1 Introduction

Year 2003 marks for the Laboratory of Computational Engineering (LCE) & Research Centre for Computational Science and Engineering (CCSE) the fourth year as a national Centre of Excellence with truly international staff of about 70 members and 10 different nationalities. This international flavour is further strengthened through a joint affiliate centre between CCSE and Wolfson College of Oxford University with the state of the art cluster-computing facilities and with two full time researcher located in Oxford and concentrating on Advanced Computational Science and Engineering (ACSE) research. The affiliate centre hosts every year 2-3 visiting scholars from CCSE to interact with Oxford scientist for further researcher training.

LCE & CCSE research 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 Computational information technology the areas of interest are Modelling and Data-Analysis, Machine Vision, and Complex Systems. In Computational materials research the areas of interest are Biophysics and Statistical Mechanics, Modelling of Structure and Growth of Materials, and Nanotechnology and Coherent Quantum Systems. In Cognitive science and technology the areas of interest are Psychophysical Research, Neurophysiological Research, Artificial Person, and Brain Computer Interface.

Recently the fourth field of research was added to our repertoire, namely Computational Systems Biology which is linked to research in Modelling and Data-Analysis, Complex Systems, and Biophysics and Statistical Mechanics. This serves also as a new addition to our educational curriculum, such that we now offer three majors: Computational Engineering, Cognitive Technology and Computational Systems Biology. All of them are part of the new Bioinformation Technology study programme, which LCE has played a key role in developing and establishing. With nearly 300 applicants for 40 student places it turned out to be the most popular among all the engineering programmes in Finland and its curriculum is developed in collaboration with related faculties and laboratories of University of Helsinki. In addition, especially in the area of Computational Systems Biology a number of 3-4 year research projects funded by the Academy of Finland, National Technology Agency of Finland and European Comission have been started in 2003 with groups in Biomedicum (University of Helsinki) and groups abroad.

Some of the 2003 highlights were: 1) Professor Adrian Sutton was elected to a Fellowship of the Royal Society (FRS) of United Kingdom, 2) Dr. Iiro Jääskeläinen was appointed as the Professor of Cognitive Technology in LCE for 2003-2007, 3) Dr. Mikko Karttunen running the group Biophysics and Statistical Mechanics was appointed as the Academy Fellow, 4) Dr. Michael Patra having worked as post-doc in LCE won European Union Marie Curie Fellowship for one and a half years to continue his research in LCE, and 5) Dr. Karttunen’s group together with Dr. Ilpo Vattulainen’s group from Physics Laboratory was selected as one of HUT’s Young Centre of Excellence for 2004-2005.

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**

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<td>Jääskeläinen Iiro</td>
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<td>Kaski Kimmo</td>
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<td>Lampinen Jouko</td>
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<td>Sutton Adrian</td>
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<td>Tulkki Jukka</td>
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**Adjunct Professors (Docents/Visiting Professors)**

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<td>Barrio Rafael</td>
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<td>Prof. (Technical University of Budapest, Hungary)</td>
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<td>Tirri Henry</td>
<td>Prof. (University of Helsinki)</td>
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**Secretaries**

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<td>Järvenpää Aino</td>
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**Senior Researchers**

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<td>Ahveninen Jyrki</td>
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<tr>
<td>Brandt Sami</td>
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Finnegan Simon
Kumpula Jussi
Lamminen Antti
Mali Olli
Nieminen Tapio
Riihimäki Jaakko
Sainiemi Lauri
Sundqvist Juho
3 List of Courses

Courses in the Laboratory of Computational Engineering

- S-114.100 Computational Science (3 cr)
- S-114.200 Special Course in Computational Engineering (4 cr) P
- S-114.210 Individual Project in Computational Engineering (2 cr)
- S-114.215 Special Project in Computational Engineering (2-5 cr)
- S-114.220 Spatial Cognition and Biomimetic Robot Navigation (2cr) P
- S-114.230 Individual Studies on Computational Engineering (1-6 cr) P
- S-114.240 Seminar on Computational Engineering (2 cr)
  
  Topic: Mathematical modeling and methods in natural sciences & engineering

- S-114.245 Laboratory Seminar on Computational Engineering (2 cr) P
- S-114.250 Special Course in Computational Science (4 cr)
- S-114-310 Introduction to Modelling and Information Theory (2 cr)
- S-114.325 Physics III (S) (2 cr)
- S-114.425 Physics III (Sf) (4 cr)
- S-114.500 Basics for Biosystems on the Cell (3 cr)
- S-114.501 Introduction to Bioinformation Technology (2 cr)
- S-114.504 Basics of Molecular and Cell Biology (4 cr)
- S-114.600 Introduction to Bayesian Modelling (2 cr)
- S-114.710 Perception and Production of Speech (4 cr)
- S-114.740 Special course on Communication and Cognition (2 credits)
  
  Topic: Methods of Cognitive Neuroscience
  
  Topic: Design and Statistical Analysis of Functional MRI Studies

- S-114.750 Systemic Psychophysiology (1cr)
- S-114.V Concepts in Nanomaterials (2 cr)
- S-114.V Correspondence-based face and object recognition (1 cr)

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

- Timo Koskela *Neural Network Methods in Analysing and Modelling Time Varying Processes*
- Mirta Rodriguez *Signatures in Superfluidity in Atomic Fermi Gases*

Licentiate of Technology

- Virpi Junttila *FEM-Modeling of Gas-Structure Interaction in MEMS*

M.Sc. - Diplomas

- Teppo Häyrynen *Quantum transport in the ballistic and Coulomb blockade regimes*
- Sini Merikallio *Available solar energy on the dusty Martian atmosphere and surface*
- Jari Mäkinen *Modeling ultrasonic transmission in boundary layer*
- Ville-Petteri Mäkinen *Parallel Linear Inversion Tomography*
- Laura Laitinen *Neuromagnetic somatomotor signals in brain-computer interfaces*
5 Research Projects

5.1 Computational Information Technology

Research in computational information technology concentrates on modelling and analysing complex physical, technical and economic processes and systems. We carry out method development and application oriented research on advanced probabilistic and information theoretic methods. Application areas include statistical modelling problems, pattern recognition, machine vision, data mining and intelligent human-machine interfaces.

5.1.1 Statistical Modelling and Computer Vision

Bayesian Methodology

Researchers: Aki Vehtari, Simo Särkkä and Jouko Lampinen

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).

The model assessment research is based on the decision theoretic approach of examining predictive distributions and the relative values of consequences of using the models. The main emphasis in model assessment research is how to estimate the predictive performance of complex models and how to estimate the associated uncertainties in these estimates. Our research is based on cross-validation ideas, because 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 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.

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.
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 prior model that defines the variations of the feature locations. The eigenshape model corresponds to determining the covariance matrix for the feature locations, which is learned in bootstrap fashion by matching a large number of images by simpler prior models.

We also have constructed efficient MCMC samplers for drawing samples from the posterior distributions of the feature locations, mainly using Gibbs and Metropolis sampling. Currently we are studying a sequential Monte Carlo approach which will greatly increase the speed of the sampling process. In sequential matching we match the features one after another, using the information about the locations of the previously matched features to aid in the matching of new features. Figure 1 illustrates the object shape model by showing the first few eigenshapes and Figure 2 shows an example of the sequential matching process.

Figure 1: Leading eigenshapes of faces, learnt from a set of training images. The face on the left has been morphed according to the eigen shapes, into positive direction (upper row) and negative direction (lower row). It can be seen that components 2 and 3 are related to rotations of the head, while components 1, 4, and 5 are shape-related.

Figure 2: Sequential feature matching. The red dots mark the drawn locations of the current feature, while the green dots are the previously drawn features. The shape (yellow lines) is computed from the object model given the drawn features.
Image segmentation by MCMC methods

Researchers: Timo Kostiainen, 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 in further processing of the image, for example in object recognition.

The use of a probabilistic approach and numerical Markov chain Monte Carlo (MCMC) methods have recently produced promising results in image segmentation. The approach is based on defining a statistical texture model for the image. The stochastic MCMC algorithm is a top-down process in which a very large number of proposal samples are generated and their likelihoods are evaluated against the texture model. Evaluation of the proposals is computationally intensive, and the complexity depends on the quality of the proposal samples.

We have developed methods for producing efficient proposal samples to reduce the computational complexity. We do this by utilizing the bottom-up information that the image probability model provides, as well as cues such as edges. In Figure 3, the advantage is illustrated by comparing the method to the case where no bottom-up information is used.

Figure 3: Efficient proposals vs. random proposals. Left: result of our segmentation method after 179 samples. Center: result of segmentation without bottom-up information in the same processing time (365 samples). Right: evolution of the posterior probabilities in the MCMC chains with (continuous) and without (dashed) bottom-up information.

The results of the MCMC algorithm are in the form of a large number of weighted samples from the posterior distribution. In many statistical analysis problems the distribution can be easily interpreted in terms of descriptive statistics. In the case of image processing, the result is a set of different segmentations of the image, which is awkward for visualization and further processing. Analysis of the posterior distribution is another part of this work.
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. They have applications in a wide variety of early vision tasks including edge detection, orientation analysis, texture analysis and stereo vision. 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. This property is known as ‘steerability’.

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. However, the steerability of Gabor filters is only approximate, and the accuracy depends heavily on the parameters and the number of different orientations in the bank.

We intend to apply the results to pose-invariant face recognition, where the variability of features due to orientation is a central problem. Using steerability, a simple and computationally efficient measure of feature similarity which is invariant to rotations in the image plane may be developed.

Figure 4: Steering Gabor filter bank into arbitrary orientations. First and second row portray Gabor filters in the spatial domain, and third and fourth row show the same filters in the frequency domain. Leftmost and rightmost columns correspond to known orientations in a bank of five different orientations. The four intermediate filters have been computed via analytical steering, and they approximate exact Gabor filters in the corresponding orientations very well both in spatial and frequency domains.
Sequential Monte Carlo Methods in Multiple Target Tracking

Researchers: Simo Särkkä, Toni Tamminen, Aki Vehtari and Jouko Lampinen

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

The main topic of the project was data association, which makes multiple target tracking much harder task than single target tracking and it also rules out usage of basic Kalman and Extended Kalman filters. In multiple target tracking, the algorithm has to estimate which of the targets produced the measurements, before it is able to use the measurements in actual tracking. In this project we developed new Rao-Blackwellized Monte Carlo data association algorithm, which efficiently solves the joint data association and tracking problem.

The secondary topic of project was modeling of negative information. In a target tracking system physical sensors report measurements only when they receive some kind of signal, which can be further processed into a measurement. In the single-sensor case all we can do is to use these signal-induced measurements. However, when there are multiple sensors measuring from the same origin (e.g. the radar of a target), and some sensors can detect this signal and some cannot, our information is increased by knowing the fact that some sensors could not detect the target. This is called negative information.

