

Fraunhofer CHALMERS Research Centre Industrial Mathematics

Annual Report 2007



FCC Fraunhofer-Chalmers Research Centre for Industrial Mathematics

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Cover

In a project with AstraZeneca R&D Mölndal we have developed a framework for modeling and simulation of atrial fibrillation, which is the most common form of heart arrhythmia. The figure shows the distribution of different cell types on the surfaces of the left and right atrium in a heart model used for studying the effects of inhibiting single or multiple ionchannel types, cf pages 43 - 44 (courtesy of AstraZeneca).

Illustrations

To illustrate our research on pages 12 - 47 we use pictures of flowers in the spirit of the Swedish Linnean year 2007, see also the inner back cover.

Annual Report 2007

Fraunhofer-Chalmers Research Centre for Industrial Mathematics, FCC

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Preface



FCC operates in Chalmers Science Park.

Also 2007 the Centre managed to maintain the income level three million euros established the year before, again with a positive net.

Together with our partners Chalmers and the Fraunhofer industrial mathematics institute ITWM we cover a wide range of applications. In 2007 the project exchange was about one million euros with each partner including basic project funding.

The Gothenburg Mathematical Modeling Centre (GMMC) run by Mathematical Sciences 2006 – 2010 with a budget of two and a half million euros and the Vinnex Centre run by the Wingquist Laboratory 2007 – 2016 with a budget of seven and a half million euros are two prestigious Swedish strategic initiatives at Chalmers where FCC participates.

The diagrams below show the development of the centre in terms of income and staff.

Staff – man-years

□ Students Fraunhofer and Chalmers 37,8 37,5 Partners Public projects **FCC** Industry project 3 083 3 028 5,0 7,5 5,3 27,5 27% 29% 5,7 2 371 25,9 4,7 2 127 2 0 3 4 4,0 21,0 3,1 34% 24% 3,1 1,5 39% 35% 24% 27,2 24,6 18% 49% 19,7 50% 18,8 17,0 42% 43% 38% 2003 2004 2005 2006 2007 2003 2004 2005 2006 2007

Income – kEUR

The profile of the Centre is controlled by its income structure. The result of 2007 is well in line with the Fraunhofer financial model, i e, the project volumes from industry (50%), public financiers (21%), and Fraunhofer and Chalmers (29%) are well in balance.

We have an attractive staff, as became apparent by three senior members leaving the Centre during the year for new positions, two of them abroad. At the same time we are delighted about also making several valuable recruitments.

The department Geometry and Motion Planning, working in close co-operation with the Chalmers Wingquist Laboratory, has established

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an income level well above one million euros. The activities 2007 include the start of a third Vinnova MERA project on paint simulation, rapidly growing income from path-planning software licences, and substantial joint development with the ITWM department Dynamics and Durability.

The department Computational Engineering and Design has expanded its work on multi-physics applications which require coupled electromagnetic and fluid dynamics simulations, in particular through projects with Swedish and other European industrial partners together with the ITWM departments Optimization, Transport Processes, and Flow and Material Simulation. The department runs a strategic cooperation with Chalmers on simulation-based optimization through GMMC.

The department Reliability and Risk Management has started a three-year joint project on load analysis for automotive applications with Chalmers Stochastic Centre, Fraunhofer ITWM, SP Technical Research Institute of Sweden, and six European truck manufacturers from Germany, Italy, the Netherlands, and Sweden. In finance and insurance we have built software platforms for Asset Liability Management, Robust Portfolio Optimization, and Collateral Debt Obligations together with ITWM.

The department Systems Biology and Bioimaging has continued to grow by adding substantial industrial (pharmaceuticals) and public (EU and GMMC) income to our long-term grant from the Swedish Foundation for Strategic Research SSF.

I thank my co-workers at FCC for your excellent work and my colleagues at Chalmers and Fraunhofer ITWM for our fruitful collaboration. From 2001 we have started 230 projects, 200 of which have been completed and 30 of which are running, with companies and organizations of different size and from different branches.

Finally I thank my colleagues in the Swedish Society for Applied Mathematics and the Swedish Institute for Applied Mathematics – STM and ITM. These organizations have now been dissolved after having secured the successful startup of FCC. It has been an honour and a great pleasure to work with you for many years!



Uno Nävert, Director of FCC.

Göteborg in April 2008

Ino Naverto Uno Nävert

Director

Profile

Mathematics has become a key technology for industrial innovation since mathematics is behind all work in the virtual world.



Project mix by income.

The Fraunhofer-Gesellschaft and Chalmers have founded FCC to undertake and promote scientific research in the field of applied mathematics to the benefits of Swedish and European industry, commerce, and public institutions. To do so the Centre undertakes scientific research and marketing financed by the founders and by public institutes, and works on projects defined by companies on a commercial basis.

FCC is an example of a bottom-up strategy to build the European research space. First we define a small network of closely (daily) cooperating research institutes. To solve concrete problems from companies from all over Europe, we then create optimal teams built out of this network. We do this in the field of mathematics, which is a key technology for industrial innovation, lying behind all work in the virtual world, e g, simulation for prediction, control, optimization, and risk assessment.

By the end of 2007 the staff was twentysix full-time equivalents, including five scientific advisers from Chalmers, each one working 10 percent to 20 percent of full time at FCC.

FCC undertakes scientific research financed by its founders and by public institutes.



Departments by income.

Scientific competence

The Centre undertakes scientific research projects and marketing of scientific results financed by its founders and by public institutes. Respecting the confidentiality of data from customers, the Centre encourages the publication of results. FCC supports efforts to use its research for educational purposes at all levels at Chalmers as well as at other educational institutions in Sweden and Europe. FCC sponsors PhD work, if the subjects are of basic interest for the research in the Centre. FCC keeps contact with the worldwide community of applied mathematicians by active participation in conferences and by inviting guest scientists.

In 2007 the Centre has received public grants from SSF (Swedish Foundation for Strategic Research), Vinnova (Swedish Agency for Innovation Systems), and EU (Network of Excellence Biosim, coordinated action YSBN).

Entrepreneurial competence

The Centre served twentyeight industrial clients in 2007. One of the largest customer was the Swedish Society for Applied Mathematics, STM, a consortium of companies with business in Sweden. A list of industrial and public clients is shown on page 7.

Experiences from Fraunhofer show that small and medium size companies constitute an important market for an industrial mathematics institute. The number of SME projects at FCC is however still only marginal.

In 2007 the Centre has served international industrial clients from Germany, Italy, Japan, and the Netherlands.

Professional networking

The Centre has a very close relation to its founders Chalmers and Fraunhofer ITWM, cf pages 8 - 11, exchanging staff members, cooperating in projects, by joint participation in European projects, by connecting Swedish clients with ITWM and vice versa, and by stimulating the co-operation between Swedish industry and other Fraunhofer institutes.

In order to fulfil its tasks optimally, the Centre co-operates with competent scientific groups at universities and elsewhere, and promotes research and education in industrial mathematics at institutions outside the Centre, cf pages 12-13, 20-21, 28-29, and 38-39.



Financial mix

The financial model distinguishes between three income sources: project financing from the founders, industrial project income, and public project income. These three should be in reasonable balance.

Since start, the industrial and public project volume has increased more than expected in the original business plan. As a result of this, the relative project financing from the founders has decreased from 44 percent in 2001 to 29 percent in 2007. FCC works on projects defined by companies on a commercial basis.

FCC in close co-operation with Chalmers and Fraunhofer shall be a leading international partner in industrial mathematics.

FCC earns approximately 30% from its founders, 50% industrial income, and 20% public income.

Acknowledgements

The Centre is a Swedish foundation established by Chalmers and the Fraunhofer-Gesellschaft. The decision has been based on a business plan prepared by the Swedish Institute for Applied Mathematics (ITM) and Fraunhofer-Institut für Techno- und Wirtschaftsmathematik (ITWM).

The Swedish Society for Applied Mathematics (STM) and the former Swedish National Board for Technical and Industrial Development (NUTEK) have supported FCC taking over ITM operations.

The Swedish Foundation for Strategic Research (SSF) has played an essential role by giving support of one million euros for a public project whereby a research team in Systems Biology and Bioimaging has been established at the Centre.

In 2005 Fraunhofer and Chalmers decided to continue their commitments for the next five years 2006 - 2010.

Clients and Partners

Since its start in 2001, FCC has successfully co-operated with enterprises of different sizes and from many branches. Those clients and partners, who have accepted to be cited, are, among others:

- ABB
- ABB Robotics
- ABB Power Technologies
- Adam Opel GmbH (DE)
- Aerotech Telub
- Albany International
- AP2 Second Swedish National
- Pension Fund
- AstraTech
- AstraZeneca R&D Alderley Park
- AstraZeneca R&D Mölndal
- AstraZeneca R&D Södertälje
- Atlas Copco Rock Drills
- Bergaskolan
- Bombardier Transportation
- BTG Pulp and Paper Sensors
- Chalmers
- Chalmers Industriteknik
- Consorzio Politechnico
- Innovazione (IT) DAF Trucks (NL)
- Daimler-Chrysler (DE)
- Delphi (JP)
- Efield AB
- Elforsk
- Elmo Leather
- Ericsson
- Faurecia Exhaust Systems
- FOL
- Fortum Power and Heat OY
- Fraunhofer ITWM (DE)
- Front Capital Systems
- General Motors (DE)
- IIR Sweden
- InNetics
- Innovativ Vision
- Iveco (IT)
- IVF Industriforskning
- Jernkontoret
- Chalmers • Fraunhofer ITWM (DE)
- University of Copenhagen
- University of Gothenburg
- University of Kaiserslautern
- EU Biosim / DTU (DK)

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- EU Visicade / Fraunhofer IGD (DE)
- ITM
- Swedish Energy Agency, STEM

- KP Pension and Insurance
- MAN (DE)
- Micropos Medical
- NMCT
- Novo Nordisk (DK)
- Optimization Partner Stockholm
- PLANit Sweden
- Poseidon Diving Systems
- PSA Peugeot Citroën (FR)
- Saab
- Saab Automobile
- Saab Communication
- Saab Ericsson Space
- Saab Microwave Systems
- Safe Technology
- Saint-Gobain Sekurit Scandinavia
- Sandvik Steel
- SCA
- Scania
- SEM
- Simula Research Laboratory AS (NO)
- SKF (Sweden and NL)
- STM Forskningsservice
- SP Technical Research Institute of Sweden
- Spotfire
- StoraEnso Corporate Research
- Swedish Insurance Federation
- Sydkraft
- TetraPak
- Uddcomb
- Universitetssjukhuset MAS
- Volvo Aero Corporation
- Volvo Car Corporation
- Volvo Powertrain
- Volvo Truck Corporation
- Volvo 3P
- University of Linköping
- University of Lund
- University of Rostock
- Technical University of Denmark DTU
- The Royal Institute of Technology
- Swedish Foundation for Strategic Research, SSF
- Swedish Governmental Agency for Innovation Systems, Vinnova

Year 2007

- Albany International
- AP2 Second Swedish National Pension Fund
- AstraTech
- AstraZeneca R&D Alderley Park
- AstraZeneca R&D Mölndal

Fraunhofer ITWM (DE)

General Motors (DE)

Chalmers DAF (NL)

• Daimler (DE)

• Delphi (JP)

• Efield

• InNetics

• IVF

Scania

• SEM

SKF

STM

of Sweden

• Stora Enso

lveco (IT)

• MAN (DE)

Saab Automobile

Saab Communication

• Svensk Verktygsteknik

Volvo Aero Corporation

Volvo Car Corporation

Volvo Truck Corporation

Chalmers GMMC / SSF

Chalmers Vinnex / Vinnova

Universities of Copenhagen, Gothenburg, Kaiserslautern,

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Fraunhofer ITWM (DE)

Linköping, Rostock, DTU

• EU

ITM

SSF

Vinnova

SP Technical Research Institute

Fraunhofer-Gesellschaft



Professor Helmut Neunzert, ITWM, Honourary doctorate at Chalmers 2007 Vice Chairman of FCC.

www.fraunhofer.de www.itwm.fraunhofer.de The Fraunhofer-Gesellschaft is the largest organization for applied research in Europe.

