation and scale.
The centre consists of a unique texture (small whitish-grey bubbles). The surrounding main part of the body consists of rings radiating out from this centre. The difficulty arising in this particular case is that the main body is strongly isotropic, i.e. standard region-based textons will produce different responses around the body, despite the entire area clearly consisting of the same texture. A further problem is the change of illumination due to the lighting coming from one side and the corals being raised, i.e. casting shadows on one side. We address the lighting-issue by using local energy operators, and extracting phase-information which is contrast/lighting invariant. The rotation-invariance issue is still an open problem. These textured regions are then used to determine the boundaries which are used to control the deformable model (consisting of 'energy' terms, one related to the inherent deformation, the other one to the fit to the data). Once the deformable model has been fitted, information about the size of the coral can be extracted. (in each image, a ruler will be photographed as part of the scene in order to provide scale information). A future application will be to match a scene containing coral from one time-instant to another, thus providing information about the change over time. Initially, this comparison is performed manually.
Wetting effects at a grain boundary; statics and dynamics

Researchers: D. B. Abraham\textsuperscript{1}, Ville Mustonen\textsuperscript{1,2} and A. J. Wood\textsuperscript{1}

\textsuperscript{1} Department of Physics - Theoretical Physics, University of Oxford
\textsuperscript{2} Laboratory of Computational Engineering, Helsinki University of Technology

We study the statics and dynamics of a two-dimensional Ising lattice system with a grain boundary in the middle. The grain boundary can be introduced by weakening the vertical bonds of the lattice by a factor $b \in [0, 1]$. By imposing Dobrushin boundary condition and keeping the system below bulk critical temperatures, an interface is formed (see figure 59). With the grain boundary there are two competing configurations for the interface to adopt; a straight interface with an angle $\phi$ and a zig-zag configuration which consists of two fluctuating sections of interface which are connected along the centre line by a further interface pinned to the defect line, see figure 60. We demonstrate that the crossover between these two is manifested by a phase transition which we call the Geodesic-to-zig-zag (GZZ) transition.

Furthermore we study the relaxation of the system using continuous time Monte Carlo with Kawasaki dynamics. The system without a grain boundary relaxes using capillary fluctuations, whereas in the case of a grain boundary mass transport through defect line dominates the relaxation process. This means that by introducing a defect line into the system one is able to confine the mass transport to the minimum energy pathway. To draw an analogy to the precursor film phenomenon in the dynamics of wetting, one can say that the grain boundary acts effectively as a substrate with a chemical potential favouring spreading.

We also consider the Horizontal-Solid-on-Solid (HSOS) formulation of the problem and show how the phase diagram of the full problem can be recovered in a appropriate scaling limit. The HSOS formulation enables us to study the dynamics of the problem analytically via Langevin equation. Again the main results of the full problem are recovered.

![Figure 59](image1.png)

Figure 59: System without a grain boundary has an interface crossing the system in angle $\phi$.

![Figure 60](image2.png)

Figure 60: System with a grain boundary adopts a dog-leg configuration below the transition temperature.
6 Research Activities