Figure 5 shows an example of classical bearings only multiple target tracking problem, which frequently arises in context of passive sensor tracking. The particles in the figures are used for visualizing the distribution, such that the particles are a random sample drawn from the posterior distribution estimate. The actual posterior distribution estimate is a mixture of Gaussians, which is hard to visualize directly. The prior distribution is on purpose selected such that all the four crossings of measurements from the two sensors contain some probability mass, and the distributions of targets are two-modal as can be seen in Figure 5, causing so called ghost phenomenon as false detections.

Figure 5: Initially (left) half of the prior probability mass is located on the ghost sensor measurement crossings and in the beginning of tracking (middle) the multi-modality of posterior distribution can be clearly seen. After a while (right) the posterior distribution changes uni-modal due to restrictions set by the dynamic model.

12
Monitoring the Condition of Sewer Network

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

The aim of the project is to develop methods for the analysis of video sequences that are scanned by a robot moving in the sewer. The project is done in co-operation with the VTT Building and Transport and is funded by TEKES. The work can be 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 especially challenging because of the large variation in surface texture. We have applied several line detection algorithms for the detection of cracks in the pipe surface and joints between pipe sections. The method illustrated in Figure 6 is based on forming an approximate Hessian for each pixel in the image. The Hessian has a large positive eigenvalue where there is a dark line in the image; these are crack candidates. Post-processing includes thresholding with hysteresis and thresholding by feature size.

![Figure 6: Crack detection results. (a) Original image of 'unwrapped' pipe surface. (b) Detected cracks and joints.](image)

The information of 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. In the project we have 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 7 illustrates. Next, after solving the problem of calibration, we will be able to use known multiple view techniques to track points through the image sequence and to reconstruct them. However, there are still many practical and computational problems to be solved before a reliable reconstruction is obtained.

![Figure 7: 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)
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 view point. We have been contributing e.g. by developing a robust estimator that has been proved optimal in the sense of consistence with similar assumptions to the ordinary maximum likelihood estimator. The estimator has been applied, for instance, in two-view geometry and its uncertainty estimation with both affine and projective camera models. Other contributions include novel statistical reconstruction algorithms and a probabilistic formulation for the two-view, epipolar constraint (Fig. 8).

Figure 8: A point in the left corner of the mouth is selected in the left image of a stereo image pair (not shown here). (a) The maximum likelihood robust estimate for the epipolar line (dashed) and the estimated, conventional confidence intervals of the epipolar line. (b) Probability distribution characterising the probability that any point the second image is on the true epipolar line. This is, in fact, a probabilistic representation for the epipolar line where the uncertainty of the estimated epipolar geometry has been taken into account. (c) One thousand independent samples drawn from the probability distribution. (Original image copyright belongs to INRIA-Syntim.)
Optimizing the Web Cache

Researchers: Timo Koskela, Jukka Heikkonen, and Kimmo Kaski

Web caching is a technique where Web objects requested by clients are stored in a cache which is located near the clients. Subsequent requests for the same object are then served from the cache, improving the response time for the end users, reducing the overall network traffic, and reducing the load on the server.

Figure 9 (on the left) shows how the requests from the clients are routed through the proxy, which fetches the objects and stores them to cache. Since the storage space of the cache is limited, an important problem in optimizing cache’s operation is to decide which strategy to use in replacing the cache objects. Typically heuristic rules, such as the LRU (replace the least recently used object) are used for the purpose. Our proposed model predicts the popularity of each object by utilizing syntactic features collected from the HTTP responses and from the HTML structure of the document. Replacement strategy can then be optimized by taking the predicted object popularities into account.

In a case study, about 50000 HTML documents were classified according to their popularity by using linear and nonlinear models. Results showed that linear model could not find correlation between the features and document popularity. Nonlinear model gave better results, yielding mean classification percentages of 64 and 74 for the documents to be stored or to be removed from the Web cache, respectively.

The gained performance improvement was demonstrated by simulations with two common heuristic replacement rules, the LRU and the GDS. Object requests were generated with an analytical model, in order to take different object popularity and object size distributions into account. Figure 9 (on the right) shows the average hit rate (portion of the objects delivered straight from the cache) in the LRU case. The LRU-C utilizes the classification results for the cache objects, and provides a significant improvement in hit rate for all realistic cache sizes.
The On-line Adaptive Brain-Computer Interface

Researchers: Jukka Heikkonen, Laura Laitinen, Janne Lehtonen, Tommi Nykopp and Mikko Sams

Brain Computer Interfaces (BCIs) are intended for enabling both the severely motor disabled as well as the healthy people to operate electrical devices and applications directly with brain activity. Our approach bases on an artificial neural network that recognizes and classifies different brain activation patterns associated motor tasks. By this means we pursue to develop a robust classifier with short classification time and, most importantly, a low rate of false positives (i.e. wrong classifications). Figure 10 demonstrates a BCI in use.

Our group is especially interested in the neurophysiological basis of BCIs. We believe that before the signals can be classified they need to be well understood. We are especially interested in the activation of the motor cortex. Like most BCI groups, we measure the electric activity of the brain using electroencephalography (EEG). In addition to EEG, we measure the magnetic activity of the brain with magnetoencephalography (MEG). MEG signals are more localized than EEG signals and thus give us more accurate information about the brain activity related to, e.g., finger movements. We study the signals, e.g., using time frequency representations (TFRs) and pick out important features from them. Figure 11 shows an example of a TFR.

During year 2003 we collected data on attempted finger and hand movements from quadriplegic people using combined MEG and EEG. The research was done in Low Temperature Laboratory in collaboration with Käpylä’s kuntoutuskeskus. We have developed a Matlab-based BCI platform for offline as well as online use. The platform is not dependent on measuring device or operating system. It could be used as fast prototyping tool for testing different BCI signal analysis as well as feedback methods. We intend to build online EEG-BCI using this platform and later MEG-BCI. In the field of the signal analysis sequential classification was introduced. Preliminary results show significant improvement in comparison to many previously used methods.

Figure 10: The user has an EEG cap on. By thinking about left and right hand movement the user controls the virtual keyboard with her brain activity.

Figure 11: TFR of a MEG sensor over the motor cortex. The activation of the brain is plotted with the time information on the x-axis and the frequency information on the y-axis. Subject began to move his right finger at time zero. Strong activation in the 10-30 Hz range can be detected after the movement has ended.
5.1.2 Complex Systems

Systems of nature, society or man-made are constituted of highly interconnected parts on many scales, the interactions of which result in complex or emergent behaviour. Examples of this kind of complex systems are financial markets, traffic flow, networks of biology, economics, web, society etc., and chemical or biological reaction-diffusion systems to mention a few. The processes of such a complex system occur simultaneously at different scales, and the intricate behaviour of the system depends also on its constituents, units or agents in a non-trivial way. Examples of intricate behaviour include for example self-organisation, self-adaptation, and structure or pattern formation etc., which can be studied using various statistical physics, information theory, statistics and game theory methods involving computational modelling and computer simulations. Our research on complex systems focuses on modern Econophysics including financial analysis, risk analysis, tree and graph analysis, and adaptive multiagent games, complex pattern formation with Turing’s reaction diffusion systems, small world type random networks.
Dynamic Phenomena on Complex Networks
Researchers: Jari Saramäki, Kimmo Kaski

Networks composed of interlinked elements are ubiquitous in Nature – neural networks, social networks, the Internet, networks of epidemic spreading, metabolic networks in cells. However, the mathematical methods for studying such networks have been developed only recently, and in particular dynamic phenomena on such networks still remains a subject with lots of unanswered questions. We study these phenomena from a computational and theoretical perspective. One of our focus areas is developing models of spreading on such networks. These may be used to explain various dynamic phenomena, ranging from the spreading of fads and ideas on social networks to epidemics caused by biological viruses, as well as propagation of excitatory patterns on brain-like neural networks. As an example, we modeled spreading of influenza-like, randomly infectious diseases on dynamically changing spreading networks, and obtained excellent fits to real-world epidemic data. The model also allows predicting the development of an epidemic at its beginning stages. We have also discovered stable oscillations of excitations on two-dimensional small-world networks. Here, an excited network node may excite its neighbors, if these are in a susceptible state. Excited nodes become refractory, and can be excited again only after some period of time. Figure 12 depicts propagation of excitation on such network. After the initial wave of excitations has passed, the process is “re-ignited” through a small fraction of long-range connections in the system. This process could be related to those giving rise to spontaneously emerging cortical rhythms. Furthermore, one should note that the process itself is similar to that of epidemic spreading of diseases, reflecting the fact that many seemingly unrelated natural processes result from similar types of simple mechanisms taking place on complex networks.

Figure 12: Propagation of excitations on a two-dimensional small world. Panel (a) indicates amount of excited nodes as function of time; red circles show times at which the snapshots (b)-(e) where taken. In the snapshots, yellow pixels indicate excited nodes, black those susceptible to excitation and red those in a refractory phase. After some nodes become excited (b), excitation rapidly spreads across the network (c,d). Then, refractory nodes start to “cool down” (e), enabling another excitatory cycle.
**Taxonomy of Financial Assets**

Researchers: Jukka-Pekka Onnela, Anirban Chakraborti, Kimmo Kaski, Janos Kertesz

* Budapest University of Technology and Economics

Network theory provides an approach to complex systems with many interacting units, where the details of the interactions are of lesser importance. In the financial market companies interact with one another, creating an evolving complex system. These complicated interactions are reflected in temporal correlations of asset returns and flows of capital.

We study certain properties of these networks numerically, where the nodes correspond to stocks and the edges to correlation based distances between them. As studies based on random matrix theory have shown, a large majority of eigenvalues of empirical correlation matrices fall within the spectrum predicted for random matrices, i.e. they are predominantly noise. A central issue, therefore, is to prune these systems so that preferably only information is retained.

The goal of our work is to improve our understanding of interdependencies, clustering and dynamics of the financial market. One approach is to construct a minimum spanning tree of edges. We have demonstrated that this leads to a scale-free network, where the scaling exponent is fairly stable over time, except for crash periods, which are characterized by a lower exponent. During crash periods the tree shrinks both topologically and in terms of its overall length. We have also demonstrated how the stocks of the minimum risk Markowitz portfolio lie practically at all times on the outskirts of the tree. Another approach is based on agglomerative clustering, which seems to capture well the clustering present on the market. We have compared some properties of empirical graphs with those of random graphs, for which results are well known. It is postulated that deviations from theoretical predictions are indicative of genuine information. As expected, the market behaves very differently from random graph models.

![Figure 13: Snapshots of financial networks. Left: MST approach. Right: Agglomerative clustering approach.](image)
**Gibbs versus non-Gibbs distributions in money dynamics**

Researchers: Marco Patriarca, Anirban Chakraborti* and Kimmo Kaski

* Dept. of Physics, Brookhaven National Laboratory, USA.