The Fraunhofer-Gesellschaft undertakes applied research of direct utility to private and public enterprise and of wide benefit to society. Its services are solicited by customers and contractual partners in industry, the service sector and public administration. The Fraunhofer-Gesellschaft maintains roughly 80 research units, including 56 Fraunhofer Institutes, at over 40 different locations throughout Germany. A staff of some 13000, predominantly qualified scientists and engineers, works with an annual research budget of 1.3 billion euros. Roughly two thirds of this sum is generated through contract research on behalf of industry and publicly funded research projects. The remaining one third is contributed by the German federal and Länder governments, partly as a means of enabling the institutes to pursue more fundamental research in areas that are likely to become relevant to industry and society in five or ten years' time.

The Fraunhofer-Gesellschaft is also active on an international level: Affiliated research centers and representative offices in Europe, USA, Asia, and in the Middle East provide contact with the regions of greatest importance to present and future scientific progress and economic development.

The Institut für Techno- und Wirtschaftsmathematik, ITWM, in Kaiserslautern became a Fraunhofer institute on January 1, 2001. ITWM has continued its exceptional development and has now (2007) a budget of 12.4 million euros and a staff of 177 persons including 112 scientists, 46 PhD students, and 19 employees of the central services. The Institute further engages 120 reseach assistents, 34 trainees, and 8 apprentices. Its Director is Professor Dieter Prätzel-Wolters.

The ITWM is organized into eight units, which reflect key competence fields: Departments in Transport Processes, Flow and Material Simulation, Models and Algorithms in Image Processing, Adaptive Systems, Optimization, Financial Mathematics, Dynamics and Durability, and the Competence Centre High Performance Computing and Visualization.

Professor Helmut Neunzert is responsible for international affairs at ITWM. FCC originates from his vision of a European institution operating in the Fraunhofer spirit.

Co-operation

FCC and ITWM are, more and more, growing together. Many projects are transferred in both directions - the flow is, in 2007, quite in balance, as it is altogether almost a million euros, which passes the border. But, of course, projects are not only given to the partner, but quite some projects were dealt with together, cf below.

The advantage of operating as one unit is clear: with a total of more than one hundred scientists FCC and ITWM offer a real power in industrial mathematics; it certainly belongs to the largest and most competent institutions for industrial mathematics in Europe.

Computational Engineering and Design

FCC and ITWM run joint projects on electromagnetics and fluid dynamics multi-physics, fibre flow modelling, and optimization by similarity clustering, cf page 12-19.

Geometry and Motion Planning

ITWM has developed improved methods for the simulation and visualization of robot cable motion and transient cable dynamics, cf page 32-35. FCC and ITWM run a joint project on surface inspection, where we develop an automatic grading system for leather manufacturing, cf page 37.

Reliability and Risk Management

FCC and ITWM run a joint project on load analysis for automotive applications with six European truck manufacturers, cf page 23. We have run several joint projects in finance and insurance, where we have developed theory and tools for asset liability management and robust portfolio optimization, cf page 27.

Systems Biology and Bioimaging

FCC and ITWM work together in a project on transport in Glial cells, cf page 41.





Chalmers



Professor Peter Jagers, Chalmers, Chairman of FCC.

www.chalmers.se www.math.chalmers.se The Chalmers University of Technology (Chalmers tekniska högskola) was founded in 1829. It is a non-profit, non-governmental university. With its 8500 students for engineering and architecture degrees, and almost 1000 PhD students it is one of Sweden's two leading technology universities.

Most of Chalmers' resources come from contracts with the state of Sweden (72%), but Chalmers also has strong support from nongovernmental research organizations (17%) and industry (11%). The annual (2007) turnover is 240 million euros. Two thirds of the budget are alotted to research and to graduate studies. With its staff of 2137 full time equivalents, including 175 full professors, the University has strong and well-known departments in most fields of science and engineering.

Chalmers has made special efforts to integrate mathematics into a broader scientific and technological perspective. Strong activities in stochastics and numerical and modelling mathematics have emerged. Thus, besides activities in the various mathematical fields, Chalmers Applied Mathematics comprises three more specialized centres.

Professor Peter Jagers was the President of the Chalmers Faculty Senate 1993 - 2002. He brought up the idea of engaging Chalmers in a joint venture, when the Fraunhofer-Gesellschaft started to look for Swedish partners. He also represented Chalmers in the subsequent negotiations.

Co-operation

A key element in the operation of FCC is its close co-operation with Chalmers.

This co-operation is mainly organized through scientific advisers and affiliated experts. Each adviser and expert typically spends between 10 and 20 percent of full time at the Centre. In 2007 there were four advisers and one affiliated expert representing optimization, stochastics (fatigue life), bio imaging, and mechanical engineering (product and production).

Here we describe three particularly successful areas within the cooperation:

Geometry and Motion Planning

Chalmers started the Wingquist Laboratory in October 2001 as part of Mechanical and Vehicular Engineering to increase the collaboration with Swedish industry and to concentrate research in strategic areas. The laboratory conducts interdisciplinary research within the field of virtual verification of product and production concepts.

FCC and Wingquist have a very close co-operation in geometry and motion planning focusing on product and production system modelling, robust design and variation simulation, and flexible production and automation systems, cf pages 28 - 35.

Statistical Fatigue of Materials

Chalmers and FCC have together built up a strong operation in fatigue life and load analysis, with industrial income 2001 - 2007 from Swedish (895 kEUR), Dutch (50 kEUR), French (165 kEUR), German (100 kEUR), and Italian (65 kEUR) companies. The total industrial income 2007 was 250 kEUR.

The strategy has been to consider the fatigue group as one unit jointly supported by Chalmers and FCC. In that way, problems from industry are imported into the academic work and research results are exported to industry. This two-way communication has proved fruitful for the students at Chalmers, including students from industry hosted at Chalmers and FCC, as well as for the industrial partners, cf pages 22 -25.

Gothenburg Mathematical Modelling Centre GMMC

In December 2005 the Swedish Foundation for Strategic Research (SSF) decided to finance seventeen strategic centres including the Gothenburg Mathematical Modelling Centre (GMMC).

The research programme includes (1) Optimization and modelling, (2) Risk, reliability, quality, and (3) Biomathematics. In 2007 the focus of FCC has been on (1) combustion engine and antenna optimization, (2) parameter estimation, model reduction, particle tracking and gel structure modelling, and (3) reliability and quality through variation mode and effect analysis, cf page 18-19, 22-25, 38-47. VINNOVA has decided on a ten year grant to Chalmers of 700 kEUR per year 2007 - 2016 for the Wingquist Laboratory Excellence Centre for Efficient Production Realization. Its director is Professor Rikard Söderberg.

"The establishment of FCC has made it possible for the fatigue group to host competence for solving particular industrial problems as well as for doing purely academic work."

Professor Jacques de Maré Chalmers Mathematical Sciences, Scientific adviser FCC

SSF has decided on a five year grant to Chalmers of 500 kEUR per year 2006 - 2010 for the Gothenburg Mathematical Modelling Centre GMMC. The director of GMMC is Professor Holger Rootzén.

Computational Engineering and Design

Modern product design and process operations are heavily based on computational mathematics through work in the virtual world. Traditional hands-on engineering is replaced by systematic approaches based on computer simulations, which provide insight in the design phase without the need for expensive measurements. The department of computational engineering and design does mathematical modelling of physical phenomena that can be described by partial differential equations (PDEs). Novel methods and engineering tools are developed which enable efficient solution of complex system of PDEs, making real industrial problems tractable to scientific analysis and simulation-based optimization.

The work is organized in three areas:

- Electromagnetics
- Fluid Dynamics
- Optimization

In electromagnetics we are an implementation partner of the company Efield that commercializes the software that was developed in the national research and code development project GEMS. The software constitutes an excellent platform for research as well as for performing consultancy projects. We have good connections with the Swedish telecommunication industry and projects are performed together with the Swedish Industrial Association for Applied Mathematics (STM). The research in fluid dynamics is focused on fibre flows, fluid-structure interaction and multi-physics applications requiring coupling of fluid dynamics and electromagnetics solvers. New simulation tools are being developed for the Swedish automotive industry for product and process optimization by fast and accurate thickness prediction of spray painting and sealing.

In optimization the research is focused on simulation-based optimal design and multiple criteria optimization. This includes development of novel optimization algorithms, coupling of simulation and optimization software and development of decision support systems that integrate multiple criteria optimization and simulation.

Contact

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Linnean Class IV plant: Pétrea volúbilis L, queen 's-wreath, the family Verbenáceae – verbena plants. The genus has 30 species and has its origin in the West Indies and tropical Americas. Pétrea is named after James Robert Petre (1713-1742), the eighth baron of Petre, who was responsible for the introduction of Caméllia japonica among other things. He was a great lover of the art of gardening and general botany and the owner of large parklands in Thorndon, Essex, England. Volúbilis means "meandering." (Stockholm University, Greenhouse, Department of Botany, 2004)

Co-operation

During 2007, the successful collaboration with the department of Geometry and Motion Planning at FCC has been strengthened through a joint project on virtual paint-shop.

Also the collaboration with the departments of Transport Processes and Optimization at Fraunhofer ITWM has grown by working on joint projects.

Acknowledgement

In 2007 the department received substantial funding from Vinnova and the Swedish Foundation for Strategic Research (SSF) through the Gothenburg Mathematical Modeling Centre (GMMC).

The Computational Engineering and Design Research Group

- Fredrik Edelvik, PhD, Associate Professor, Head of Department
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- Erik Höök, MSc Engineering
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- Andreas Mark, Lic
- Robert Rundqvist, PhD
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Adam Wojciechowski



Ann-Brith Strömberg



Michael Patriksson

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Electromagnetics

The rapid increases in computer power and the development of efficient numerical methods have facilitated computer simulation of complex electromagnetic propagation and interaction phenomena. This is an emerging technology in application areas such as wireless technology, antenna analysis, electromagnetic compatibility, micro electronics, radar signature and medicine.

The activities in electromagnetic simulations at FCC are based on the software suite developed in the national research and software development project GEMS (General ElectroMagnetic Solvers), PSCI project 24082-62591. FCC's participation as sub-contractor in GEMS has brought the center to the forefront in electromagnetic simulations. FCC is an implementation partner of the recently founded company Efield AB that commercializes the GEMS software and contracted to perform further development. FCC markets efield® to new customers as well as performing consultancy projects using the software.

In 2007 the FCC group in computational electromagnetics was heavily involved in the preparation of the first release of efield®. In a research project funded by the industrial consortium STM alternative integral formulations for dielectric and lossy materials were investigated. This novel work resulted in orders of magnitude faster convergence for the multilevel fast multipole method (MLFMM) compared to the original solver. Within GMMC we initiated efforts on multi-objective antenna optimization.

Linnean Class X plant: Caesalpínia gillièsii (WALL EX HOOK) D. DIETR., bird-of-paradise bush, the family Fabáceae – leguminous plants. Caesalpinia L. is a genus with 150 tropical and subtropical species that is named after the Italian Cesalpino (1519-1603). He was the personal physician of Pope Clement VIII but was also a philosopher and botanist. In De Plantis (1583) he maintained that plants were composed of bark and marrow, a division that was particularly interesting to Linnaeus. Gilliésii is named after the Scotsman and naval surgeon John Gillies (1792-1834)), who was interested in botany and collected plants in Chile and Argentina. (Playa las America, Tenerife, March 2005)

The efield® software

The efield[®] software is a result from a successful collaboration between Swedish academia and industry. FCC has played an important part in the development of the software and is currently performing further development contracted by Efield AB. The activities during 2007 have mainly been preparation work for the first releases and improvement of the MLFMM solver for dielectric materials.