6.1 Visits to the Laboratory

- Yurii Alexandrov, Prof., Russian Academy of Science, Russia.
- Rafael Barrio, Prof. Autonomous University of Mexico, UNAM, Mexico.
- Giorgio Bonmassar, Dr., Harvard Medical School, USA.
- Gemma Calver, Dr., Oxford Centre for Functional Brain Imaging, University of Oxford, UK.
- Ruth Campbell, Prof., University College London, UK.
- Anirban Chakraborti, Dr., Brookhaven National Laboratory, USA.
- Holland Cheng, Prof., Division of Biological Sciences, University of Carolina, USA and Karolinska Institute, Sweden.
- Michael Coady, Dr., Groupe d’études des protéines membranaires, Université de Montréal, Canada.
- Martin Dobšík, M.Sc., Brno Technical University, Czech Republic.
- Burkhard Dünweg, Prof., Max-Planck-Institut für Polymerforschung, Germany.
- Sir Roger Elliott, Prof., University of Oxford, UK.
- Guðmundur Haraldsson, Prof., University of Iceland, Iceland.
- Erin Hayes, M.Sc., Northwestern University, USA.
- Nobuyasu Ito, Prof., Dept. Applied Physics, The University of Tokyo, Japan.
- David Landau, Prof., University of Georgia, USA.
- Philip Maini, Prof., University of Oxford, UK.
- Nikolas Provatas, Prof., Department of Materials Science and Engineering, McMaster University, Canada.
- Jorma Rissanen, Prof.Emer., IBM Research Center, Almaden, USA.
- Christopher Roland, Prof., North Carolina State University, USA.
- Mohsen Sabouri, Dr., Virginia Polytechnic Institute and State University, USA.
- Celeste Sagui, Prof., North Carolina State University, USA.
- Julian Shillcock, Dr., Max Planck Institute of Colloids and Interfaces, Potsdam, Germany.
- Peter J. Slotte, Prof., Åbo University, Finland.
- David Tomanek, Prof., Michigan State University, USA.
- Susumu Uchiyama, Dr., Osaka University, Japan.
- Jamie Wood, Dr., University of Oxford, UK.
- Kin Wah Yu, Prof., the Chinese University of Hong Kong, China.

6.2 Visits by Laboratory Personnel

Sami Brandt

Michael Frydrych
- Brno Technical University, Czech Republic
  - 9.-16.6.2004
  - 28.-31.12.2004
- Aristotle University of Thessaloniki, Greece, 25.-28.8.2004
Iiro Jääskeläinen
- Massachusetts Hospital - Massachusetts Institute of Technology - Harvard Medical School Athinoula A. Martinos Center for Biomedical Imaging and Georgetown University Medical Center. March 19-25, 2004, Charleston, MA, USA.
  - Talk: "What" and "where" - dynamic parallel processing of sound novelty and object characteristics in the human auditory cortex.

Kimmo Kaski
- Department of Physics, Simon Fraser University, Vancouver, Canada, 10-11 and 16-17 November, 2004.
  - Invited talk: Turing systems, models of biological morphogenesis.
- The Institute of Theoretical Physics, Chinese Academy of Sciences, Beijing, China, 2-4 November, 2004.
- Institute of Physics, Budapest University of Technology and Economics, Hungary, 5-8 October, 2004.

Mikko Karttunen
- Dept. of Physics, Oakland University, Rochester (MI)
- Dept. of Biophysics, Jagiellonian University, Krakow (POL)
- Finnish IT Center for Science, Espoo (FIN)
- Dept. of Physical Chemistry, Stockholm University (SWE)

Timo Kostiainen

Jukka-Pekka Onnela
- Professor Albert-László Barabási, Department of Physics, University of Notre Dame, IN, USA, November 2004.
- Professor János Kértesz, Department of Theoretical Physics, Budapest University of Technology and Economics, Hungary, September 2004.

Marco Patriarca
- Department of Mathematics at King’s College, London, July 2004.
  - ESD COST-P10, short term visit fellowship.
- Institute of Theoretical Physics, Tartu University, October, 2004.

Aapo Nummenmaa

6.3 Participation in Conferences and Seminars

Sebastian von Alfthan
- XXXVIII Annual Conference of the Finnish Physical Society, March 18-20, 2004, Oulu, Finland
  - Talk: Clusters of amorphous Si in crystalline Si: stability and collapse

Toni Auranen
Fredrik Boxberg
- 27th International Conference on Physics of Semiconductors
  - Poster: Polarization-dependence on the Gain in Quantum Well Lasers.

Sami Brandt
  - Talk: Motion Without Correspondence from Tomographic Projections by Bayesian Inversion Theory
- 17th International Conference on Pattern Recognition (ICPR 2004), Cambridge, U.K., August.
  - Talk: On the Probabilistic Epipolar Geometry

Anu Huttunen
- XXXVIII Annual Conference of the Finnish Physical Society, 18-20 March, 2004, Oulu, Finland
  - Talk: Band structures of photonic crystal slabs.