We study simple models of money conserving economy, in which $N$ agents can exchange money in pairs. At every "time step", a pair $(i, j)$ is randomly chosen, and the agent money amounts $m_i$ and $m_j$ undergo a variation,

$$
\begin{align*}
    m_i &\rightarrow m_i' = \epsilon (m_i + m_j), \\
    m_j &\rightarrow m_j' = (1 - \epsilon)(m_i + m_j),
\end{align*}
$$

where $\epsilon$ is a uniform random number in the interval $(0, 1)$. This system relaxes toward an equilibrium state with a Gibbs distribution $f(m) = m^{-\lambda} \exp(-m/m)$ (curve $\lambda = 0$ in the Figure), where $m$ represents the average money. However, if agents save a fraction $\lambda > 0$

![Figure 14: Numerical data (dots) and fitting functions (continuous lines) of equilibrium money distributions for different values of the saving propensity $\lambda$.](image)

(saving propensity) Eqs. (1) become

$$
\begin{align*}
    m_i &\rightarrow m_i' = \lambda m_i + \epsilon(1 - \lambda)(m_i + m_j), \\
    m_j &\rightarrow m_j' = \lambda m_j + (1 - \epsilon)(1 - \lambda)(m_i + m_j).
\end{align*}
$$

(2)

Our numerical simulations lead to the final equilibrium distributions shown in Fig. 14. We also found the corresponding exact solution for an generic value of $\lambda$, with $0 < \lambda < 1$, by fitting the results of numerical simulations, which reads

$$
P_n(x_n) = \frac{x_n^{n-1} \exp(-x_n)}{\Gamma(n-1)} \equiv \gamma_n(x_n).
$$

(3)

This is a $\gamma$-distribution $\gamma_n(x_n)$ for the variable $x_n = m/(m/n)$, where $n(\lambda) = 1 + (3\lambda)/(1 - \lambda)$. The fitting curves for the distribution (continuous lines for $\lambda \neq 0$) are compared with the numerical data in Fig. 14.
Agent based models, which try to describe features in real-world complex systems, have become more popular during the last years. Thanks to the increasing computing power, it is possible to execute simulations for ever complicating models, although the complexity is not a favourable quality as regards to the understanding of the hided, fundamental factors in a phenomenon under interest.

An interesting, simple and powerful model including many features present in real world complex systems is a minority game. At each time step, the players of the game have to decide between two alternatives, say whether to choose side A or B, and those who, after the decisions, happen to belong to the minority win. This simple game exposes many interesting features that have been extensively studied in recent years. Our contribution to the development of this game, is the introduction of genetic adaptation. We allow agents to use genetic manipulations to cross their strategies in order to find good ones. This added feature describes better many real-world situations, where one is required to fight for ones survival. It is not enough to be good or best at one time, but one has to improve and fight all the time. Examples that prove the need of this continuous developing can be found from business, academy, sports, biology, evolution, ... The intelligence leads to interesting changes compared to the basic minority game. Especially, the system as a whole strives towards a state that maximizes the utility of the whole community. This invisible hand effect has its analogies in real world, for example in commodities price forming process.

Figure 15: Normalized fluctuations describe the society utility in minority games: lower values mean higher utility. Learning mechanism leads to a considerable improvement in efficiency compared to the basic game.
Pattern Formation in Turing Systems

Researchers: T. Leppänen, M. Karttunen, K. Kaski, and R.A. Barrio*

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In 1952 one of the greatest mathematicians of the 20th century, Alan Turing proposed a system of reaction-diffusion equations describing chemical reactions and diffusion to account for morphogenesis, i.e., the development of patterns, shapes and structures found in nature. The recent growth in computing resources has enabled numerical simulations of Turing systems, which has brought a great deal of knowledge concerning their properties. These complex systems have been used in explaining, e.g. patterns on animal coatings (mammals, fish, butterflies).

We study numerically structures generated by the Turing mechanism in two and three dimensions. We investigate the dependence of the resulting structures on the system parameters, transitions between these structures, growth from two to three dimensions and percolation of chemicals in the system. In addition, we are interested in the effect of random noise on developing structures, since it is very important from the point of view of biological applications. We use linear stability analysis and nonlinear bifurcation analysis to study the pattern selection in the system analytically.

The goal of these studies is to gain insight into the properties of Turing systems and to facilitate developing biological growth models based on Turing systems. For applications, it is very important to have a better insight of the morphological characteristics of Turing systems in order to be able to implement the required qualitative features to the model in a biologically plausible manner. Figure 16 shows two typical three-dimensional Turing structures, namely the lamellar and spherical morphologies.

Figure 16: The morphologies observed in three-dimensional Turing systems are the lamellar phase with twisted grain boundaries (left) and the spherical phase with organized droplets (right). The visualization has been carried out by plotting the isosurface of the chemical concentration data.
Statistical Analysis of Asset Returns

Researchers: Juuso Töyli, Laszlo Kullman*, Kimmo Kaski, Janos Kertesz*
* Budapest University of Technology and Economics

Asset returns have traditionally been modelled with methods based on the normal distribution. However, the empirical returns are characterised by stylized facts that imply non-normality. The stylised facts include heavy tails thus the empirical distribution is leptokurtic, the variances are auto-correlated although returns are not (except for very small intraday time scales), large and small returns are clustered, and there are jumps and crashes although these are typically asymmetric so that the magnitude of crashes is larger than that of jumps. Despite of these stylized facts, the shape of the distribution approaches normal distribution when the time interval is increased and the monthly returns are generally regarded as normally distributed. These characteristics suggest that the return generating stochastic process is non-linear, time dependent, and complex.

During the past century several model has been suggested but there seems to be no unanimous view. These models can be divided in time-independent and time-dependent categories. Well-known time-independent models include normal distribution, Lévy distribution, truncated Lévy distribution, generalised Lévy distribution, Student t, mixed diffusion jump, mixture normal distribution, and mixture distributions. Time dependent models contain autoregressive heteroscedastic models, stochastic volatility models assuming the volatility as stochastic process, and models based on chaos theory resulting in complex dynamics. These current models are not nevertheless able to capture the dynamics of empirical returns and the results are contradictory. The possible time-dependency of the shape of the distribution has also mainly been ignored.

The research has so far concentrated on the understanding of the return generating process. We have developed toolboxes to fit and simulate data according to the well-known time-independent models. It seems that they are able to capture the long-term distribution but not the structure of the process. We have also studied the effect of different dependencies, linear and non-linear, on the shape of the distribution and generating process. Along with these, the possible biases resulting from different terms of measurements have been researched. Finally, we have studies the changes in the return generating process when the time interval grows. Currently, it seems that the models we have used cannot completely capture the dynamics of the market. Therefore, we have also started to build artificial market in order to understand the role of micro agents in return generation process and to understand the underlying dynamics.

Statistical Analysis of Small World Networks

Researchers: Jani Lahtinen, János Kertész† and Kimmo Kaski
† Budapest University of Technology and Economics

The small world networks are graphs, which albeit having a large amount of vertices still on average retain small distance between individual vertices relative to traversal of links. Such networks are for example the internet, WWW, stock market trading interlinking, biochemistry signaling and metabolism in protein systems, epidemics, formation of polymers, tranportation systems or interlinked systems of social interactions. Cascading failures occur when failure of few agents initiate a domino effect of collapsing a large number agents. These massive breakdowns can be analyzed with simple models of sandpiles of Bak, Tang & Wiesenfeld, which resemble collapsing effect on sandpiles.
5.2 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.
In structural biology, electron tomography is used in reconstructing three-dimensional objects such as macromolecules, viruses, and cellular organelles to learn their three-dimensional structures and properties. The reconstruction is made from a set of transmission electron microscope (TEM) images which may be obtained by tilting the specimen stage by small angular increments (single axis tilting). In order to successfully perform the 3D reconstruction in electron tomography, transmission electron microscope images have to be accurately aligned or registered. The alignment problem can be posed as a motion estimation problem that can be solved by using geometric computer vision methods.

Previously, we have developed two methods where the registration is automated. Most accurate alignment can be achieved if conventional colloidal gold markers are used. In contrast to the manual picking, our method collects the gold beads automatically by using recent techniques of computer vision. For cases when it is not possible to use gold particles, we have proposed an alternative method that is based on tracking high curvature points of the intensity surface of the images. Results show almost as good performance as we have obtained by using fiducial markers (Figure 17). The development of the alignment algorithms is still going on for better accuracy and to take computational aspects into consideration.

Figure 17: Stereo image pair of a reconstructed microvillus where the image series has been aligned by tracking certain interest points of the image intensity surface.
cryo-EM Single particle reconstruction

Researchers: Vibhor Kumar, Jukka Heikkonen, and Peter Engelhardt

Three dimensional model reconstruction of macromolecules from Cryo electron microscopic images is being seen as a good alternative to study viruses and protein structures. In comparison to X-ray crystallography of protein cryo-EM study is not so expensive so this is being considered as good method for solving structure of proteins specially proteins which are hard to crystallize such as membrane proteins. It can also be used to validate the X-ray crystallographic structure of proteins. The 3D reconstruction is made from a large set of cryo electron microscope images of the specimen. In order to successfully perform the 3D reconstruction, right specimens should be picked from the cryo-EM micrographs and properly preprocessed and accurately aligned or registered. The particle picking problem can be approached with different techniques.

We have developed methods to pick the particle from the filtered micrograph. These methods work even in the presence of high noise to signal ratio in micrograph. In addition to this we are doing 3D reconstruction of macromolecules. We did 3D reconstruction of N protein of Hantavirus in order to study its structure and function. We are now finding new and efficient way to do high resolution 3d reconstruction. For this we have already proposed filtering of cryo-Em images and in order to find a good method for finding orientations of the specimen images and to reconstruct the 3d model we are looking some alternatives as maximum entropy method, clustering and accurate averaging.

![Figure 18](image1)

(a) shows the picking(yellow) of circular projections of KLH protein and subsequent refining of results by gabor filter (light blue) and histogram(red) based methods ; (b) A 3d model of Hantavirus N protein reconstructed from cryo-EM micrograph
Signal denoising with Minimum Description Length principle

Researchers: Jukka Heikkonen, Vibhor Kumar, Janne Ojanen, Jorma Rissanen

The need for high-throughput assays in molecular biology places increasing requirements on the applied signal processing and modelling methods. The effects of undesirable noise in the measured data must be somehow modelled and removed if we want to extract information about the studied data generating machinery. An efficient denoising method enables smaller details to be extracted reliably in high-throughput applications, where cost effectiveness demands minimization of the reaction volumes.

Denoising can be done in a quite elegant and efficient way by the Minimum Description Length (MDL) principle, which treats and separates noise from the useful information as that part in the data that cannot be compressed. This MDL denoising method requires no ad hoc parameters or knowledge of the noise characteristics. It provides a basis for high-speed automated processing systems without requiring continual user interventions to validate the results as in the conventional signal processing methods.