The software is used for antenna design, electromagnetic compatibility, radar signature and microwave applications. The solvers are based on formulations in both time domain and frequency domain. A key feature is the use of hybrid methods. In frequency domain a Method of Moments, MoM, boundary integral solver is coupled to a physical optics solver. In time domain an unstructured finite element method is coupled to a finite difference method. The underlying idea of the hybrid methods is to take advantage of the strengths of the individual methods without suffering from their weaknesses and thereby substantially increase the spectrum of solvable problems.

Improved integral formulations for dielectric bodies in MLFMM

In the frequency domain solver, the integral formulation for dielectrics is very ill-conditioned. This is a problem in particular when iterative methods are used since the iterative process converges slowly if it converges at all. This is of crucial importance since this fact limits the use of the fast multipole method to problems with only perfect electric conductors. The industrial consortium STM has funded a project where alternative integral formulations have been investigated.

A particularly challenging problem is to combine dielectric material with metal. In figure 2 the surface currents and in figure 3



Figure 1. Induced surface currents on the ESA Swarm satellite when the left antenna element (one of the two cups on top of the satelite) is transmitting electromagnetic waves. The efield® multilevel fast multipole method (MLFMM) solver has been used (illustration from Efield AB).



Figure 2. Surface currents on Eikon, modeled as a metallic object with radar absorbing material on the leading edges, after a radar pulse has hit the aircraft. A multilevel fast multipole method (MLFMM) has been used.

the bistatic radar cross section for the UAV Eikon with radar absorbing material on the leading edges are presented. Results for the old solver based on the Rumsey reaction formulation (PMCHWT) are in figure 3 compared to results for which the PMCHWT formulation is combined with the Müller formulation. The old implementation suffered from a non-optimal scaling of the equations. Furthermore, a careful analysis of eigenvectors and eigenvalues lead us to a novel combination of equations in the Müller formulation. As seen in the figure the effect on convergence is dramatic.



Figure 3. Comparison of bistatic radar cross section for the UAV Eikon with radar absorbing material on the leading edges computed by the two standard formulations and the new solver based on an improved integral formulation, respectively.

Fluid Dynamics

In industrial systems, like paper making, energy production, or other manufacturing facilitites, understanding the physics of fluid dynamics holds one key to drastically improving the process with respect to production speed, environmental impact, or production cost.

Although single phase fluid flow has many scientifically challenging questions that are still open, flows in industrial systems often include complications such as the presence of more than one phase, interactions between the fluid flow and its boundaries or some other direct link connecting the flow solution with the solution of a different problem. These three aspects of CFD – multiphase flow, fluid structure interaction and flow with multiphysics coupling respectively, are the main interests and core competences of the CFD group at FCC.

Our activities during 2007 within the CFD field have concerned filters, fibres and droplet sprays. Much of the work has been devoted to creating simulation tools for the applications in question, tools that are built around advanced use of commercial CFD codes or around in-house codes. To support these activities the FCC group in CFD expanded with a specialist in development of CFD software during 2007. In addition, in several projects we have a close collaboration with the departments of Transport Processes and Flows and Material Simulation at our partner Fraunhofer ITWM.

Linnean Class VIII plant: Fúchsia x hýbrida HORT. EX SIEB. & SOSS, hybrid fuchsia, the family Onagráceae – willowherb or evening primrose plants. The first fuchsia was probably discovered around 1695 by the French botanist Father Charles Plumier during his third expedition to South America. He found it on Santo Domingo and described it in his book, Nova Plantarum Americanum Genera, wich was published in 1703. He named it Fúchsia Triphýlla Flore Coccinea. Fúchsia has been named after the German physician and botanist Leonhart Fuchs (1501-1566). Hybrida is derived from hýbridus, wich means of mixed races or bastard, and the names was therefore used for a great number of cultivars. (Stockholm University, Greenhouse, Department of Botany, 2004)

Copyright: photo Helene Schmitz, text Pia Östensson

Paper forming simulations

In 2006 and 2007, FCC and ITWM together with Albany International took the first step towards a simulation tool for paperforming fabrics. Individual and arbitrarily curved fibres were simulated under different operating conditions as they settled and formed networks on two different forming fabrics. The results showed that the method works for simulating initial forming patterns in the papermaking process. Development of software and simulation techniques continues in 2008.

CFD Solver

During 2007 FCC has developed an inhouse CFD-solver. The code is written in C++ and is based on Finite Volume discretisation on unstructured grids using the SIMPLE algorithm. It can handle turbulent, transient and weakly compressible flows on arbitrary geometries. The code has been compared to Open Foam and Fluent with good results in solution accuracy as well as computational time. Apart from single phase CFD the code can also handle Lagrangean particle tracking with two-way momentum coupling, meaning that introduced particles affected by the fluid flow as well as influencing the flow.

Virtual Painting

FCC is, in a Vinnova project in collaboration with SAAB Automobile, Volvo Car Corporation, and the Industrial Research and Development Corporation (IVF), developing tools for predicting paint thickness in the process of painting car bodies using pneumatic and electrostatic paint applicators. The recently developed in-house software tool which is based on fast and efficient algorithms for tracing particles, and solving for Efield and fluid flow, shows very good potential for applications in the virtual paint area.

The process of painting a car using an Electrostatic Rotary Bell applicator (ESRB) involves atomization and charging of paint droplets in a rapidly rotating device - the



Figure 1. Simulations of initial paper forming patterns on a forming fabric from Albany International.



Figure 2. Free falling particles in a benchmark simulation of lid-driven cavity flow. The images show fluid streamlines coulored by velocity and local mean particle velocity arrows coloured by number density of particles. The left image represents a case with weak momentum coupling between the phases and the image to the right represents a case with stronger momentum coupling.

bell. The droplets are forced towards the target using a combination of shaping air from the applicator and an electrostatic field between applicator and target.

Apart from the particles being influenced by E-field and air flow, the air flow is influenced by the paint particle motion as well as shaping air and the rotating bell, and the E-field is slightly influenced by the charged particles in the domain. The problem is thus coupled in many ways as well as inherently transient, since the applicator is moving throughout the domain. This puts high demands on the solution algorithm in order to achieve feasible computation times for a realistic problem.

In the beginning of 2008, FCC is putting the final touches on a software demonstrator for virtual ESRB painting coupled to the FCC path planning software.



Figure 3. Side view of a spray of simulated paint leaving an ESRB. The arrows represent droplet local mean velocity and they are coloured by the local number density of droplets.



Figure 4. Sequence of images from a simulation of painting a standard test plate with an ESRB paint applicator. The colouring of the plate represent thickness of paint, and the lines are field lines of the Efield.

Optimization



In the last decades the engineering sciences have seen a massive break-through of computer assisted methods. This enables virtual testing of products and processes prior to expensive physical testing and validation which, in turn, opens the door for applying modern optimization techniques in the design process. Mathematical optimization methods, tailored for specific application areas and customer demands on precision and robustness, provide efficient search strategies, which improve this process. In many applications trade-offs between different criteria such as costs and quality indicators are necessary. At the department of Computational Engineering and Design the activities are focused on

• Optimization of products and processes with respect to multiple criteria

We perform research on robust multi-objective optimization algorithms which are applied to the optimal design of engineering systems in application areas such as electromagnetics, fluid dynamics and solid mechanics. To facilitate an automated design process, decision support systems that integrate multiple criteria optimization and simulation are developed.

• Maintenance planning

In many industries the costs for spare parts are very high and also the maintenance activity itself may generate high costs in terms of, e.g., lost production. Maintenance planning often combines statistics and optimization techniques. The optimization and fatigue groups at FCC and Chalmers mathematics study efficient methods for the maintenance of aircraft engines in a joint research project.

Workshop

On December 3-4 2007, FCC and GMMC organized the workshop "Robust multiobjective design optimization with simulation" at Chalmers Science Park, Göteborg. The workshop gathered fifty researchers and developers from different fields within academia and industry, primarily from the Nordic countries, to discuss the state-of-the-art and future challenges in solving these problems.

The topics of the presentations ranged over computational processes for aircraft optimization, interactive decision support for in industrial processes, topology optimization in flow problems, and microwave tomographic imaging, among others.

Linnean Class V plant: Hoya subquintuplinervis MIQ, Hoya or wax plant, the family Asclepiadáceae – milkweed plants. There are approximately 70 species of the genus Hoya from China to Polynesia. The genus was named after Thomas Hoy (c. 1750-1829). He was the gardener of the Duke of Northumberland at Syon House. Syon House is located by the Thames River just opposite Kew Gardens. (Stockholm University, Greenhouse, department of Botany, 2005)

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Decision support based on simulation and multi-criteria optimization

This three year project was part of a base program with the industrial consortium STM. The goal was to develop a prototype tool that integrates multiple criteria optimization and simulation and that visualizes solutions in an interactive decision support tool. Several case studies have been investigated and a first version of the prototype optimization tool, consisting of a number of modules for mathematical modeling, simulation computations, optimization algorithms, and visualization, has been developed. The optimization algorithms can be adapted to one or multiple objectives and to various mathematical properties of the design models. Different simulation environments can be used and the results can be visualized in the optimization objective space as well as in the space of the simulation model.

Combustion engine optimization

It is nowadays possible to simulate the physical and chemical processes inside combustion engines by appropriate software and high performance computers. These simulations can predict, for example, fuel consumption and emissions of soot and nitrogen oxides. By varying the design parameters of the engine, different configurations of these can be simulated and their performances compared. We use global and local optimization algorithms in combination with simulations to find Pareto optimal design parameters with respect to several goal functions.

To construct a combustion engine is a complicated and multi-objected task since it is for example desirable to have low fuel consumption, high effect as well as low emissions of NOx and soot. The engineers can greatly benefit from having access to the best possible software tools during this process. A tool for multi-objective optimization of combustion engines is useful to gain insight into the complicated relationship between the physical entities involved in the



engine design and design-dependent entities such as NOx, soot and fuel consumption. Ultimately it can be used to improve the engine design.

In the project, which was performed in co-operation with GMMC, Volvo Car Corporation and Volvo Powertrain, we developed new optimization routines and best practice for combustion engine optimization based on computational fluid dynamics.

Product configuration with respect to multiple criteria

The industry is increasingly characterized by specialization and customization; specifications and equipment must be tailored to suit each particular service task. The main focus is on optimizing product features to give each customer the best product with respect to effectiveness, safety, quality and environmental impact – all with the intention of minimizing product lifetime costs. Therefore many products are available in an enormous number of variants in order to fulfill these demands on features and diffe-

A front axle installation of a truck. Different combinations of frames, axle beams, leaf springs, steering arms, etc lead, to a large number of possible configurations. The simulation shows the temperature variation during the compression-combustion-expansion process in a diesel engine. Spray and droplet formation can also be seen during the multiple fuel injections.

rent missions, operating environments, and product utilizations. Beside these demands the product must fulfill internal company demands that secure an efficient development and manufacturing process.

In co-operation with Volvo 3P the PhD student Peter Lindroth is developing a framework for finding optimal sets of truck configurations. The problem of deciding "what is a good product configuration" (i.e., design solution) for a certain purpose has multiple criteria, and the goal for the production and sales is typically formulated as the maximization of safety, transport efficiency, quality, diving performance, and environmental friendliness. The specific goal of the project is to define a framework for the product configuration problem and to apply this framework to a reference case based on a selected segment of truck configurations. The framework combines internal demands and demands given by the customers. It also comprises the main features of multi-criteria decision support.