Ilkka Kalliomäki
  - Talk: Image analysis of aggregates for concrete quality modeling

Mikko Karttunen
- APS March Meeting, 2004, Montreal, Canada
- XXXVIII Annual Conference of the Finnish Physical Society, 18-20 March, 2004, Oulu, Finland
- Multiscale modelling: membranes and alcohols. Nordita Workshop on Statistical Physics, Soft Matter and Biological Physics, 28-31 August, 2004, Copenhagen, Denmark

Kaisa Kautto
- CARAMEL-ELENA carbon nanotube meeting, 30-31 August, 2004, Helsinki, Finland.
  - Poster: $C_{10}$ is not determined by distributing points uniformly on a sphere.

Kimmo Kaski
- AAAS 2004 Annual Meeting, 11-16.2.2004, Seattle, USA.
  - Talk: Predicting development of epidemics with a dynamic small world model.
- 1st International Workshop Hangzhou 2004 on Simulational Physics, 4-8 November, 2004, Hangzhou, China.
  - Talk: Financial Market - A Network Perspective

74
Timo Kostiainen
- Autumn Seminar of the Pattern Recognition Society of Finland, 22 November, 2004, Oulu, Finland.
  - Talk: Mobile robot - a testbed for computer vision research

Janne Lehtonen
- 2nd International Brain-Computer Interface Workshop and Training Course, 17-18 September, 2004, Graz, Austria
  - Poster: Brain Computer Interface Platform

Ville Mustonen

Aapo Nummenmaa

Tommi Nykopp
- 2nd International Brain-Computer Interface Workshop and Training Course, 17-18 September, 2004, Graz, Austria
  - Poster: Sequential Classification of Finger Movements from MEG Recordings

Jukka-Pekka Onnela
- International Conference on Complex Systems, May 2004, Boston, MA, USA.

Marco Patriarca
- Kääriku Estonian Autumn School of Physics, 8-10 October, 2004 Kääriku, Estonia
  - Lecture course: Introduction to Molecular Dynamics.
- 17th Marian Smoluchowski Symposium on Statistical Physics, 4-9 September, 2004, Zakopane, Poland.
- Institute of Theoretical Physics, Tartu University, Estonia, October, 2004.

Johanna Pekkola
  - Poster: Pekkola, Ojanen, Autti, Möttönen, Tarkiainen, Jääskeläinen, Sams: Primary auditory cortex activation by visual speech
  - 123rd Anniversary of Duodecim Symposium
  - Talk: What happens in the brain when you listen to music?
  - Talk: Primary Auditory Cortex Activation by Lip-reading: and fMRI Study at 3 Tesla

Maria Sammalkorpi
  - Talk: Ion-Irradiation-induced stiffening of carbon nanotube bundles
- Poster: Ion-Irradiation-Induced Load Transfer in Single-Walled Carbon Nanotube Bundles and Multi-Walled Carbon Nanotubes
- Talk: Carbon Nanotubes at LCE: Simulation Studies of Structural and Mechanical Properties

Mikko Sams
- 8th International Congress on Spoken Language Processing., Octover 4-8, 2004, Jeju, South-Korea
- Talk: Neurocognition of speech-specific audiovisual perception

Abstracts:
- Lehtonen, J., Nykopp, T., Heikkonen, J. and Sams, M. Brain computer interface plat-

Jari Saramäki
  - Poster: The Intensity and Coherence of Motifs in Weighted Complex Networks.
- Nordic Workshop on Networks, 16-18 December, 2004, Copenhagen, Denmark.

Margareta Segerståhl
- International Conference on Complex Systems, May 2004, Boston, MA, USA.
  - Oral presentation: Coupling sexual reproduction and complex multicellularity.
  - Poster: Coupling sexual reproduction and complex multicellularity.