Our analysis of the denoising problem in 1-D signals such as mass spectrometry, capillary electrophoresis genotyping and DNA sequencing signals as well as in 2-D cryo-EM images shows that the MDL denoising method produces robust and intuitively appealing results sometimes even in situations where competing approaches perform poorly.

![Figure 19: Left: The original cryo-EM image of PRD1 virus. Right: The result of MDL based denoising.](image)

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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.

Since the development of the DNA microarray technique in the mid-90s, there has been an enormous increase in gene expression data from several organisms. 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 lapses, that the current models do no take into account.

Because real regulatory networks in living cells are not that well characterized, models have to be verified with artificial data. Our first goal is to make expression data simulator capable of producing synthetic data that captures the known features of gene regulation. The research so far has concentrated on recurrent neural network models of gene regulation.
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 20: Capillary array electrophoresis genotyping workflow.
Modeling of Bacterial Metabolism

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

Laboratory of Bioprocess Engineering, HUT

The interest in computational methods in biological applications has recently been increasing greatly. This is, in part, due to a need to quantitatively integrate biological knowledge that is diverse and mostly qualitative. We have started this mission, as a part of a larger systems biology effort, by formulating a model of glucose metabolism of a lactic acid bacterium Lactococcus lactis.

Our model characterizes 24 enzymatic reactions involved in the metabolic pathway. The reaction rate equations depend on the concentrations of 31 metabolites and 131 kinetic parameters. The rate equations and the stoichiometry of the reaction network form a system of ordinary differential equations that is solved with Matlab. The problem with this approach is that the parameters have been collected from a number of articles and thus they are not directly comparable. In the future we wish to test our model with direct experimental data.

The model is handy e.g. in designing knock-out mutant strains of the bacteria. It predicts how the carbon fluxes change if an enzyme is deleted. These knock-out mutants are a common tool in biotechnology when the fermentation characteristics of these bacteria are engineered. The model also gives us more insight into the control of metabolism at enzymatic level and it is an excellent starting point for more advanced models.

Figure 21: The interplay of enzymatic reactions dictates the carbon fluxes in the cell. It is in our interests to direct the flux towards economically desirable products by combining our knowledge of systems biology and bioprocess engineering.
Genetic and Environmental Causes of Nephropathy in Type 1 Diabetes

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

* Folkhälsan Research Centre, Biomedicum Helsinki

Diabetes is a complex disease that has both hereditary and environmental background and it is unlikely that there is a single gene dictating the incidence. Therefore it is imperative that we apply a multifaceted and holistic approach in identifying the most significant risk factors.

The FinnDiane study, headed by Doc. Per-Henrik Groop from the Folkhälsan Research Centre, aims for the identification and early detection of diabetic complications. So far, the research group has accumulated clinical information of about 4000 type 1 diabetic patients and 1500 relatives in Finland. At the moment, a genome wide scan of some 120 selected families is in progress, so we will have a unique data in the world and an excellent opportunity to learn more about the disease and its complications.

Maintaining and analysing the huge database is a difficult task. It is no longer enough that we associate one gene to a particular phenotype, we have to be able to go beyond this first level of organisation and find larger patterns and clusters of susceptibility. LCE has the key role of providing the expertise and know-how in both data visualisation and statistical analysis.

Diabetes is turning into an epidemic in the developed world – at the moment there are over 30,000 type 1 and 200,000 type 2 patients in Finland alone. The FinnDiane study is focused on the type 1, which is characterised by an autoimmune reaction against the insulin producing cells in the pancreas. As a result, an affected person becomes rapidly dependent on external source of insulin.

After about 20 years of T1D, a third of the patients have or are in the process of developing kidney disease. Complications are the most dangerous aspect of diabetes, since they are mostly irreversible and very costly in every sense of the word. Furthermore, at present day, we lack a reliable early diagnosis method that would facilitate efficient prevention and treatment.

![Figure 22: Pedigrees with diabetes and complications.](image-url)
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 this apparent dichotomy is to be hoped for. Thirdly, the germ cells are 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 for a better analysis of 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 from an unconventional analysis of germ cell identities show a surprising way to link sexual reproduction and multicellular development. This allows us to model a new level of biological organization between cell biology and complex multicellularity. It integrates different biological disciplines with systems analysis and modeling and enables us to look at many biological phenomena from a new perspective.
5.3 Computational Materials Research

In LCE & CCSE the Computational Materials Research activity covers various aspects of materials physics such as soft and biomaterials, structure and growth of solid materials, and nano- and quantum systems, in the groups of Biophysics and Statistical Mechanics, Modelling Structure and Growth of Materials, and Nanotechnology and Coherent Quantum Systems, respectively.

5.3.1 Atomic Level Modelling of Structure and Growth of Materials

The research of our group is concerned with the study of structural properties of and growth phenomena in solid materials. All studies rely on microscopic modeling, in which the interatomic 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 and various nanostructures – e.g. thin films, quantum dots 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 purpsoes. 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.
**Strain relief in mismatched heterostructures**

Researchers: Antti Kuronen, Marco Patriarca, and Kimmo Kaski

We study the conditions for nucleation of dislocations in lattice-mismatched heterostructures, which have recently risen a great interest due to their technological importance. In particular, we study the effect of lattice misfit, overlayer thickness and surface structure on the dislocation nucleation. To this aim we use simulation programs with a graphical user interface coupled to a molecular dynamics and minimum energy path determination code. In Fig. 23 the effect of surface structure on the dislocation nucleation activation energy in a 2D system with misfit $m = -3.5\%$ is shown. The stress concentration caused by the defects on the surface (notch or step) lowers the activation energy $E_B$ considerably. We study misfit induced

![Figure 23](image)

Figure 23: Left: Three different systems used to study the effect of surface structure on the dislocation nucleation barrier. Right: Minimum energy paths for dislocation nucleation for the three systems depicted on the left.

dislocations by changing continuously the misfit, rather than temperature or the applied stress. This technique allows one to observe clearly the transition from a perfect crystal to a state with one or more dislocations and vice versa. This is shown in Fig. 24 (right), where the internal energy at $T = 0$ is plotted as a function of the misfit $m$. We observe a hysteresis effect, due to the activation barrier for dislocation nucleation.

![Figure 24](image)

Figure 24: Left: Sample structure made up of a quantum dot and a substrate. Colors are according to potential energy. Right: Internal energy versus $\alpha_2/\alpha_1 = m + 1$, where $m$ is the misfit and $\alpha_k$ the lattice constants.
Clusters of amorphous Si in crystalline Si: stability and collapse

Researchers: Sebastian von Alfthan, Adrian Sutton, Antti Kuronen and Kimmo Kaski

We have studied the thermal stability of small spheres of amorphous silicon embedded in crystalline silicon using atomistic computer simulations. We use a molecular dynamics simulations to follow the time dependent behavior of these clusters. In order to study this problem we have developed a novel method for automatically identifying the position of the amorphous-crystalline interface at different time-steps.

We calculate the surface and bulk energies of amorphous clusters and also study the dynamical behavior of the interface between the amorphous and crystalline phases at different temperatures. This enables us to calculate the mobility and activation energy of the interface movement. Using these results we can predict the long time behavior of larger clusters at room temperature. Also the atomistic structure of the interface and the process by which the growth happens is of interest. We identify some typical features by which the growth happens such as a ledge growth mechanism and the formation of prefered atomic planes at the interface.

Figure 25: A slice of a system with an amorphous cluster is depicted at three different time steps when simulated at a temperature of 1250 K.
Dislocations in FCC Metals: Peierls Stress and Interaction with Defects

Researchers: Péter Szelestey, Marco Patriarca, and Kimmo Kaski

A [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. We use atomic level, Molecular Dynamics simulations, with the aid of the previously developed Embedded Atom potentials and visualization and tracking methods, in order to proceed along two distinct research directions.

**Mobility**: An essential factor affecting the mobility of dislocations is the Peierls potential, the periodic potential experienced by a gliding dislocation, due to the discrete nature of the crystal. Under external stress, dislocation motion in the Peierls potential represents a complex problem, especially for a dissociated dislocation, as its structure changes during motion. We have studied this phenomena using for the case of a screw dislocation. We considered various configurations with different separation distances and analyzed its implications for low temperature plastic behaviour.

**Interaction with defects**: Another research direction is aimed to study the interaction of a moving dislocation with sessile defects. We are particularly interested in vacancy-formed defects, such as Frank’s dislocation loops and stacking-fault tetrahedra. On one hand, these defects represents obstacles for the moving dislocation, act as pinning sites, and on the other hand, the defects can undergo transitions due to intersection with a moving dislocation.

![Figure 26: Snapshots of a stacking-fault tetrahedron (pyramid shaped object) intersected by a dissociated screw dislocation. The two partials can be identified by the blue, originally straight lines. The screw dislocation moves from the left to the right side. Only atoms in the core region are visualized.](image-url)
Modeling of thin semiconductor films

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

*Center for Simulational Physics, The University of Georgia, Athens, GA, USA

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. These systems are strongly influenced by the strain-related effects and long-range elastic interactions which requires using large-scale simulation methods. Our approach is to use empirical potentials in connection with advanced Monte Carlo techniques which allows us to reach sufficiently large system sizes (up to 100000 atoms). Moreover, temperature dependence is inherently included in the simulations.

Semiconductor surfaces are often difficult to study because these systems are characterized by complicated energy landscapes, and consequently conventional algorithms can easily get trapped into metastable states. 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 27 shows a snapshot of a relaxing Si island surrounded by addimers. All red particles are mobile and can migrate on the surface.

![Figure 27: Relaxation of a Si island 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).](image)
Mechanical Properties of Carbon Nanotubes

Researchers: Maria Huhtala, Jussi Aittoniemi, 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, on local strain and defects. For composite and device development it is essential to understand how these structural changes affect the properties and our work strives after shedding some more light on the occurring phenomena. Current projects include studies of carbon nanotube local bending and buckling and studies of irradiation induced defects in carbon nanotube strength, load transfer and inter-shell friction. The tools employed are both classical molecular dynamics and dynamical tight binding methods. Figs. 28 and 29 show examples of the defect structures which have been studied.