Reliability and Risk Management

Understanding the impact of uncertainty and quantifying and managing risk to secure and optimize reliable operations, products, and systems are important issues for most industry and societal sectors.

The department develops mathematical models of products and processes, emphasizing a sound balance between model complexity, uncertainty, and optimality, providing key competences in mathematical statistics, stochastic processes, and combinatorial optimization.

Our focus is on two areas briefly described below and later illustrated by some examples of industrial projects.

Fatigue Life and Load Analysis

Many failures of engineering structures are caused by the fatigue of metals. Numerical solvers of partial differential equations can calculate mechanical stresses and strains into great detail. However, the knowledge of the actual loads on the structure in service is usually very vague. In addition, fatigue damage must be predicted for the whole specified service life of the structure. Lacking detailed information about material imperfections and geometry, the engineer is forced to use simple empirical models for the fatigue damage evaluation, and compensate by large safety factors, which unfortunately often are based on experience and not rationalized in a robust way. Statistical methods are needed for a rational development of sound safety factors based on both measurements and on historical experience.

Finance and Insurance

In Sweden and EU there are a number of initiatives, e.g., Basel II and Solvency II, to define common rules for banks, insurance companies and pension management agencies, aiming at strengthening the security of the clients with respect to risk. In the financial industry more and more complex derivatives and instruments appear. Trade means need to hedge for currency risks and fluctuating commodity prices, including electricity prices on deregulated markets. Rational operations call for asset-liability management tools based on sound risk measures.

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Linnean Class XIX plant: Cirsium vulgare (SAVI) TEN., bullthistle, the family Asteráceae-composite plants. Cirsium is comprised of 250 species from the northern temperate zones and temperate America. The Greek word kirsion and the Latin word cirsion both refer to a kind of thistle. Vulgáre means common. (Lisslö Farm, Norrtälje, 2005)

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Co-operation

We collaborate closely with Chalmers Mathematical Sciences, Fraunhofer ITWM, and SP Technical Research Institute of Sweden.

Acknowledgement

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Fatigue Life

Fatigue from a Statistical Point of View

The strategy of the fatigue group is to develop new methods for fatigue assessment in industrial practise. Statistical methods can help to build a complete picture of the reliability of mechanical constructions with respect to fatigue resistance, and hence show where it is most efficient to take steps to improve the quality of a product. Within this overall perspective, the FCC fatigue group in particular focuses on the following areas:

• Modelling of fatigue life. We develop and make use of statistical methods for fatigue life prediction for spectrum loads, as well as methods for estimation of the fatigue limit, especially in connection to defects.

• Analysis of service loads. We use the theory of stochastic processes, rainflow count analysis, and work on questions concerning on-board logging, acceleration of fatigue tests, and the relation between laboratory tests and service loads.

• *Reliability and robust design.* The load and the strength variables may be combined in a statistical reliability approach, where the design targets can be evaluated.

Scientific projects

Since 2006 the group has participated in one part of the Gothenburg Mathematical Modelling Centre (GMMC). The work aims at merging different reliability tools into a common framework, useful for industrial practice, which will be published as a Wiley book.

In February 2007 Magnus Karlsson defended his PhD thesis, which was carried out at Volvo Trucks and Chalmers in close connection to FCC. The project was dedicated to the problem of load analysis of truck customers.

Industrial projects

Two projects have dominated our work during 2007, namely the three-year project to write a Guide to Load Analysis for the six European truck manufacturers, and a project for SKF regarding analysis of the fatigue strength of bearing steel. Other industrial projects have been evaluation of fatigue tests for Astra Tech, statistical support for measurement uncertainty evaluation at SCA, and statistical review of methods for Stora Enso.

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Linnean Class IX plant: Perséa americána MILL., avocado, the family Lauráceae – laurel plants. The genus Perséa is comprised of 200 species which were originally tropical. The avocado tree is 15 to 20 meters high with evergreen leaves which resemble laurel leaves. The flowers are small and grow in clusters. The tree produces thousands of flowers where roughly one flower in 5,000 will produce fruit. In 1753 Linnaeus gave the avocado the name Laurus perséa, but in 1768 Phillip Miller (1691-1771) placed the avocado in the genus Perséa and named it Perséa americána. Both the Greek Persea and the Latin Persea arbour mean tree from Persia. The avocado comes from the Aztec word ahuacacuauhitl, wich means testicle tree. The Spaniards shortened it to aguacate and the English to avocado. The avocado was considered to be an aphrodisiac which made it popular among the Indians and the Spanish colonizers. (El Jardín de Aclimatación de La Orotava (The Orotava Botanical Garden), Puerto de la Cruz, Tenerife, 2005)

Guide to Load Analysis for Automotive Applications

The goal of this three-year project that started in 2007 is to develop a Guide to Load Analysis, especially oriented towards truck applications. The guide will provide a toolbox of useful methods within different areas of load analysis. The project is run by FCC, with Dr Pär Johannesson as the project leader, in collaboration with Mathematical Sciences at Chalmers, SP Technical Research Institute of Sweden, and Fraunhofer ITWM. The project is financed by the six European truck manufacturers, namely Daimler, DAF, Iveco, MAN, Scania, and Volvo.

Background

In fatigue design of mechanical components and systems there are two main variables, namely, the load the component is exposed to, and the strength of the component. The ultimate goal for the manufacturer is to make a design that exactly meets the needs of the customers, neither too strong nor too weak. The requirements need to be converted into for example a certain small risk of failure, a proper safety factor, or an economical expected life. In order to make a robust design it is as important to have good knowledge about the properties of the customer loads, as it is to have good knowledge about the mechanical behaviour of the material and structure in question. The development of information technology and its integration into vehicles has given new possibilities for in service measurements. Further, the design process is also changing where the development is moved into the computer. Both these tasks require a refined view on load analysis and lead to a renewed interest in load analysis.

During the year of 2006 an initial oneyear project was carried out, with the aim to prepare the ground for a Guide to Load Analysis. The project included an investigation of the current practice and future needs within load analysis, together with a survey on the state-of-the-art in load analysis for automotive application.

Development of the Guide

The task of the project is to write a Guide to Load Analysis for Automotive Applications, following the structure:

Part I. Introduction Part II. Methods for load analysis

- Cycle counting methods.
- Frequency based methods.
- Methods for multi-input loads.
- Load editing and generation of time signals.
- Models for random loads.
- Response of mechanical systems.
- Load variation and reliability.

Part III. Load analysis in view of the vehicle design process

- Evaluation of customer loads.
- Derivation of design load specifications.
- Validation of systems and components.

The Guide will give an overview of existing methods in the area of load analysis, where the most important methods will be described in detail. Further, several seminars will be given at each company with the aim to introduce the Guide. The focus of the Guide should be to give understanding to pre-competitive mathematical and statistical tools in load analysis. The purpose, use, and benefits of such a guide to load analysis are manifold: (1) It should include basic methods, such as rainflow cycle counting, in order for it to be a guide for new engineers in the area, (2) It should also include advanced methods that may not be in regular use yet, but could be potentially useful for the engineering practice, (3) It should explain which methods to use for which applications, pointing out their relevance, merits and disadvantages, (4) It should result in new engineering methods that are based on existing mathematical and statistical methods, (5) It should serve as a common knowledge base that would make it easier for industrial collaborations, e.g. between truck manufacturers and suppliers.



Front row: Pär Johannesson (FCC), Manfred Streicher (MAN), Bengt Johannesson (Volvo), Sascha Feth (ITWM), Michael Speckert (ITWM), Martin Olofsson (Volvo), Sara Lorén (FCC). Back row: Magnus Karlsson (Volvo), Thomas Svensson (FCC), Igor Rychlik (Chalmers), Anders Forsén (Scania), Roland Müller (Daimler), Nina Kirchner (ITWM), Bas Perdok (DAF), Christof Weber (Daimler), Jacques de Maré (Chalmers), Gustav Willén (MAN), Peter Nijman (DAF).

Fatigue Limit and Inclusions

Many fatigue properties of materials are governed by the defect contents in the material, either at the surface, or in the interior. Especially for hard steels the fatigue limit is coupled to the size distribution and the intensity of non-metallic inclusions. The idea of the weakest link model gives the conclusion that the most detrimental defect will decide the actual fatigue limit for a component or specimen. However, the most detrimental defect is not necessarily the largest one since a large defect may be exposed to a small local stress and a small defect to a large local stress.

The distribution of the maximum inclusion size in a material may be estimated in three different ways, namely

- 1) by Extreme Value Analysis (EVA), where the maximum inclusion size in different control areas are measured,
- 2) by fatigue tests, where the detrimental inclusion is experimentally found, and
- 3) by ultrasonic testing, where inclusions in a scanned volume may be observed, and their sizes measured.

The final application of interest is the maximum inclusion size in a large volume representing the stressed volume in a component. This volume may be a thousand times or larger than the tested volume in the EVA case. When using ultrasonic testing larger volumes may be scanned, resulting in a smaller degree of extrapolation. For fatigue tests the stressed volume of the specimen may be in the same order as for a component.

There are statistical problems both in estimating the defect distribution from measurements, and in the translation from the defect distribution to the fatigue limit of a component. During the last year we have worked on investigating the relation between defect content and the fatigue limit for components with non-homogeneous stress distributions. Especially, for the inverse problem, treating point 2 above, we have developed methods for estimating the defect size distribution from fatigue tests with non-homogeneous stress states, e.g. rotating bending tests, and uniaxial test procedure of notched specimens, see figure 1.

This area of problems has been studied in different projects for SKF during the recent years. We have also invested in internal projects and established a close co-operation with SP within the relation between defect contents and fatigue limit, especially in connection to finite element calculations.

An application

From a fatigue test using a uniaxial test procedure with an hourglass specimen, the inclusion size distribution is estimated under the assumption that it follows an extreme value distribution. Further, the Murakami

relation between the fatigue limit and the maximum inclusion size is used. From the estimated parameters in the extreme value distribution it is possible to calculate the distribution of the most detrimental inclusion for other stress conditions and component shapes, see figure 2. The interest is often the inclusion sizes in a large volume as mentioned above. From the estimated parameters it is possible to see how the maximum inclusion size increases with increasing volume under the same stress condition, see figure 3. From the Murakami relation between the fatigue limit and the maximum inclusion size it is possible to calculate the fatigue limit distribution from the inclusion size distribution for the corresponding stress conditions and component shapes, see figure 3.



Figure 1. The test procedure is uniaxial with a notched specimen, giving a non-homogenous stress distribution. This illustrates that the largest defect need not be the most detrimental one, since the local stress may be small in this example blue.





Figure 2. Probability density functions for the maximum inclusion size in a volume under different stress conditions and component shapes.

Figure 3. Fatigue limit distribution estimated from a uniaxial test with an hourglass specimen, the red line. The blue line uses the estimated defect distribution from the uniaxial test, but transformed to the fatigue limit for a rotating bending stress distribution. The green lines are the fatigue limit under homogenous stress condition and two different volumes.

Courses for practising engineers

An important part of the fatigue group activities is to give courses for industry. Several different courses have been developed during the years.