Toni Tamminen
  - Talk: Bayesian object matching with Markov chain and sequential Monte Carlo.
  - Talk: A Bayesian occlusion model for sequential object matching.

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

Michael Frydrych:
- Member of Hatutus, Pattern Recognition Society of Finland.

Ilkka Kalliomäki:
- Member of Hatutus, Pattern Recognition Society of Finland

Mikko Karttunen:
- Member of the Finnish Physical Society
- Member of the American Physical Society
- Member of the Biophysical Society

Kimmo Kaski:
- Fellow of American Physical Society
- Member of Association for Computing Machinery
- Fellow of the Finnish Academies of Technology
- Fellow of the Institute of Physics, UK
- Member by invitation, Academica Europaea
- Fellow of Finnish Academy of Science and Letters
- Supernumerary Fellow, Wolfson College, University of Oxford, UK

Jouko Lampinen:
- Finnish Pattern Recognition Society, Hatutus (member of IAPR)
- International Neural Network Society, INNS
- Member of the board in the Finnish Brain Research Society

Maria Sammalkorpi:
- Member of Finnish Physical Society

Toni Tamminen:
- Member of the Pattern Recognition Society of Finland.

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
- Member of the Finnish Pattern Recognition Society

6.5 Other Activities

Mika Ala-Korpela has acted as
- Reviewer in
  - Annals of Medicine

Toni Auranen has acted as
- Reviewer in
  - IEEE Transactions on Robotics

Sami Brandt has acted as
- Reviewer in journal:
  - Pattern Recognition Letters

Anu Huttunen has acted as
- Reviewer in Journal
  - Optics Communications

Ilkka Kalliomäki has acted as
- Reviewer in Journal
  - IEEE Transactions on Pattern Analysis and Machine Intelligence

Mikko Karttunen has acted as
- External examiner
  - MPhil thesis, Chinese University of Hong Kong, China
- Reviewer for NWO (the Netherlands Organization for Scientific Research)
- Reviewer in journals
  - the 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

- Interviews

- **Alcohol on cell membranes**, biological physics research at Helsinki Univ. of Technology, Helsinki University of Technology press conference and live webcast, May 13, 2004
  - in Tekniikka & Talous, Finland: 'Biophysics is aiming to the top', Feb. 26, 2004. Weekly newspaper on technology and economy, circulation about 105,000 with about 180,000 readers (according to an annual national marketing survey).

Jouko Lampinen as acted as
- Opponent of doctoral thesis:
  - University of Oulu, Dept. of Electrical and Information Engineering
- Official reviewer of doctoral thesis:
  - University of Kuopio, Dept. of Applied Physics
  - University of Oulu, Dept. of Electrical and Information Engineering
- Organizing committee member in international conferences:
  - European Symposium on Artificial Neural Networks, ESANN 2004
- Reviewer in Journals:
  - IEEE Trans. on Neural Networks
  - Neural Networks
  - Neurocomputing
  - Journal of Electronic Imaging
  - IEE Proceedings on Radar, Sonar and Navigation
  - Iasted Journal of Control and Intelligent Systems

Maria Sammalkorpi has acted as
- Reviewer in Journal
  - Physical Review B

Mikko Sams has acted as
- Reviewer in Journals
  - European Journal of Neuroscience
  - NeuroImage
  - Journal of Cognitive Neuroscience
- Member of Editorial Board in
  - Tiede (Finnish popular science magazine)
  - Polysteekki
- Member of
  - Academy of Finland’s preparatory committee for Research program for Neuroscience

Aki Vehtari has acted as
- Member of the board in Pattern Recognition Society of Finland, Hatutus
- Reviewer in journals
  - Journal of the American Statistical Association
- Journal of Computational and Graphical Statistics
- IEEE Transactions on Neural Networks
- Neural Networks
- Neurocomputing
- International Journal of Neural Systems
7 Publications