![Figure 28: Vacancy reconstructions in a single-walled (17,0)-tube. From the left: single vacancy (one atom missing), double vacancy (two atoms missing) and triple vacancy (three atoms missing).](image1)

![Figure 29: Two views of a covalent inter-shell bond in a multi-walled (5,5)@(10,10)-nanotube. For example, two adjacent vacancies can form such a bond.](image2)
5.3.2 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 \textit{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).
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 30: 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 31: Formation of a vesicle. Time goes from left to right, top row illustrating the vesicle from outside and bottom row from inside.
This project addresses the synthesis, characterization and modelling of self-assembling biomolecular systems based on lipids and their complexes with proteins. The variety, stability and relative ease of synthesizing these systems offer considerable potential for the development of novel electronic, magnetic and optical device technologies. We shall explore the experimental and theoretical principles underlying the synthesis and electronic properties of a well-targeted subset of these materials. We have chosen to focus on polymerized superstructures of phospholipid vesicles and cytochrome c. The cytochrome c is a very well characterized stable peripheral protein. We have recently found that the liposomes undergo a self-assembly process in the presence of cytochrome c forming bundles of threads in rope-like polymerized structures. Both cytochrome c and several naturally occurring lipids, as well as man-made lipid derivatives, are commercially available in pure form. Such derivatives include those functionalized groups that lead to the formation of very large stable polymerized structures. It is the combination of the self-assembly, functionalization and stability of these materials that make them attractive candidates for the replacement of semiconductor device technologies over the next decade.
5.3.3 Research on Semiconductor Quantum Structures, Bioelectronics and Physics of New Information Technologies

Quantum dots (QD) and quantum wires (QWR) are compound semiconductor or metallic structures that confine electrons or holes or both in a potential box having a dimension of few tens of nanometers. These semiconductor structures have exceptional optical and transport properties, which makes them ideal for fundamental research as well as highly potential platforms for nanotechnological, bioelectronics and biotechnology applications. In the enclosed project descriptions we describe few topics that have been in focus during 2003.

All projects include extensive domestic and international collaboration with the following laboratories: Optoelectronics Laboratory, HUT, VTT Electronics, Instituto Nazionale di Fisica della Materia, University of Lecce, MegaGauss Laboratory, University of Tokyo, Inst. of Industrial Science, University of Tokyo, Center for Terahertz Science, USCB. On national level there is a close collaboration with VTT Microelectronics, University of Jyväskylä and University of Oulu.

As a new field we have started research of low power biomorphic neural circuits based on floating gate MOS and SET transistors. 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.

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.

We have investigated cold atomic Fermi-gases which can be used for studying important quantum many-body effects such as superconductivity. Cold atomic gases may also serve as a source of atoms in quantum information processing applications. Recent focus has been in the study of superfluidity and its detection by optical means. This research is done in collaboration with the University of Innsbruck, Austria, with Nordita, Denmark, and with the Loomis Laboratory, University of Illinois, USA. We have also participated in the University of Jyväskylä-based experimental research on the idea of using superconducting Josephson junctions as the basic processing element of a quantum computer.
Modelling of nanoscale semiconductor devices

Researchers: Fredrik Boxberg, Roman Terechonkov and Jukka Tulkki

The commercial integrated electronics is mainly based on silicon (Si), while compound semiconductors (CS), e.g. gallium arsenide (GaAs), are used in very special applications. For example, light detectors and 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 Si and CS. The motivations are lower power consumption, faster operation and smaller device size.

We have studied a CMOS fabrication technique for Si quantum wires (QWRs). Figure 34A shows schematically a Si QWR (turquoise color) embedded in silicon dioxide (SiO$_2$). These kind of QWRs could easily be integrated in commercial integrated circuits. We have modelled the growth process of SiO$_2$ on the QWRs and its effect on the fabricated devices. Great strain-induced effects on the electronic properties were found. These effects alone could in principle ruin the operation of the devices. So far it has not been possible to fabricate high quality Si QWRs and we argue that one reason is the oxidation-induced strain field.

Currently the main topic of research are the electronic and optical properties of CS devices. We are studying the possibility to fabricate both laser devices and single photon devices (e.g. needed for future quantum information technology). We have been working on quantum wells (QW), QWRs and quantum dots (QDs). Figure 34B shows an 8 nm thick corrugated QW (the hatched layer) with a corrugation period of 13 nm. The corrugation confines the carrier density into wires. The wire-like carrier densities are shown with turquoise in Fig. 34B. Moreover, we have been studying indium arsenide (InAs) QDs embedded in a GaAs matrix both with and without a covering layer. A typical QD structure is shown in Fig. 34C. The turquoise region corresponds to the InAs QD.

Figure 34: Schematic drawings of (A) a Si QWR embedded in SiO$_2$, (B) a corrugated InGaAs quantum well and (C) a covered InAs QD island. The turquoise areas correspond to the active region of the device, i.e., high charge carrier density. The red bars correspond to 50 nm in (A) and (C) and 25 nm in (B).
We are developing general tools for strain analysis, band structure calculations and optical models. The final aim is to model photonic devices starting from the structural properties and ending up with properties like the light amplification in the device. For this purpose we need to simulate the strain field, the electronic structure and the recombination of carriers.

The strain in the modelled structures is due to different lattice constants of the epitaxially combined materials. The strain is of the order $10^{-2}$. Hence, the devices can be built with hardly any dislocations and we know that the strain is completely elastic. However, the strain affects the electronic structure remarkably and it cannot be omitted from the calculation of electronic and photonic properties of quantum structures. The assumption of a dislocation-free structure is one of the corner-stones of our model. The strain and the piezoelectric field in these structures affects the position and the inter band coupling of the energy bands. The strain calculations are based on the elastic continuum theory. The full treatment of the strain in compound semiconductors leads to an electro-elastic coupled problem where the strain is coupled to the piezoelectric field. This coupling is due to the ionic atomic structure of III-V compound materials. The effect is absent in purely one material semiconductors like Si or Ge.

The optical properties rely completely on the underlying electronic bands, which are influenced by the device geometry and crystal orientation. From the electronic structure one can model properties like photon recombination rates, polarization of the emitted light and light amplification. One could in principle extend this model to describe also some basic dynamic photonic processes.
**Electronic structure calculations.**

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.

There are only two methods to obtain the band structure: either experimental or theoretical approaches. Development of the computers has made possible to compute semiquantitative band structure for compound semiconductors.

Band structure calculations are computationally very intensive. Therefore we have developed parallelized computer algorithms to solve the finite difference eigenvalue problem. Our computer code gives us 8-band eigenvalues and eigenfunctions for quantum well, quantum wire and quantum dot structures.

The 8-band $k \cdot p$ model used in our calculations is based on combining a Shrödinger equation based series expansion of the wave function with an experimentally determined parameters. In addition to the experimental data, one also uses information from band structure calculations of the related bulk semiconductors Fig. 35.

![Diagram](image)

Figure 35: On the left: The calculation procedure diagram. On the right: The electron density distribution for conduction ground state band (step-like quantum wire case).

In our project we are interested in the electronic states near the band edge. For this case, the $k \cdot p$-method gives reasonable results. The size of the matrix to be diagonalized can be up to million by million. This enforces us to use many processor computers and partial spectrum eigenvalue solver library. The PARPACK library allows us calculating the eigenvalues and eigenvectors Fig. 35 under the minimum RAM requirements.
Modelling optical components for access networks

Researchers: Jani Oksanen and Jukka Tulkki

With the long haul network backbone transformed into an optical information highway, the transfer capacity is mostly limited by the electronic bottlenecks in the access and metropolitan area networks. The undisputed success of the optical fibres in the network backbone encourages to resolve the bottlenecks by passing to optical solutions in the other parts of the networks as well. This solution, however, requires all-optical components which do not exist commercially (or at all) at present.

Metropolitan area networks include a large number of separate connections, which makes fast switching devices and inexpensive laser transceivers essential. The goal of this project is to create models and new ideas for the devices needed in expanding the optical network.

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) and 3) the use of quantum cascade lasers in free space optical communications. At the moment we are focusing our attention on an all-optical inverter, that could enable fast optical logic with reasonable input powers. The inverter shows promising characteristics for low input signal bitrates (up to $\sim 10^12$). At higher bitrates it experiences some stability problems we’re hoping to overcome.

Theoretical models and simulations allow profound insight in the device operation, within the framework of the accuracy of the model and its assumptions. 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.

![Schematic representation of the linear optical amplifier including a waveguide and a vertical microcavity with highly reflecting distributed Bragg reflectors (DBR).](image)

Figure 36: Schematic representation of the linear optical amplifier including a waveguide and a vertical microcavity with highly reflecting distributed Bragg reflectors (DBR).
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) and Green’s function methods within the Landauer-Büttiker formalism to calculate the conductance in selected two- and three-dimensional channels. To compare these two methods we calculated the conductance of a 2D T-stub (see the inset of Fig. 37(a)). 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].

Figure 37: (a) The conductance of the a-stub. The shape of the T-stub is shown in the inset. The waveguide is \( w = 10 \) nm wide and the size of the stub is \( 10 \) nm \( \times \) \( 10 \) nm. The zero of the energy axis corresponds to the ground state energy of the lead: \( E(n = 1) = \frac{\hbar^2 \pi^2 n^2}{(2m^* w^2)} \approx 75 \) meV, \( m^* = 0.05 m_0 \). (b) Calculated conductance of the QPC at \( T = 0K \) and \( T = 1.5K \).

In a single electron transistor (SET) a small conducting island is connected to a source and drain by tunnel junctions. In a tunnel junction a thin layer of insulator separates two conductors (e.g. thin silicon dioxide layer between doped silicon areas). If the junction area is small and the temperature is low the movement of an electron can be blocked by charging energy of the island (i.e. the thermal energy of an electron is smaller than the coulomb energy required to transfer the electron into the island). This is known as the Coulomb blockade phenomenon. If small voltage is applied between drain and source an electron can tunnel into the island rais-
ing the Fermi energy of the island and preventing other electrons tunneling into it until either
the applied voltage is increased or an electron is tunneled out of the island. Furthermore the
number of excess electrons in the island can be controlled with a gate electrode which shifts
the energy levels of the island.

Figure 38: Energyband diagram of a double junction system. In the left figure all applied voltages are
set to zero and no current flows through the SET. In the right figure electrons can tunnel into the island
and out of it because the excited state of the island due to the Coulomb charging lies between the Fermi
energies of the left and right leads.

We have simulated the functionality of an SET based exclusive-OR (XOR) logic gate with
SIMON (SIMulation Of Nano-structures), a software which makes use of Monte Carlo and
Master equation methods for calculations. The two gates of the single electron transistor are
the input nodes of the XOR gate and the source of the SET represents the output node.

Figure 39: The switching characteristics of XOR gate at T = 40 K. The drain-source voltage is
V_{DS} = 10 mV, the tunneling junctions have parameters C = 10^{-10} F and R_T = 10^5 Ω and the gate
capacitances are C_{G1} = C_{G2} = 2 \times 10^{-18} F.
Researchers: Teppo Häyrynen and Jukka Tulkki

Due to limitations set by the power consumption and algorithm design new ideas and techniques has to be applied in the integration of ever-growing number of electronic components on a single chip. Parallel processing at the system level is one way to increase computational power. Single electron transistors (SET) may offer another way. SET circuits are a challenge for system design because of their sensitivity to fluctuating background charge and the requirement for low temperature. However, SETs might be used in fast and power efficient signal processing circuits. Especially neural approach is a promising methodology to bypass the setbacks of SETs.

Our goal is to implement the energy efficient processes of signaling in biological neurons to electronic circuits. Our purpose is to develop equivalent circuit models for a single neuron as well as for a synapse interacting between neurons. Furthermore our goal is to model a group of interacting neurons.