- Statistics for loads, fatigue, and reliability. This course is given as four half-days, where each half-day is based on an industrial problem given by the industry. The course has now been given several times, in 2007 at Volvo Trucks, following the lecture notes "Problemdriven Statistikkurs - Belastning, utmattning och tillförlitlighet" by Pär Johannesson and Jacques de Maré.
- Course in spectrum fatigue. This three days course has been given three times in co-operation with the SP Technical Research Institute of Sweden in Borås. The course is based on the idea that fatigue design should be performed on loads resembling the service situations. In most applications the amplitude of the loads varies with time, and the component is exposed to a spectrum of different amplitudes. The topic is often referred to as spectrum fatigue. The course covers 1) planning and execution of load measurements; 2) load analysis and editing; 3) fatigue tests for spectrum loads; 4) statistical evaluation of spectrum tests and construction of design curves.
- *Measurement uncertainty.* This three days course has been given at Volvo Trucks, and is based on the lecture notes "Nio tumregler och två kungsvägar för att behärska mätosäkerhet" by Thomas Svensson.

Supervising PhD students

Below we describe two PhD projects where the students passed their examination in 2007.

Modelling of truck loads

The automotive industry problem of customer correlation is represented in our work by the PhD project for Volvo Trucks, where Magnus Karlsson was supervised by Thomas Svensson, Jacques de Maré and Pär Johannesson. The project was dedicated to the problem of load analysis of truck customers and includes modelling of vehicle cornering, fatigue assessment of components sensitive to lateral loads, random process modelling and statistical design of field data measurements. Magnus defended his PhD thesis "Load Analysis for Fatigue Assessment of Vehicles - a Statistical Approach" on February 23, 2007, and the content is described by Magnus.

"As the demands on transport efficiency increases, the vehicle industry is, to a greater extent than before, tailor-making vehicles to customers. This means that the design task is also becoming more important as over-dimensioning may lead to less loading capacity and worse fuel economy, and under-dimensioning may lead to component failures, which in turn can cause loss of performance. Getting proper knowledge about the strength of components, and the loads they are subjected to, is therefore essential.

Also, the loads vary due to several sources of variation: The operating environment differs from one truck to another. The vehicle utilisation, i.e. how the vehicle is driven, causes variation. For trucks also the transport mission will have an impact, as e.g. the gross combination weight will be different. Moreover, the specific features of the vehicle will affect the loads that a component is subjected to since the external loads are transferred dynamically in the vehicle.

An important trend in the vehicle industry is to move fatigue considerations into earlier stages of the design process. In these stages, the vehicle only exists as a computer model. It is then necessary to have a model for the external loads coming into the vehicle.

In my PhD thesis at the department of mathematical statistics at Chalmers University of Technology I developed a parametric model to describe the lateral loads that the vehicle is subjected to. By studying how the parameters in the model vary depending on the driver, the market and the road type, it is possible to get a deeper understanding for the loads and how important the different sources of variation are."

Maintenance of jet engines

In a joint project for Volvo Aero two PhD students have worked on optimization of maintenance schemes for aero engines. One part of the project is devoted to statistical aspects on optimal maintenance, and the PhD student Johan Svensson was supervised by Dragi Anevski at Chalmers together with Jacques de Maré and Thomas Svensson. Johan defended his PhD thesis "Survival Estimation for Opportunistic Maintenance" on June 1, 2007.

Magnus Karlsson after the conferment of the doctors' degree



Finance and Insurance

Finance and insurance offer a wide range of mathematical challenges. Finance, especially the options and futures markets, needs to model interest rates, stocks, bonds, real estate – to name but a few – in order to derive fair prices for its wide selection of products. Insurance faces issues such as estimation of mortality and risk, fair pricing of insurance contracts, pension plans and so on.

One of the aims of the ongoing Solvency II initiative is to move towards a more realistic valuation of assets and liabilities. In many cases, existing systems are based on conservative assumptions about interest rates, population dynamics etc, which in turn generate implicit safety margins meant to guarantee solvency levels. The realistic valuation approach, it is hoped, will be more transparent and ensure greater robustness against adverse economic scenarios, thus in the long run strengthening the insurance industry as a whole.

For banks, a similar regulatory system is already in place in the form of Basel II. Solvency II is built along the same lines, reflecting the increasing overlap between the two industries.

Both sets of regulations are divided into three pillars. Under pillar one, the regulators encourage the development of company specific risk models. One possible way of attacking this problem is through the development of ALM/DFA models, which may be used in stress or scenario testing, but also as part of the development process for new products.

FCC and our associates, having a strong understanding of the underlying mathematics complemented by practical modelling experience, offer expertise for financial and insurance institutes in Sweden and across Europe. Together with our partners Chalmers and Fraunhofer ITWM we have developed theory and software for Asset Liability Management, robust portfolio optimization, and credit derivative pricing.

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Linnean Class III plant: Hórdeum sp., barley, the family Poáceae – grasses. Hórdeum L is a genus with about 20-40 species, at least three of which were cultivated in Europe as early as the Stone Age. Among the kinds most commonly cultivated today are barley with two or six rows of grain. Barley is the hardiest of the cereal grains and can be cultivated up to the 70th latitude and at elevations as high as 4800 meters above sea level. Barley does not contain gluten and does not rise very well and is therefore used as fodder and in the production of malt, among other things. The word hórdeum is Latin and means barley. (Puerto de la Cruz, Tenerife, 2005)

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SimIns - an ALM/DFA platform

FCC, in co-operation with the Swedish Insurance Federation through the industrial consortium STM, has developed a stateof-the-art modelling platform for Asset Liability Management (ALM)/Dynamic Financial Analysis (DFA). The platform aims at simplifying the modelling construction process and providing a basis for company specific risk models. Another important goal is to further the interest of actuarial mathematics and econometric modeling in general.

The aim of ALM-studies is in fact manyfold. It is of interest to analyze the current market conditions and see how changes, so called stress-tests, will impact existing long-term strategies. Further, combining the simulations with an optimization algorithm may lead to important insights regarding changes in investment policies and new benchmark portfolios. It is also possible to evaluate how new and proposed rules and regulations may influence one specific company or, on a macroscopic level, the economy of an entire industrial sector.



Traditionally, companies, pension-funds and other investors do not perform these simulations themselves, but rely on the results of external consultants. A consequence of this is that the simulation model, from the customer's point of view, is perceived as a black box. Further, these external models are usually not able to cater to the specific needs by the different companies. The SimIns platform, complete with optimization and portfolio strategy plug-ins and a set of example models, has been distributed amongst the Federation members.



Robust portfolio optimization

The fundamental question of portfolio optimization is quite natural: How do we trade in the stock market in the best possible way? However, this is not easy to answer. It is widely known that when classical optimal portfolio strategies are applied with parameters estimated from data, the associated portfolio weights become remarkably unstable and volatile. The predominant explanation for this is the difficulty to estimate expected returns with sufficient accuracy.

Recently, a new approach has been developed at Chalmers which gives stable and robust estimates of expected returns. These expected returns are particularly well suited for use in portfolio optimization.



We parameterize an n stock Black-Scholes model as an n factor Arbitrage Pricing Theory model where each factor has the same expected return. Hence the non-unique volatility matrix determines both the covariance matrix and the expected returns. This approach gives stable and robust estimates of expected returns. The investor can impose his or her views on the market, either for individual stocks or for groups of assets, by selecting a volatility matrix which suggests expected returns of the stocks that he or she believes are reasonable.

The example below shows the outcome for a portfolio of three stocks. The optimal strategy is applied out-of-sample, and the model parameters are estimated from a window of 18 months of data, which is updated each month.

FCC has completed a project with The Second Swedish National Pension Fund, AP2, and Chalmers to develop the new methodology for robust portfolio optimization described above. The results are very promising for circumventing the well-known stability problems associated with many of the standard mean-variance portfolio strategies.



Price development for three individual stocks and wealth process based on ranks for Markowitz´ optimal strategy (thick green line; unstable) and the robust strategy (thick blue line).

Seminars

The ALM/ DFA modeling platform SimIns and the Excel platform RoPox for Robust Portfolio Optimization were presented at seminars in Stockholm in May and November 2007.

Geometry and Motion Planning

Many products such as car and truck bodies, engines, medical prosthesis, mobile phones, and lumbering equipment depend visually and functionally on its geometry. Since variation is inherent in all production, consistent efforts in styling, design, verification and production aiming at less geometrical variation in assembled products is necessary to achieve easy-to-build highquality products. Also, the demand on short ramp up time and throughput in the manufacturing industry increases the need of effectively generate and visualize collision-free and optimized motions in the assembly plant. During 2006 the department of Geometry and Motion Planning have successfully developed methods, algorithms and tools supporting these activities within three main subjects

- Geometry Assurance
- Path planning and Robotics
- Surface Inspection

In particular, the FCC software tool Industrial Path Solutions for automatic path planning of collision-free motions has been successfully used by our partners in the automotive industry to solve geometrically complex manufacturing problems in mere minutes instead of hours or days. The strength of the mathematical algorithms in combination with the easy user interface has allowed the path planning technology to be spread outside the expert teams of simulation engineers. The IPS path planning technology is now also part of the master education in virtual production at Chalmers.

An industrial and scientific challenge of car body manufacturing is to guarantee geometrical quality and factory throughput during spot welding. To solve this problem FCC has started to develop algorithms integrating line balancing, sequencing and coordination of operations with our path planning technology, see Virtual Geometry, Path Planning and Station Logic.

Today, many assembly problems are detected too late in the product and production realization, involve cables, hoses and wiring harness. The reason for this is the lack of virtual manufacturing tools supporting real time simulation of flexible parts and motions. The FCC technology developed together with ITWM has been successfully implemented as a IPS Cable Solver module, see Simulation and Path Planning of Flexible Parts.

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Linnean Class I plant: Canna índica L, Indian shot, the family Cannáceae-canna plants. There are some 8-10 species of this, the only genus of the family Cannáceae originating in the tropical or subtropical Americas. The Greek kanna or Latin canna means tube, rush, reed. The word can be traced far back in time to languages spoken in the areas around the Tigris and the Euphrates. The original meaning of índica was "from India". Canna edúlis – arrowroot or achira as it is called in South America, is known for its root stalks rich in starch and is used among other things for making a flour similar to the one made from arrowroot (Maránta arundinácea L). Moreover, Canna edúlis is now considered to be the same species as Canna índica. (Stockholm University, Greenhouse, Department of Botany, 2004)

Co-operation

During 2007, the successful collaboration with Winqquist Laboratory at Chalmers has been further strengthen by the collaboration within Wingquist Vinn Excellence Centre. Also the collaboration with the Industrial Research and Development Corporation (IVF), and the ITWM departments Dynamics and Durability and Image Processing, has grown by working together on common projects.

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Geometry Assurance

Geometry-related quality problems are often discovered during the assembly process when parts are about to be assembled and do not fit as expected. Often the reason is geometrically sensitive product and production concepts that have not been verified enough due to lack of powerful analysis tools. A design or production change at this stage is very costly and does almost always result in delays in market introductions with lost revenue as a consequence. Therefore, FCC in corporation with the Wingquist Laboratory at Chalmers and the

Swedish Institute of Production Engineering (IVF) operates to support a systematic reduction of variability in processes and products in the following key areas:

- Robust design and variation simulation
- Inspection planning preparation
 and optimization
- Statistical process control and root cause analysis

Linnean Class XXI plant: Euphórbia dendroides L., tree spurge, Euphorbiáceae - spurge plants. Euphórbia is the largest plant genus with approximately 2,000 species in the entire world. The name exists in both Greek and Roman literature as the Latin euphorbia and the Greek euphorbion. The species epithet dendroides means tree-like. (El Jardín de Aclimatación de La Orotave (The Orotava Botanic Garden), Puerto de la Cruz, Teneriffa 2005)

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Robust Design & Variation Simulation

The key idea behind Robust Design is to make the product as insensitive to variation or disturbance as possible, to make it withstand potential uncertainties in the manufacturing process or changes in the operating environment. We use statistical Monte Carlo simulation, sensitivity analysis and contribution analysis from our partner RD&T Technology to make the product insensitive to manufacturing and assembly tool variation. This reduces the need for costly physical prototypes and test series, see figure 1.