Figure 40: In the parallel conductance model the plasma-membrane of a neuron consists of cross-membrane proteins which operate as ionchannels and a double layer of lipids. Ionchannels can be modeled with (voltage dependent) conductances and the double lipid layer of lipids with a capacitance.

In biological neurons a signal is carried by ions, mainly by $K^{+}$-, $Na^{+}$-, $Cl^{-}$- and $Ca^{2+}$-ions, producing a current trough the plasma-membrane and along the neuron. Thus the neurons can be dealt as an electrical components. The starting point of the study is a transmission line formalism for modeling the signal propagation in a neuron. A well known model for the plasma-membrane of neuron is the so called parallel conductance model. In this model the cross-membrane proteins that operate as ionchannels are modeled with parallel conductances and the double layer of lipids is modeled with a capacitance. Furthermore the cytoplasm of a neuron can be modeled with a resistance. Currently we are developing a dynamical model for the plasma-membrane of a neuron. Our objective is to take into account the essential properties of biological neurons.
Photonic Crystals

Researchers: Anu Huttunen and Päivi Törmä*
* Department of Physics, University of Jyväskylä.

Photonic crystals are periodic dielectric structures. The periodicity creates bandgaps for light, i.e., light in a certain wavelength region cannot propagate in the photonic crystal. The periodicity, and thus the bandgap, can be in either one, two or three dimensions. Two-dimensional photonic crystals embedded with defects could be used e.g. as waveguides for integrated optics and a defect inside a three-dimensional photonic crystal can act as a microcavity. Photonic crystals are a very attractive solution to various problems in telecommunications and may become the key material for integrated optics.

We study thin slabs of one- and two-dimensional photonic crystals. We show that varying the boundary material results in changes in the band gap and that this effect can be utilized for reflecting light traveling along a one-dimensional photonic crystal slab by changing the boundary material abruptly (see Fig. 41). We have suggested that in two-dimensional photonic crystals, the same effect could probably be used for guiding of light by patterning the boundary material. We also study photonic crystal structures made of Kerr-nonlinear material.

![Figure 41: (a) Energy density profiles of a Gaussian pulse in a photonic crystal slab at different times. The frequency of the pulse can propagate in the photonic crystal when boundary material is air, but falls into a band gap when boundary material is GaAs. This can be seen from the intensity profile as the pulse is reflected. (b) The fraction of the energy density of a Gaussian pulse that is reflected inside the slab from the point where the boundary material above and below the photonic crystal slab changes from air to a material with dielectric constant $\varepsilon_b$. Solid line indicates dielectric boundary materials and dots indicate metals: gold, silver, and aluminum.](image)

We also study photonic band gap fibers regarding ultra-fast optical systems. The cladding layer of photonic band gap fibers is periodic in the plane of the fiber cross-section. The goal is to design and demonstrate efficient amplification of optical pulses in photonic crystal fibers with amplifying medium. Tight optical confinement can be achieved in photonic crystal fibers by proper design of the geometry leading to enhanced amplification. Also dispersive and nonlinear effects are very different from conventional optical fiber.
Cold Degenerate Atomic Fermi Gases

Researchers: Mirta Rodriguez, J. Kinnunen\textsuperscript{1}, P. Pedri\textsuperscript{2}, L. Santos\textsuperscript{2} and Päivi Törmä\textsuperscript{1}

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The remarkable achievement of Bose-Einstein condensation (BEC) in alkali gases has stimulated the trapping and cooling of also the Fermionic isotopes.

Atomic gases can be efficiently and accurately manipulated. They are dilute and weakly interacting thus offering the ideal tool for studying fundamental quantum statistical and many-body physics.

The most prominent phenomena for the fermionic samples is the experimental realization of a superfluid Fermi gas. Novel forms of fermionic superfluidity in alkali gases have been reported during the present year. Fermionic superfluidity happens at low enough temperatures due to the attractive interaction between the atoms trapped in different hyperfine states.

We are studying different manifestations of superfluidity in these novel systems:

1) We have proposed the use of on-resonant light to probe the order parameter in order to detect the superfluid transition by analyzing the atomic current.

2) A purely quantum transport phenomena such as Bloch oscillations can also be observed in these Fermi gases when they are loaded in a periodic optical potential. We have analyzed the bloch oscillations both in the normal and superfluid regime and proposed the different value of the amplitude of the oscillation as a signature of superfluidity.

Fermi-Bose and Bose-Bose mixtures are one of the central topics in the field of atomic gases. We have considered the scissors mode in these multicomponent systems.

Figure 42: Fermi sea of neutral atoms at $T = 0$ loaded into a magnetic or optical one-dimensional harmonic trap.
5.3.4 Medical physics: Radiation Dosimetry at Cellular Level

Researchers: P. Välimäki*, A. Kuronen, S. Savolainen* and J. Stepanek†
*Helsinki University Central Hospital, Finland
†University of Zurich and Paul Scherrer Institute, Switzerland

New promising methods in cancer treatment like radioimmuno and neutron capture therapies provide new challenges to dosimetry. Contrary to the therapies exploiting external beam, radiation distributions in these new methods are generally highly non-uniform. Since there exists at the moment no means to measure the doses absorbed by the patients from internally deposited radionuclides, the only way to proceed is to develop theoretical methods to estimate these doses.

One remarkable, but mostly disregarded factor in analytical microdosimetry is the cell cluster model to which the dosimetric calculation itself is applied. Three dimensional cell cluster models have so far been quite simple consisting mainly of clusters of spheres largely due to insufficient computing capacity. On the other hand the cell-level dosimetry field has lacked totally the verification of the cluster models against biological reality. We are currently developing a new method to overcome both of these deficiencies. As the basis for the modelling the method uses realistic cell related microscopy data of the tissues. Dose calculations in the realistic cell cluster makes it possible to verify the usefulness of the currently used cell cluster models and to further estimate the effects of the cell shape, the cell size variation and the spatial distribution of the cells in the cell-level dosimetry.
5.4 Cognitive Science and Technology

Cognitive Science and Technology Group studies neurocognitive mechanisms of human communication and develops methods for brain signal analysis. Perceptual mechanisms are studied in psychophysical experiments, in which various aspects of the stimuli as well as subject’s mental state are manipulated. On the basis of the results 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. We are also developing an Artificial Person (AP), a model of the communicating human being. AP provides us a well-controlled audiovisual speech stimulus for basic research but may also be used in various applications. Together with Computational Information Technology group we are developing Brain-Computer interfaces. This research is described in section 5.1.1.

5.4.1 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 priming’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.

Modelling of audiovisual speech perception The above results as well as others have been modelled with the Fuzzy Logical Model of Perception (FLMP) developed by Massaro and co-workers, and it fits the results well. The FLMP assumes that phonetic categorization occurs independently in both audition and vision. The final phonetic percept is modelled as a maximum likelihood integral of the two unimodal percepts. We have extended the FLMP to account for the effect of audio signal-to-noise ratio, as illustrated in Fig. 43. We have also applied the FLMP to the illusory flashes described above. Also here, the model fits the data well.

We have investigated the role of over-fitting in the FLMP’s good fits. Over-fitting occurs when a model is too general. It will then fit the noise in the data rather than the structure.
Over-fitting models tend to fit the data well but perform poorly at predicting new data. Cross-validation exploits this. By fitting the model to only a subset of the data and testing it on another subset the predictive ability of the model is tested. Cross-validation reveals that the FLMP does indeed over-fit.

We have developed a new model of audiovisual integration termed Linear Feature Integration. This model assumes that integration of acoustical and visual feature vectors occur prior to categorization as a weighted vector sum. We have applied LFI to the illusory flashes described above and obtained poorer fits but better cross validation results than obtained with the FLMP. This supports that LFI may be an appropriate model that does not over-fit the data.

**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 44). 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 /u/. 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 /u/), as compared with congruency (e.g., visual and auditory /u/), significantly activated the Broca’s area, the prefrontal cortex and the superior parietal lobule 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.

Figure 44: 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.

**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 45). Common activation areas to presentation of auditory and visual vowels were observed in the left Insula, the Broca’s area, the lateral premotor cortex, and the inferior parietal area as well as the right superior temporal gyrus/sulcus. Significantly stronger activation for visual than auditory speech was observed in the left motor and sensory areas, inferior parietal lobule, posterior cingulate gyrus and visual sensory specific areas. Significantly stronger activation for auditory speech, in turn, was observed in the left lingual gyrus, the left insula, anterior cingulate bilaterally and auditory sensory specific areas. 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, specifically focusing to the primary auditory cortex (See figure 46). 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 neurons 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.47). 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.

Figure 47: The effects of auditory and visual adaptor stimuli on subsequently presented auditory cortex N100m responses to auditory phonemes. Auditory phonemes preceding the target phonemes caused significant decrease in response amplitudes. Visual phonemes (articulations) presented before the auditory phonetic stimuli caused significant suppression of the auditory responses, which was significantly less than by the auditory adaptors.

**Processing of sine-wave speech in the human brain** We studied in collaboration with the University of Oxford whether there are speech-specific regions in the human brain by using sine-wave speech (SWS) stimuli. Typically, naïve subjects perceive SWS stimuli as strange (non-speech) sounds. However, when subjects are told that SWS stimuli can be heard as speech, they typically start to perceive the stimuli phonetically. We used fMRI to investigate how subject’s knowledge on the nature of SWS stimuli affects their neural processing. The experiments were conducted in the FMRIB Centre in Oxford. Our findings suggest that posterior region of the left superior temporal sulcus would be a speech-specific processing site in the human brain.
5.4.2 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, 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.48). These studies were conducted at our collaborative laboratory, the Massachusetts General Hospital - Harvard Medical School - Massachusetts Institute of Technology Athinoula A. Martinos Center for Biomedical Imaging in collaboration with Drs. Jyrki Ahveninen, Tommi Raij, Sari Levänen, Matti Hämäläinen and John W. Belliveau.
5.4.3 Artificial Person

Researchers: Martin Dobšík, Michael Frydrych, Andrej Krylov, Jari Kätsyri, Pertti Palo, Mikko Sams

In social interaction, 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 evidence that the speech perception improves significantly also with computer animated audio-visual speech synthesizers, talking heads. Facial expressions are an important dimension in face-to-face communication. They may accentuate spoken information, convey additional information or regulate conversation between several speakers. Non-verbal body language, which also involves facial expressions, has been claimed to compose as much as 65% of human communication. 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 have developed a toolkit for real-time animation of Finnish-speaking 3D talking head, "Artificial Person". We have paid special attention in improving the quality of audiovisual
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. 49). The Artificial Person is able to express six basic emotions (anger, disgust, fear, happiness, sadness and surprise) and their combinations.

![Graph showing identification percentages for expressions of actors in different datasets.](image)

Figure 50: Identification percentages for expressions of actors in different datasets.