Inspection Planning and Analysis

Inspection planning refers to the activity to gather information about variation in individual parts, processes, assemblies and assembly equipment, in order to control the manufacturing process and to be able to give feed-back to a number of activities in the geometry assurance process. Today inspection planning is almost always solely based on experience and can be improved significantly by using mathematical and statistical analysis. We develop methods and support tools for intelligent inspection preparation. The motive is to gather as much information about the product and the process as possible with minimum number of inspection points, see figure 2.

Statistical Process Control and Root Cause Analysis

Today routine measurements in the industry are often made on-line during the production process. Statistical process control (SPC) is a set of quality tools aimed at reducing variability utilizing these measurements. For manufacturing processes of simple parts, patterns on a control chart may provide enough diagnostic information to an experienced operator to pin point the root cause. However, experience shows that many SPC attempts fail to produce meaningful results



Figure 1. Colour Coding, based on sensitivity analysis, of the Volvo S80 Car Body. Areas sensitive to dimensional variation are indicated with red colour (courtesy of Volvo Car Corporation).







Figure 3. A multi-fixture assembly where a number of parts are assembled. From left to right: Assembly, production data, multivariate statistical process control, root cause analysis, assembly fixture fault, simulated effect of correction (courtesy of Saab Automobile).

because the lack of diagnostic support for the effort. Therefore, we develop statistical methods to make root cause analyses on the product to find and correct problems in the manufacturing and assembly process. The motive is fast identification and correction of problems and increased knowledge about product/process correlation, see figure 3.

Path Planning

Automatic Path Planning for Rigid Bodies and Industrial Robots

Despite that modern industries use virtual prototypes to replace physical prototypes, visualize assembly processes and program industrial robots off-line, the full potential of the virtual factory is not reached. Programming of motions and paths for robots and equipment is still done manually, since the existing support for automatic path planning is very limited. Another limitation is the geometrical accuracy between the virtual model and the physical reality. Therefore, geometrical tolerances need to be considered during path planning. This is a first step, going from nominal to production adapted virtual models and hence connecting the production loop including styling, design and manufacturability.

Virtual verification of that products can be assembled and later on disassembled for service purposes is an important part of geometry simulation in the manufacturing industry. Methods and software for automatically generating collision free assembly paths are therefore of great interest. Also, off-line programming of robots and coordinate measurement machines used in the factory lead to hard problems for the simulation engineer when trying to manually find collision free paths between points, with that of minimizing cycle time and joint wear. Therefore, FCC operates to support the following path planning applications:

- Assembly visualization / verification/design
- Assembling with robot
- Welding and sealing
- Coordinate measurement
 machine
- Load balancing, sequencing and coordination of robot operations

Linnean Class XIV plant: Clerodéndrum ugandense PRAIN, butterfly bush or Ugandan clerodendrum, the family Lamiáceae – labiate plants. This Clerodéndrum species originates, as the species epithet indicates, from Uganda. Clerodéndrum has long been included in the family Verbenáceae-verbena plants, however it is now included in the family Lamiáceae. (Stockholm University, Greenhouse, Department of Botany, 2005)

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Assembly Visualization/ Verification/Design

This project with our partner Volvo Car Corporation has resulted in simulation software for automatic path planning, viewed in figure 1. The software is based on a virtual 3D model describing the kinematics and the geometry in the assembly cell, interacting with a collision tester.

For small sub-assemblies as well as final assemblies, simulations give valuable support when evaluating new concepts and comparing alternative solutions. Also different assembly sequences can be compared and verified. As a result, product functionality and manufacturability can be improved.



Figure 1. Is it possible to assembly the tunnel bracket? The FCC path planner finds a solution in less than 2 minutes. Even an experienced simulation engineer will struggle for days with this assembly verification (courtesy of Volvo Car Corporation).

Assembling with Robot

In addition to collision avoidance and kinematic constraints, automatic robot programming involves minimization of cycle time, robot wear and joint forces. Efficient path planning and reachability analysis is also beneficial when comparing station layouts choosing robots and designing tools, grippers, and fixtures, see figure 2.



Figure 2. In this station, the driving unit is assembled into the car body. Due to the narrow door opening, the clearance is very small and programming without support from a path planner is difficult. This demo application developed by FCC finds a solution in 3 minutes (courtesy of Volvo Car Corporation).

Path Planning and Sealing of Car Body Seams

This project with our partner Volvo Car Corporation has resulted in simulation software for automatic path planning of Robotized sealing applications. In the sealing station, robots spray the sticky sealing mass along, for instance, spot welded seams. By covering the seams, dirt and water cannot come into the chinks and cause corrosion. The sealing also has a sound insulating effect. In the first step, the algorithm finds several different collision-free motions applying the sealing mass along each seam. In the second step, collision-free motions are generated in such way that an optimal sequence connecting one solution for each seam is obtained, see figure 3.



Figure 3. Automatic path planning and optimisation of a sealing station (courtesy of Volvo Car Corporation).

Coordination/Interlocking of Multi-Robot Manufacturing Cells

In many manufacturing operations, e.g. spot welding of car bodies, several robots needs to share the same workspace. To coordinate and avoid collisions the robots are synchronized by defining interlocking points along the robot paths. At an interlocking point it is checked whether the program can continue without the risk of collision or not. If the risk of collision is present the program halts until this is no longer the case. Programming of interlocking points is today done on-line, as current simulation software lacks support for automatic generation and validation. This project with our partner Volvo Car Corporation has resulted in interactive software providing methods and algorithms for minimizing interlocking related time-loss through an efficient use of interference zones, see figure 4.



Figure 4. Where and when shall the robots wait for each other in order to avoid collisions and minimize cycle time (courtesy of Volvo Car Corporation)?

Virtual Geometry, Path Planning and Station Logic

The goal of this project is to create a cost-effective and quality-assured assembly process for complex products. Today, geometry assurance, robot path planning and line balancing are carried out partly manually and isolated with limited transparency. Therefore, this project integrates variation simulation, path-planning, sequencing and line balancing with station logic to generate an integrated and cost-effective manufacturing process where product quality and cycle time can be evaluated and optimized for



Figure 5. New virtual methods and tools for geometry assurance, path planning and station logic allow for a more efficient production and preparation (courtesy of Volvo Car Corporation). different product and production systems. A PhD student within Volvo Cars industrial PhD program is specially working with integration and interfaces between the three areas. The projects will in particular show how welding point locations and sequence affects auto-body quality and cycle time.

This project is part of the Vinnova MERA program and is a collaboration project between Volvo Cars Corporation, AB Volvo, Saab Automobile AB, Scania AB, Semcon AB, Caran AB, Fraunhofer-Chalmers Centre, Wingquist Laboratory at Chalmers, see figure 5.

Fast and Memory Efficient Sweep Volume of Moving Parts

The swept volume is the space generated when a part is moved along a path. Such volumes have many applications in virtual prototyping, e.g. booking the volumes needed for different parts during an assembly operation or to find interference zones for multi-robot coordination. The sweep volume can be very complex since both the part geometry and motion can be complex. Due to this complexity the computing time and the memory needed for generating and representing the volumes has been too large to be used in practice. In this project, FCC has developed and implemented a solution that meets the high demands of manufacturing engineering when it comes to computing time and complexity of geometry models, see figure 6.



Figure 6. An assembly path and corresponding swept volume (courtesy of Volvo Car Corporation).
Non-Nominal Path Planning

One important aspect in the assembly process design is to assure that there exists a collision-free assembly path for each part. To manually verify assembly feasibility in a digital mock-up tool can be hard and time consuming. Therefore, the recent development of efficient and effective automatic path planning algorithm and tools are highly motivated. However, in real production, all equipment, parts and subassemblies are inflicted by geometrical variation, often resulting in conflicts and on-line adjustments of off-line generated assembly paths. Therefore, we have developed a new algorithm and working procedure enabling and supporting a more cost effective non-nominal path planning process for assembly operations. The basic idea is to combine state-of-the-art technology within robust design and variation simulation with automatic path planning. By integrating variation and tolerance simulation results into the path planning algorithm we can allow the assembly path going closer to areas of low variation, while avoiding areas of high variation, see figure 7.

Simulation and Path Planning of Flexible Parts

The project goal is a more efficient and quality assured production preparation of flexible parts. Examples of flexible parts in automotive industry are air pipes, fuel pipes, electrical wires, and tubes on production equipment like robots, see figure 8 - 10.

The project has generated a software demonstrator in which cables and wires of various material parameters can be simulated in real time. Forces and moments can be analyzed, cable length can be optimised, clips can be attached, and motions can be evaluated. The project results include (i) Simulation results have proven to be accurate, (ii) The software is already used in car projects, (iii) GM has decided to support the technology developed in this project as a global standard for simulation of flexible cables, and (iv) Approximately 40 engineers at Saab/GM and Volvo Cars are trained in the software demonstrator developed in the project.

The project is part of the Vinnova MERA program and is a collaboration project between Saab Automobile AB, Volvo Cars Corporation, and Fraunhofer-Chalmers Centre.



Figure 8. Examples of Compliant/flexible parts (courtesy of Saab GME).



Figure 9. Optimization of length, clip positions and effect of over length of the Radio Assembly cables (courtesy of Saab GME).



Figure 7.A driving unit assembly path taking results from variation simulation of the car body into account. Areas of high geometrical variation are avoided (courtesy of Volvo Car Corporation).



Figure 10. Force analysis of engine hose (courtesy of Saab GME).

Surface Inspection

Esthetic design has become an important factor in many branches of the production industry. The interaction between the geometrical shape and the surface quality of a product has a substantial impact on the impression conveyed by a product. Despite ever improving production processes and quality enhancing measures, all industrial production is subject to errors and defects. Since the quality requirements from the customers' part are constantly increasing, improved quality control in general is of vital importance, and in particular surface quality control.

Up to recently, the quality control of produced objects' surfaces has been done by human inspection. Even though the quality controllers usually are very experienced, variations in the inspection results occur, both between individuals, but also due to mood, fatigue etc.

An alternative is to set up an automatic surface inspection utilizing a camera system and image processing algorithms (see figure 1 and 2) to automatically detect and rate defects. A number of high-resolution cameras covering the entire object to be inspected continuously acquire images which are sent to an equal number of processing units, where modern image processing algorithms are evaluating the image data. Candidate defects are generated by some fast algorithms looking for irregularities, and these candidates are subject to a more detailed analysis verifying the existence of a defect and categorizing its type.

An automatic system has many advantages, including

• Objectivity. The inspection result for a certain object will always be the same, which is not the case for manual inspection.

• Speed. Automatic systems are usually faster than humans to find and classify defects. Furthermore, while humans have a limit, the speed of an automatic system may be improved by increasing the hardware capacity.

• On-line. An automatic system can usually be installed directly in the production line, without interrupting the production. Manual inspection must usually take place off-line, which in reality means that only a few selected samples may be inspected.

• Statistics. An automatic system supports systematic gathering of detailed statistical data over the occurrences of various defects.

Linnean Class XII plant: Lampránthus spectábilis N.E.B.R., trailing ice plant, the family Aizoáceaefig-marigold plants. The genus Lampránthus comes from South Africa and contains 180 species. The Greek lampros meaning shining or glowing, and anthos, meaning flowering, form the genus name. Spectábilis means well worth seeing and comes from spectare which is Latin and means to look at, to contemplate. (Stockholm University, Greenhouse, Department of Botany, 2004)

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Figure 1. Schematic description of an automatic visual inspection system.



Figure 2. An automatic inspection system for fabrics.

Inspection and grading of leather hides

Currently, FCC and ITWM are jointly involved in a project for developing an automatic inspection and grading system for a major Swedish leather hide manufacturer.

The task of the system is to sort hides after the tanning process into a number of quality classes, depending on the number of defects and their location on the hide. The quality class controls the degree of further processing (painting) which determines the value of the hide. If the quality is overestimated, defects may be visible after finished processing, leading to further processing and additional costs. Underestimating the quality leads to excessive painting and loss of product value. An automatic system reducing the errors and variation in the early grading may thus be very cost-efficient.

The problem of automatically classifying a hide according to quality may be divided into two steps:

• Automatic detection of all relevant defects such as scratches, insect bites, warts, and shingles eczemas, while avoiding spurious detections caused by natural irregularities of the hide (e.g. veins). Examples of defects and natural structures are shown in figure 3.

• The result of the detection algorithm is a list of defects describing their type, intensity/severity, and position on the hide. All of this is taken into account by a grading algorithm to select a quality class.

During 2007, a prototype system has been installed and is being evaluated at the main production line at Elmo.



Figure 3. Schematic image of various defect types.

Systems Biology and Bioimaging

The application of tools and techniques, borrowed from engineering disciplines such as systems and control theory, signal processing, and computer science, for studying biological and biochemical systems has received an increasing attention over the last couple of years. This is due to a number of factors such as recent advancements in measurement technology, a need for pharmaceutical companies to find alternative strategies to beat current shortcomings in early drug development and increase competitiveness, and the improved understanding of living systems due to the sequencing of genomes and characterization of the function and role of corresponding proteins. FCC provides an integrated approach to the study of biochemical and physiological processes, from the characterization of single parts to the analysis of dynamic phenomena on a systems level. The work at the department includes both biological/biomedical modeling applications as well as development of computational tools and algorithms. The department is organized in two areas:

- Systems Biology
- Bioimaging

We are currently involved in modeling projects where yeast (*Saccharomyces cerevisiae*) and oocytes (*Xenopus laevis*) are used as model organisms. Modeling of ion-channels and action potential propagation are other areas of interest, which have been studied both in the continuation of a project with AstraZeneca R&D in Mölndal, where fibrillation in atrial tissue is addressed, and in a project together with a group at the Division of General Zoology at Kaiserslautern University addressing mechanisms involved in the interplay between neuron and glial cells in the brain.

The computational tools and algorithms developed at the department can be divided in four main areas: System identification – to build mathematical models of dynamic systems based on measured data; Model reduction – to reduce the size and scope of models to arrive at models whose parameters can be estimated and validated using available measurement data; Image analysis – to automatically extract un-biased information from images using various tools from mathematics and statistics; and Software tools – to support the model building process and computational analysis of the obtained models.

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Linnean Class XVIII plant: Hyperícum perforátum L., Common St. John's wort, the family Clusiáceaethe St. John's wort plants. Perforátum means perforated or punctured, which refers to the leaf of the Common St. John's wort. The leaf appears to be full of holes when it is examined against the light. According to an old legend Hyperícum was supposed to ward off evil spirits, and the devil pierced the leaves with needle holes in revenge. (Lisslö Farm, Norrtälje 2005)

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Co-operation

We have a very close collaboration with the Swedish company InNetics. Other collaborations include joint work with General Zoology at Kaiserslautern University, Bionanophotonics at Chalmers, Cell- and Molecular Biology at Gothenburg University, and partners in the BIOSIM and YSBN projects.

Acknowledgement

The department has received substantial funding from the Swedish Foundation for Strategic Research both directly and via Gothenburg Mathematical Modeling Centre, GMMC. Furthermore, the group has received funding for the BioSim and YSBN projects from the European Commission.

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Systems Biology

Combining model based signal processing, system identification, mechanistic models, and sensitivity analysis with novel measurement platforms provides a strong competitive edge for researchers in the pharmaceutical and biotech industry. Systems biology partly addresses these things and is an emerging scientific field that aims at elucidating the properties and function of biochemical and biological systems on a systems level, e.g., how biomolecules interact and implement various functions which cannot be understood by studying the system components in isolation.

The activities in systems biology at FCC are focused around the application and development of computational methods and mathematical models of biological systems on different levels of abstraction utilizing time resolved measurement data. The research is carried out in close co-operation with both academic and industrial partners. The in-house competences are in the area of control and dynamic systems and the group has several years of experience of both software development and application of methods from systems and control theory to projects in both the engineering and pharmaceutical industry.

Our vision is to develop means to enable researchers to delineate and understand the underlying mechanisms of a disease or phenomenon at the mechanistic level, i.e., in terms of biochemical reaction or interaction networks. We focus on mechanistic models to map out and better understand a specific biological phenomenon or pathological condition.

The systems biology group at FCC also has very close collaboration with the Swedish company InNetics, the developers of the systems biology software PathwayLab.

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Linnean Class VI plant: Túlipa linifólia REGEL, narrow-leaftulip, the family Liliáceae-lily plants. There are som 100 species of Túlipa L. originating in temperate Eurasia to Central Asia. Ogier Ghiselin de Busbecq, the envoy to the Vatican at the court of Suleiman the Magnificentin Constantinople, introduced the genus in Europe in 1554 and gave it the name Tulipe, which was later Latinized by Linnaeus. He wrote in Flora Svecica that the wild tulip, Túlipa sylvéstris, starts to open its flowers at 10 o'clock while the garden tulip opens its flowers at slightly before 8 o'clock, and Linnaeus also stated there that the bulbs can be cooked in oil and pepper to make a tasty and healthy dish. (Stockholm University, Greenhouse, Department of Botany, 2005)

Modeling the Ras/cAMP/PKA Signaling Pathway - Stress Response in Yeast

In the budding yeast S. cerevisiae, the Ras/ cAMP/PKA signal transduction pathway regulates many cellular and physiological processes, such as growth, resting state and sporulation, carbohydrate and nitrogen metabolism, stress tolerance, and cell wall resistance to lyticase digestion, making the pathway central to cell life. An interesting down-stream target of the RAS/cAMP/PKA pathway are the transcription factors Msn2p and Msn4p, which during low cAMP levels enters the nucleus and activates specific gene promoter targets. The localisation of Msn2/ 4p, which can be time-resolved visually, thus becomes good reporters for the activity in the pathway. Based on different types of negative feedback regulations, the RAS/cAMP/PKA pathway has been attributed a possible role as an oscillator, responsible for the observed periodic nucleocytoplasmic shuttling of the transcription factors Msn2/4p. By inhibiting the phosphodiesterases involved in the degradation of cAMP, caffeine has the potential of modulating the characteristics of such oscillations.

This project brings together a unique mix of competences (applied physics, cell and molecular biology, mathematical statistics, image analysis and systems biology) in an area that is central to contemporary biotechnology. The partners are Prof Mikael Käll (Chalmers) and Prof Anders Blomberg (Gothenburg University). The aim is to integrate quantitative microscopy data into systems biology models that provide a deeper understanding of the processes directly involved in, but also linked to, the pathway, such as feedback loops and the modulation of oscillatory behavior. Dynamic models are being built from quantitative in vivo data in order to encapsulate obtained knowledge about causal relationships between the involved molecular species on the mechanistic level, see figure 1. Nonlinear differential equations describing the interactions between components have been formulated



Figure 1.A model diagram for the Ras/CAMP/PKA signaling pathway implemented in Pathway-Lab (top). Simulations of a model for the RAS/cAMP/PKA pathway. Sustained oscillations of the two RAS forms GDP and GTP (bottom left) and a phase plane plot of damped oscillations in RASGDP and cAMP (bottom right).

and methods from system identification will be used to utilize the available data to estimate unknown parameters and to validate different hypothesis.

Modeling Components of the Neuron-Glial Interplay

Neurons in the human brain are embedded in a web of glial cells. Contrary to earlier beliefs, glial cells are not passive bystanders to the information processing and metabolism in the brain, but respond to neuronal signaling. To understand the principles of neural activity, and diseases such as epilepsy, the study of glial cells could therefore be very important. One glial transporter, that is believed to play a pivotal role in the metabolite shuttling between glial cells and neurons, is the monocarboxylate transporter MCT1, symporting protons and monocarboxylates, such as lactate, across the cell membrane. It has been shown that the transport rate of MCT1 can be enhanced by carbonic anhydrase isoform II (CAII).



Figure 2. Kinetic model of MCT1 transport. The proton is the first substrate to bind to the transporter in this mirror-symmetric scheme.

The focus of this project has been to determine the mechanism of MCT1 transport, and how it interacts with CAII, based on a combination of electrophysiological techniques and mathematical modeling. Using ordinary differential equations (ODEs), the transport process of MCT1 is modeled as a number of interconnected states, shown in figure 2, representing a network of discrete protein-substrate configurations. From this system of ODEs, an explicit rate expression for the substrate flux has been derived by employing model reduction techniques. Simulations of the model have been compared with experimental data obtained from MCT1-expressing oocytes injected with different amounts of CAII. Results from inhibition-experiments have lead to the determination of the binding order scheme and the rate limiting step. The model also suggests that CAII increases the effective rate constants of the proton reactions, possibly by working as a proton antenna.

The project has been carried out in close co-operation with Fraunhofer-ITWM and Professor Dr Joachim Deitmer and Dr Holger Becker at the Division of General Zoology at Kaiserslautern University.

Nonlinear Mixed Effects Modeling Tools

In this project we have considered how the statistical modeling framework of nonlinear mixed effects (NLME) modeling, a.k.a. nonlinear hierarchical modeling, is used with parameter estimation methods. This framework is commonly used by the pharmaceutical industry in the analysis of pharmacokinetic and pharmacodynamic (PK/PD) models. In NLME modeling a number of individuals with different properties, in a population, are characterized.

NLME models in PK/PD analysis typically take the form of state-space models, based on ordinary differential equations (ODEs) for the state evolution and with discrete-time observations. ODEs cannot be used to take correlations in the measurement data into account, which is an often occurring phenomenon in biological data. A better choice is then to use stochastic differential equations, SDEs, which are more flexible.

The goal is primarily to estimate the parameters that describe the properties of the population, but not of each individual, given a set of measurement data. In PK/PD analysis there is typically only a few data points available for each individual, which makes the model uncertainties important in the analysis. There are three sources of randomness in NLME models with SDEs; systems noise, measurement noise, and the interindividual variation.

A maximum likelihood framework is used to estimate the population parameters. There is no general closed form expression of the population likelihood function, which must be approximated. The parameter values that best fit the measurement data are obtained by optimization of the population likelihood function. A mathematical filter, e.g. the extended Kalman filter, is used to minimize the impact of noisy data in the function evaluation.

The theory has been implemented on the Matlab platform on the form of a prototype toolbox, NLMEtools. The toolbox is based on SBtoolbox, which has previously been developed at FCC. To speed up some of the most time consuming functions, Matlab communicates with the programming language C through Matlab MEX-files. NLMEtools also provides a graphical user interface on top of the command line driven toolbox functions, shown in Figure 3. The main functions of NLMEtools are model specification, simulation, parameter estimation and visualization of the likelihood function.









Figure 3. The graphical user interface for NLMEtools.

In Silico Simulation of Fibrillation in Canine Atrial Tissue

Atrial fibrillation is the most common form of heart arrhythmia and is associated with a 5-6 fold increase in the incidence of stroke. Computer models describing the temporal evolution of the action potential over realistic atrial geometries are very useful to understand or predict the effect of drugs acting as inhibitors on single or multiple ion-channels. In particular, these models make it possible to relate the dynamics of the action potential propagation to drug effects on the single cell level. This in turn permits in silico reconstruction and investigation of phenomena like atrial flutter and fibrillation.