We started to create a digital database of emotion related facial movements, first of this kind in Finland. At the moment, the database contains static pictures and short video sequences of six basic expressions performed by two actors and Artificial Person. Both actors are certified FACS (Facial Action Coding System) coders. FACS is an objective and comprehensive system for recognizing, describing and coding facial expressions. The database has been evaluated. Preliminary results indicate that the expressions of Artificial Person, except fear, were identified as expected (Fig. 50).
5.4.4 Neuroinformatics

Researchers: Iiro Jääskeläinen, Jouko Lampinen, Mikko Sams, Kimmo Kaski

Neuroscientists, having developed sophisticated methods to investigate the brain in great detail, increasingly face the challenge of managing the enormous amounts of data and inferences drawn from them. To complicate things, the data are highly diverse, arising from chemical, biophysical, structural, morphological, physiological or behavioural sources, each having its own characteristic parameters. Data are collected at all levels of biological organization, from the genetic, cellular, and neural network levels up to the whole-brain structure and function, using sophisticated and varying technology. Neuroinformatics, standing at the intersection of neuroscience and information science, aims at ultimately making it possible for researchers to share their primary data and analysis tools for quantitative integration of different levels of knowledge by means of computational modelling.

LCE is committed to advancing neuroinformatics as recently recommended by an OECD working group that one of the laboratory’s workers, Iiro Jääskeläinen, belongs to (http://www.oecd.org/pdf/M00033000/M00033112.pdf). In practice, we have started a collaborative effort with CSC and other HUT laboratories towards creating an interoperable database for MEG data. Being one of the pioneers in MEG research globally, the HUT is a very well suited environment for testing the requirements for MEG data sharing and archiving. Additionally, we are committed to free distribution of brain signal analysis algorithms developed at LCE. A new neuroinformatics major within the study program of bio-information technology at HUT has also been set up by LCE, to offer teaching on this relatively new and exciting topic.

5.4.5 Statistical Brain Signal Analysis

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

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 relying on the data only. Some additional a priori information must be provided in order to obtain sensible results, necessitating a Bayesian treatment of the problem.

The overall aim of the research 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 propose a full Bayesian approach in the MEG inverse problem with $\ell^p$-norm priors. This model contains as special cases the minimum norm estimate (MNE) and minimum current estimate (MCE), which are both widely used in practice. The choice between MCE and MNE is completely arbitrary; our method deals with this by introducing a hyperparameter which continuously varies between the limiting cases of MCE and MNE. Instead of fixing
the hyperparameter to some value *ad hoc*, it is integrated over using MCMC methods when performing the final analysis.

![Simulated Activation](image1) ![Inverse Estimate](image2)

Figure 51: Left figure shows a simulated activation plotted on the discretized cortical white-matter gray-matter boundary viewed from the left. In the middle, an inverse estimate obtained by using the MCMC samples (shown on the right) from the posterior distribution of the hierarchical model.

We also proposed an alternative hierarchical extension of the model corresponding to the minimum norm estimate (see Fig. 51). 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. The outcome of integrating over the hyperparameters was a heavy-tailed prior distribution especially suitable for reconstructing focal brain activations.

Tentative results of the simulation studies were promising and we have started more extensive simulation and real data experiments. Means for reducing the dimensionality (the number of free parameters) of the inverse problem were preliminarily studied. This included spatial correlation models, principal component analysis, and parametric/semiparametric models for brain activation patterns. These issues will be further investigated in the future and applied to real problems of cognitive neuroscience.
5.5 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 Sience 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$^{1,2}$
$^1$ Department of Engineering Science, University of Oxford
$^2$ Laboratory of Computational Engineering, Helsinki University of Technology

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. 52 and hence difficult to segment using plain edge-detectors, we use textons to jointly segment and classify individual regions of each individual coral. Fig.53 illustrates one particular species.

Figure 52: 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 53: 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

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 54). With the grain boundary there are two competing configurations for the interface to adopt: a straight interface with an angle $\phi$ and a dog-leg 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 55. We demonstrate that the crossover between these two is manifested by a phase transition.

Furthermore we studied 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 in to 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.

![Figure 54: System without a grain boundary has an interface crossing the system in angle $\phi$.](image1)

![Figure 55: System with a grain boundary adopts a dog-leg configuration below the transition temperature.](image2)
6 Research Activities

6.1 Visits to the Laboratory

- Douglas Abraham, Prof., University of Oxford, UK.
- Yuri Alexander, Prof., Russian Academy of Science, Russia.
- Rafael Barrio, Prof., Autonomous University of Mexico, UNAM, Mexico.
- Alex Bunker, Dr., Unilever Research, Port Sunlight, UK.
- Kim Christensen, M.Sc., University of Southern Denmark, Denmark.
- Markus Deserno, Dr., Max Planck Institute for Polymer Research, Germany.
- Lei Dong, M.Sc., The Chinese University of Hong Kong, China.
- Zoltan Eisler, M.Sc., Budapest University of Technology and Economics, Hungary.
- Ralf Everaers, Dr., Max-Planck Institute for Complex Systems, Gernany.
- Gudmundur Haraldsson, Prof., University of Iceland, Iceland.
- Ji-Ping Huang, M.Sc., The Chinese University of Hong Kong, China.
- Outi Hovatta, Prof., Karolinska Institutet, Sweden.
- Giulia Iori, Dr., King’s College London, UK.
- Janos Kertesz, Prof., Budapest University of Technology and Economics, Hungary.
- David Landau, Prof., University of Georgia, USA.
- Paul Leath, Prof., Rutgers, State Univ. of New Jersey, USA.
- Sergey Lyulin, Dr., Russian Academy of Science, Russia.
- Ole Mouritsen, Prof., University of Southern Denmark, Denmark.
- Jorma Rissanen, Prof., IBM Research Center, Almaden, USA.
- Miguel Robles, Dr., Autonomous University of Mexico, UNAM, Mexico.
- Rolf Würtz, Dr., Ruhr-Universität Bochum, Germany.
- Kin Wah Yu, Prof., The Chinese University of Hong Kong, China.
- Yan-jiao Zhao, M.Sc., The Chinese University of Hong Kong, China.

6.2 Visits by Laboratory Personnel

Sebastian von Alfthan
- Invited talk: Clusters of amorphous Si in crystalline Si: stability and collapse

Michael Frydrych
- Miralab, University of Geneva, Switzerland, 4 September, 2003.

Laura Juvonen
- Center for Simulational Physics, The University of Georgia, Athens, GA, USA, 10 February - 2 March, 2003.

Iiro Jääskeläinen
- MGH-NMR Center, Boston, MA, USA, 2-11 September, 2003.

Ilkka Kalliomäki

Mikko Karttunen
- Montreal, Canada, January-February, 2003
- Invited talk at Department of Physics, McGill University, Montreal, Canada
- Invited talk at Department of Physics, Clark University, Worcester, USA
- Invited talk at Department of Physics, University of Guelph, Guelph, Canada
• Santiago, Chile, March, 2003
  - Invited talk at Department of Physics, University of Santiago, Chile.

Kimmo Kaski
• Institute de Fisica, Universidad Nacional Autonoma de Mexico, Mexico, 13-18 January, 2003

Jari Kätsyri
• MiraLab, University of Geneva, Switzerland, 4 September, 2003.

Teemu Leppänen

Riikka Möttönen

Aapo Nummenmaa
• Massachusetts General Hospital, Massachusetts Institute of Technology - Harvard Medical School, Athinoula A. Martinos Center for Biomedical Imaging, Charlestown, MA, USA, 2-9 June, 2003.

Mirta Rodriguez
• Quantum Optics group, University of Hannover, Germany, 25 May - 6 June, 2003.

6.3 Participation in Conferences and Seminars

Sebastian von Alfthan
  - Poster: Phase Separation in Amorphous Semiconductors
• 2003 MRS Fall Meeting, 1-5 December, 2003, Boston, USA
  - Poster: Phase separation in amorphous SiO.

Tobias Andersen
• Society for Neuroscience 33rd Annual Meeting, 8-12 November, 2003, New Orleans, USA

Toni Auranen
• Lääketieteellisen fysiikan ja teknikan yhdistyksen päivä, posterikilpailu, 9 January, 2003, Biomedicum, Helsinki, Finland.
  - Poster: Nonparametric statistical analysis of time-frequency representations of magnetoencephalographic data.

Anirban Chakraborti
• Unconventional Applications of Statistical Physics, 20-22 March, 2003, Saha Institute of Nuclear Physics, Calcutta, India.
  - Invited talk: M. Sysi-Aho, A. Chakraborti and K. Kaski: Biology helps you to win a game.
• 8th Annual Workshop on Economics with Heterogeneous Interacting Agents, 29-31 May, 2003, Kiel, Germany.

Martin Dobsik
• International Conference on Auditory-Visual Speech Processing, AVSP, 4-7 September, 2003, St. Joroiz, France.
Michael Frydrych
- International Conference on Auditory-Visual Speech Processing, AVSP, 4-7 September, 2003, St. Joroiz, France.
  - Poster: Toolkit for Animation of Finnish Talking Head.
Jukka Heikkonen
- RSS 2003 The International Conference of the Royal Statistical Society, July 14-17, 2003, Diepenbeek, Belgium
Maria Huhtala
  - Poster: The effects of ion-irradiation-induced defects on mechanical properties of carbon nanotubes
Anu Huttunen
  - Poster: A. Huttunen, P. Törmä: Photonic crystal slabs: effect of the surrounding material.
Laura Juvonen
- 16th Annual Workshop, Recent Developments in Computer Simulation Studies in Condensed Matter Physics, 24-28 February, 2003, Athens, GA, USA.
- The Annual March Meeting of the American Physical Society, 3-7 March, 2003, Austin, Texas, USA
  - Talk: Reconstruction and intermixing in thin Ge layers on Si(001).
Iiro Jääskeläinen
- Ninth Annual Meeting of the Organization of Human Brain Mapping, 18-22 June, 2003, New York, USA
  - Chairman in Symposium: Multi-modal investigation of the human auditory cortex
- Co-chairman in 1st Nordic workshop on Brain imaging and Neuroinformatics, 2 October, 2003, Tampere, Finland.
Aatu Kaapro
- TICPS workshop on Computational Systems Biology, 16 June, 2003, Tampere, Finland.
Mikko Karttunen
- Tieteen päivät- Science Days, 8-12 January, 2003, Helsinki, Finland.
- Hairy Interfaces and Stringy Molecules Summer School and Workshop, 13-17 August, 2003, Odense, Denmark.
- CECAM (Centre Euopeen de Calcul Atomique et Moléculaire) meeting: Self organization in (bio)molecular systems, 20-22 October, 2003, Lyon, France
  - Turku Lipid meeting, 18 November, 2003.
Kimmo Kaski
- Cesaer’s 14th General Assembly and Seminar, 23-25 October, 2003, Lyon, France
  - Talk: Life, the new Element of Engineering Sciences
- Unconventional Applications of Statistical Physics conference, 20-22 March, 2003, Saha Institute of Nuclear Physics, Calcutta, India
  - Member of organizing committee
  - Invited talk: J.P. Onnela, A. Chakraborti, K. Kaski and J. Kertesz: Does money grow on trees?
  - Co-organizer of the Symposium.
- III Brazilian Meeting on Simulational Physics, 13-15 August, 2003, Ouro Preto, MG, Brazil
  - Invited talk: Turing systems as models of pattern formation in nature.
- 2003 MRS Fall Meeting, 1-5 December, 2003, Boston, USA
  - Invited talk: Carbon Nanotube Structures and MD Simulations at the Realistic Limit

Vasily Klucharev
- Ninth Annual Meeting of the Organization of Human Brain Mapping, 18-22 June, 2003, New York, USA

Vibhor Kumar
- TICPS workshop on Computational Systems Biology, 16 June, 2003, Tampere, Finland.

Antti Kuronen
  - Poster: Dislocation Nucleation from Strained Layer Surfaces

Jari Kätsyri
- International Conference on Auditory-Visual Speech Processing, AVSP, 4-7 September, 2003, St. Joroiz, France.
  - Poster: Identification of Natural and Synthetic Emotional Facial Expressions.

Janne Lehtonen
- Neuroscience Finland 2003,22-23 August, 2003, Biomedicum, Helsinki, Finland
  - Poster: L. Laitinen & J. Lehtonen: Brain Computer Interface
- 1st Nordic workshop on Brain Imaging and Neuroinformatics, 2 October, 2003, Tampere, Finland.
- VIII Congress of the Nordic Medical Society of Paraplegia,4-7 September, 2003, Helsinki, Finland.
  - Talk: Characterisation of the sensimotor cortical activity in tetraplegics.
Teemu Leppänen
  - Talk: Robustness and connectivity of Turing patterns
- Third Annual Helsinki-Stockholm meeting on Biomolecular Modeling, 9-11 April, 2003, Helsinki University of Technology, Finland.
  - Talk: Pattern formation in Turing systems
- Current Topics in Physics Symposium, 16-20 June, 2003, Universidad Nacional Autónoma de Mexico, Mexico.
  - Invited talk: Robustness and Connectivity of Turing Structures
- A Non-linear World: The real World. Second International Conference on Frontier Science, 8-12 September, 2003, University of Pavia, Italy.
  - Poster: Robustness and Connectivity of Turing Structures.

Markus Miettinen
  - Poster: Combined Effect of Solvent Quality and Shear Flow on a Polymer Chain: A Computational Study
- Hairy Interfaces and Stringy Molecules Summer School, 13-17 August, 2003, Odense, Denmark

Ville Mustonen
  - Talk: Filling in Triangular 2d Ising model

Riikka Möttönen
- Ninth Annual Meeting of the Organization of Human Brain Mapping, 18-22 June, 2003, New York, USA

Petri Nikunen
  - Poster: Dissipative particle dynamics: From algorithms to applications

Aapo Nummenmaa
- Advanced Course in Neuroscience: from molecules to brain functions, 11-17 January, 2003, Tvärminne Zoological Station, Finland.
- MEG Intensive Course, 8-10 February, 2003, Otaniemi, Finland.

Janne Ojanen
- TICSP Workshop on Computational Systems Biology, June 16-17, 2003, Tampere, Finland
- RSS 2003 The International Conference of the Royal Statistical Society, July 14-17, 2003, Diepenbeek, Belgium
  - Poster: A New Fully Automated Allele Calling Method For High-Throughput Genotyping

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Ville Ojanen
- International Conference on Auditory-Visual Speech Processing, AVSP, 4-7 September, 2003, St. Joroiz, France.

Jani Oksanen
- 7th International Workshop on Nonlinear Optics and Excitation Kinetics in Semiconductors (NOEKS7), 24-28 February, 2003, Universität Karlsruhe, Germany.

Jukka-Pekka Onnela
- A Non-linear World: The Real world. Second International Conference on Frontier Science, 8-12 September, 2003, University of Pavia, Italy.

Marco Patriarca
- International Conference News and Expectations in Thermostatistics, 21-28, September, 2003, Capo Boi, Villasimius, Cagliari, Italy
- Poster: M. Patriarca, A. Chakraborti and K. Kaski: Gibb’s versus non-Gibb’s distributions in money dynamics.
- Frontier Science 2003 Conference A Nonlinear World: the Real World, 8-12 September, 2003, Collegio Cairoli, Pavia, Italy.
- Poster: M. Patriarca and T. Leppänen: Modelling language competition.
- Contributed talk: Visualization and tracking of crystal defects. M. Patriarca, A. Kuronen and K. Kaski
- Poster: P. Szelestey, M. Patriarca and K. Kaski: Numerical study of dislocation properties in nickel
- Poster: A. Kuronen, M. Partiarca and K. Kaski: Dislocation nucleation from strained layer surfaces.

Mirta Rodriguez
- Vortices in superfluids and supercondutors, 4-8 January, 2003, Oulu, Finland
- Poster: M. Rodriguez, G.-S. Paraoanu, P. Törmä: Vortices in trapped superfluid Fermi gases.
- XXXVII Annual Conference of the Finnish Physical Society, 20-23 March, 2003, Helsinki, Finland
- XXIX Biannual meeting of the Royal Physical Society of Spain, 7-11 July, 2003, Madrid, Spain
- Poster: M. Rodriguez, G.-S. Paraoanu, P. Törmä: Bloch oscillations and josephson effect in atomic Fermi gases.
- Quantum Challenges, 4-6 September, 2003, Falenty, Warsaw, Poland.
- Poster: M. Rodriguez, P. Törmä: Bloch oscillations in Fermi gases.

Mikko Sams
- International Conference on Auditory-Visual Speech Processing, AVSP, 4-7 September, 2003, St. Joroiz, France.
- Invited talk: Multi-modal studies of human audio-visual integration
- 43rd Annual Meeting of the Society for Psychophysiological Research, 29 October - 2 November, 2003, Chicago, IL, USA
- Invited talk: Audio-visual speech processing and attention
- 7th Finnish-Russian Winter School, 12-18 January, 2003, Tväriminne, Finland
- Invited talk: Neurocognitive mechanisms of audiovisual speech

Adrian Sutton
- Royal Society of London, on the occasion of the election to a Fellowship of the Royal Society, July 2003.
- Invited talk: Fundamental aspects of electronic conduction in nanowires.

Toni Tamminnen
- Poster: Learning an object model for feature matching in clutter.

Mika Toivanen
- TICPS workshop on Computational Systems Biology, 16 June, 2003, Tampere, Finland.

Jukka Tulkki
- Talk: Bioengineering education in HUT.
- Cesaer’s 14th General Assembly and Seminar, 23-25 October, 2003, Lyon, France
- Talk: Bioinformation technologist: A system engineer mastering ICT and life sciences

Aki Vehtari:
- Practical Bayesian Statistics 5. 28 - 31 July 2003 Milton Keynes, U.K.

Wei Zhao
- Hairy Interfaces and Stringy Molecules Summer School, 13-17 August, 2003, Odense, Denmark

6.4 Memberships in scientific societies

Sebastian von Alfthan:
- Member of Materials Research Society, MRS
- Member of Finnish Physical Society

Maria Huhtala:
- Member of Finnish Physical Society

Kimmo Kaski:
- Fellow of American Physical Society
- Member of Association for Computing Machinery
- Fellow of the Finnish Academies of Technology
- Fellow of Institute of Physics, UK.OP
• Member by invitation, Academica Europaea
• Fellow of Finnish Academy of Science and Letters
• Supernumerary Fellow, Wolfson College, University of Oxford, UK
Adrian Sutton:
• Fellowship of Royal Society, UK.
Toni Tamminen:
• Member of International Association for Pattern Recognition
• Member of the International Society for Bayesian Analysis
• Member of 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 Finnish pattern recognition society,

6.5 Other Activities

Sami Brandt has acted as
• Reviewer in journal:
  - Pattern Recognition Letters
Iiro Jääskeläinen has acted as
• Reviewer in Journals:
  - Biological Psychology
  - Clinical Neuropsychology
Mikko Karttunen has acted as
• Reviewer in Journals
  - European Journal of Pharmaceutics
  - Chemical Physics Letters
  - Chemistry and Physics of Lipids
• External thesis examiner
  - Department of Physics, The Chinese University of Hong Kong
  - Department of Physics, University of Jyväskylä
• Radio interview
  - Finnish Radio 1’s weekly science programme, May 7, 2003. Cells, membranes, their
    modeling and functions.
Kimmo Kaski has acted as
• Member of Editorial Board in
  - International Journal of Modern Physics
• Reviewer in
  • Reviewer in Ph.D. dissertation
    - Pep Mourino, Universitat Politecnica de Catalunya
Timo Koskela has acted as
• Reviewer in Journal
  - Neural Networks
Jouko Lampinen has acted as
- Opponent in Ph.D. dissertations:
  - Joni Kämäräinen, Lappeenranta University of Technology
- Member of organizing committee
  - ESANN 2003
- Member of the board in Finnish Brain Research Society
- International Project Reviewer
  - Reviewer and evaluator in mid-term evaluation of EU 5th framework IST-programme
    (4 projects)
- Reviewer in journals and conferences
  - IEEE Transactions on Neural Networks
  - Journal of Electronic Imaging
  - International Journal of Pattern Recognition and Artificial Intelligence
  - HICCS, Hawaii International Conf. on Systems Sciences

Janne Lehtonen, Laura Laitinen and Tommi Nykopp
- Appearance in YLE 1, Prisma program. September 2003.

Mirta Rodriguez has acted as
- Referee in Journal
  - Physical Review A

Mikko Sams has acted as
- Reviewer in Journals
  - Cognitive Brain Research
  - Neuroscience Letters
  - Journal of Cognitive Neuroscience
  - Scandinavian Journal of Psychology
  - Emotion
- Pre-examiner in Ph.D. dissertations
  - Sari Avikainen, Ph.D., University of Helsinki.
- Member of Editorial Board in
  - Tiede (Finnish popular science magazine)
  - Polysteeki (Journal of the Helsinki University of Technology

Toni Tamminen has acted as
- Reviewer in conference
  - 11th European Symposium on Artificial Neural Networks

Jukka Tulkki has acted as
- Chairman of the Faculty Council of the Department of Electrical and Communications Engineering, Helsinki University of Technology
- Coordinator of the Study Programme of Bioinformation technology in Helsinki University of Technology.
- Member of the Research Council of Helsinki University of Technology

Aki Vehtari has acted as
- Member of the board in Pattern Recognition Society of Finland, Hatutus
- Reviewer in journal
  - Journal of Computational and Graphical Statistics
- Reviewer in conference
  - Esann 2003
7 Publications


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