In this work we have developed a framework for modeling and simulation of electro-chemical activity in large scale cell networks. The framework allows incorporation of different geometrical models and cell models in a plug-in fashion, as well as methods for definition of myocyte fiber orientation and distribution of myocyte subtype, see figure 6. On the single cell level the myocytes are described by a set of coupled non-linear ordinary differential equations. On the tissue level the cells are connected according to monodomain assumptions, forming a network represented by a connectivity matrix defined by the geometrical model. This constitutes the basis for the full atrial tissue model, which is illustrated in figure 4. In order to ensure good scalability with respect to model complexity, i.e., the total number of differential equations to be solved, the framework has been implemented in a multi-processor environment.

Within the simulation framework, a geometric model of the canine atria has been constructed utilizing ultra sound imaging data. A realistic fiber structure and cell type distribution has also been incorporated in the model, based on extensive literature studies and consultation with clinical experts. The modeling workflow is depicted in figure 5.

The simulation framework has been used to induce fibrillation and flutter like electro-dynamic activity in cell networks and the effect of ion-channel modulation on this behavior has subsequently been investigated. Qualitatively the results are in good accordance with in vivo observations, which indicates that the approach is viable for this application and motivates further extensions and studies. The type of simulations presented in this work has great potential to provide insights into the underlying mechanisms of atrial fibrillation and flutter, as well as a basis for prediction of drug effects.



Figure 4. Modeling work flow: ultra sound image, z-stack of ultra sound images, traced curves, 3D geometry, and simulation model.



Figure 5. Outline of the developed modeling and simulation framework: network model, cell model, and connectivity model (membrane potential equations).



Figure 6. Sample distribution of different cell types on the surfaces of the atria (left). Muscle fibre orientation (right). The valves, ventricles, and connecting blood vessels are not part of the current model.

Parameter Estimation

In this project we have considered system identification of biological and biochemical systems described by differential equations. Since measurement data often is sampled at discrete points in time we are faced with a mixed continuous-discrete parameter estimation problem. A common way of addressing this problem is to add Gaussian measurement noise to the measured variables and perform a maximum likelihood estimation of the unknown parameters. However, the underlying assumption that there is no uncertainty in the proposed differential equations for the system under study is often not that realistic. A formal way of introducing a measure of this uncertainty is to consider stochastic differential equations (SDEs), which also incorporates noise terms or disturbances to account for unknown or non mechanistically modeled effects. We have studied and implemented methods for system identification for a model class described by a system of stochastic differential equations and measurements taken at discrete time instants.

The methods have been based on a prediction error minimization framework, which means that the performance of a model is being judged based on its predictive power. We have used both directly parameterized Kalman filters (DKF) and extended Kalman filters (KF) to compute the predicted output of the model. The prediction error is then formed and its size is measured in some norm, which becomes a function of the parameters to be determined as well as the available data. Parameter estimates are then computed by minimizing this measure and we have utilized gradient based methods which require the predictor structures to be differentiated. Equations for the differentiated version of the EKF equations have been derived, which has to be solved simultaneously with the original EKF equations to obtain the value of the objective function and its gradient in each step of the optimization algorithm. The method has been implemented in Mathematica, which makes it possible to both automate the process of setting up the EKF and differentiated EKF equations for a given problem as well as applying robust state-of-the art implementations of various gradient based optimization algorithms. The method has been validated on some small test examples which show promising results.

Model Reduction

Model reduction of biological and biochemical models, i.e., to reduce the complexity of large mechanistically based models to more simplified ones, is an important part of the modeling process. It becomes particularly

important when the complexity of a model does not match the amount of available data. By applying model reduction techniques a smaller model with fewer parameters and state variables, but which still captures the main features of the system to be modeled, can be derived. In this work we have extended a method for model reduction of linear reaction systems based on state aggregation (or lumping) previously developed at FCC to nonlinear reaction systems. The method is applied to both small artificial examples to illustrate its properties, as well as a large real system which is a 102 state EGF-activated MAP kinase cascade model. The developed method reduced this 102 state model with a factor of two to a model with only 48 states, which still accurately performs the same signal transduction as the original model.

Another result in this area is a novel reduction method that reduces complex rational rate expressions, such as those often used to describe enzymatic reactions. The method is a term-based identifiability analysis and one of the first methods to meet the classical engineering objective of improved parameter identifiability without losing the systems biology demand of preserved biochemical interpretation.

$$\mathbf{V}_{\max} \frac{\mathbf{A}}{\mathbf{1} + \frac{\mathbf{A}}{K_{\mathrm{A}}} + \frac{\mathbf{B}}{K_{\mathrm{B}}} + \mathbf{K} \mathbf{A} \mathbf{B}} \approx \widehat{\mathbf{V}}_{\max} \frac{\mathbf{A}}{\widehat{\mathbf{K}} + \mathbf{B}}$$

Whole Body Modeling

The development of mathematical models that can describe the overall metabolism of a human will be a milestone for biosimulation. Such models are likely to add completely new dimensions to the understanding of the dynamics of the metabolic and integrated physiological function of the human body. A framework for realistic mathematical models of whole-body metabolism has been developed at the Department of Biomedical Sciences at the University of Copenhagen, partly within the BioSim project. Such whole-body models consist of ordinary differential equations describing the kinetics of the metabolism in organs and the interaction of organs via the blood compartment. This way, the models describe the physiology of the whole body in vivo as it relates to metabolism. The approach is modular, where the modules typically are the anatomically defined individual organs of the body. In order to obtain a realistic description, the models describing the individual organs are detailed biochemical models constrained by the available experimental data on the mass balance across the organ. The data defining these constraints are stationary state fluxes and concentrations at specific, welldefined physiological states. The involved mathematical framework provides means to define whole-body models of various complexities. FCC has taken part in this project by contributing to the XML specification for organ models and whole body structure representations. Furthermore, we have implemented a part of the simulation environment for whole body models in Matlab.

Thiamine Regulation in Yeast

Thiamine metabolism in yeast is a complex dynamic system involving different processes such as thiamine uptake, utilization, biosynthesis, and gene regulation, see figure 7. This metabolic network is interesting from several points of view; it represents a model for microbial nutrient sensing and regulatory system with well defined and characterized components, it consists of a relatively small number of proteins with rather specific functions restricted to this system, and it contains genes which are under the most stringent transcriptional control known. These features make this network an attractive system to be studied using a systematic modelling approach. In fact, in the ongoing project together with the Hohmann laboratory at Gothenburg University it turned out that the modelling of thiamine uptake lead to significant new biological insights into the system.



Figure 7. Thiamine regulation - detailed view (upper). Thiamine metabolism processes (lower).

Bioimaging

Quantitative bioimaging has in the last couple of years aroused substantial interest for life science applications. In eukaryotic cells, quantitative measurements of protein expression, protein localization and protein-protein interactions are key components for a proper understanding of cell functionality. Fluorescence microscopy and the use of fluorescent protein tags, which facilitates specific labeling of proteins, is an exceptionally powerful technique for these kinds of quantitative measurements. For example, it enables visualization of localization processes, levels of expression, protein kinetics, and protein-protein interactions in real time and in vivo. at the level of individual cells. It also enables studies of protein expression variations over generations and population studies. However, since human interpretation of images is qualitative and subjective, software for objective automatic image analysis are necessary for the standardized measurements usually required in proteomics, in particular in high-throughput studies. Quantitative bioimaging and corresponding algorithms for image analysis is also an excellent setup for generating high quality data needed in systems biology modeling projects.

At FCC we develop image analysis methods for automated quantitative analysis of images. The applications are for example automated tracking of cells or particles in time-lapse sequences of images and high-throughput screening of protein expressions in large populations. We also conduct research to understand diffusion mechanisms of solutes in polymer-based hydrogels. Here inference of the statistical properties of 3D gel microstructures are extracted via image analysis of 2D transmission electron images. Then the diffusive behavior of thousands of molecules in reconstructed versions of the 3D gels is analyzed and compared with experimental results.

Our goal is to provide mathematical and statistical tools to application fields that produce images where quantitative measurements can, or could be, conducted. The first step typically involves image analysis methods but in order to reach true quantitative understanding of the studied phenomenon, assorted methods from statistical learning and/or simulation studies are usually required. Our present collaborating partners come from various academic institutions, research institutes, and industry.

Contact

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Linnean Class XXIV plant: Cyrtómium falcatum (L.F.) PR., Japanese holly fern, Dryopteridáceae wood fern plants. There are about 15 species in the genus Cyrtómium from North America, Asia and Africa. The genus name is derived from the Greek kyrtoma which means bend and the species epithet falcatum refers to the sickle-like shape. (Stockholm University, Greenhouse, Department of Botany, 2005)

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Quantitative Cell Studies

We collaborate with the Center for Biophysical Imaging at Chalmers, for developing algorithms and computer software for quantitative in vivo imaging. For the image analysis algorithms used, the emphasis lies on robust methodologies which enables long time-lapse studies of protein localization, migration, and inheritance over several cell cycles, as well as high through-put screening of protein functionality of a large number of gene-disrupted cells. During the last couple of years FCC has developed a software demonstrator CellStat equipped with graphical user-interface (GUI) for automated recognition and tracking of yeast cells from transmission microscope images, combined with quantification and localization of GFP-tagged proteins using fluorescence microscopy. A screen-shot of the main window of the software can be seen in the right-most panel of figure 1.

Gel Structure Modeling

Understanding the diffusion mechanisms of solutes in polymer-based hydrogels is important for the development of many industrial applications. In the pharmaceutical industry for instance the future most likely involves more sophisticated delivery systems. In order to decrease the time it takes for new drugs to reach the market it is from a drug delivery point of view very important to understand the intrinsic coupling between the physical properties of the solute/drug and the structure of the surrounding matrix in which the solute/drug is incorporated. Fundamental understanding of diffusion



Figure I. Bright-field image (left) and the corresponding fluorescence image (middle) of a GFP-tagged fluorescent protein in a population of yeast cells. The main window (right) of the software developed at FCC for quantitative cell analysis. Here, cells which contain high local concentrations of the fluorescence protein are colored red.

mechanisms in polymer gels is important also in other applications such as hygiene materials. Here the swelling rate depends to a large extent on the flow and diffusion rates of small solutes into a polymer based material.

A method for identifying the three-dimensional gel microstructure from statistical information in transmission electron micrographs has been developed by FCC in cooperation with SIK (the Swedish Institute for Food and Biotechnology), the Department of Mathematical Statistics and Department of Chemical and Biological Engineering at Chalmers. The micrographs, see the left part of figure 2, are projections of stained strands in gel slices. The gel strand network is modelled as a random graph with nodes and edges, and parameters in the model are estimated by a Markov chain Monte Carlo method. A three-dimensional network is then simulated from the model and the right part of figure 2 shows a 3D rendering from such a simulation.



Figure 2. Left: part of a TEM micrograph from a stained Sepharose gel. Right: screen shot from a 3D rendering of the simulated gel network.

Adaptive simulation of particle diffusion in complex geometries and structures

In connection with the gel structure modeling project, we also run a project on simulation of diffusing particles and molecules in complex 3-D geometries such as gel networks estimated from the TEM images. For this we have developed an adaptive time-stepping solver for stochastic differential equations (SDE). The surrounding geometry acts as obstructing medium for the diffusing molecule and the solver can take care of more general kinds of particlestructure interactions using interaction potentials, as well as reflection and adsorption. Here, it is of interest to be able to predict the diffusive behavior (e.g. mobility, stability) of the molecule-structure pair, where either one, or both, is designed for a specific purpose. The estimated diffusion coefficients are validated by comparing with diffusion coefficients measured via an experimental method called NMR diffusometry.

The adaptive time-stepping method for SDE is also of interest when solving SDEs in general. In the future we will adapt and use this method in other projects within FCC where appropriate and needed. An example of such a project is the Nonlinear Mixed Effects Modeling Tools project.

Årsredovisning

för tiden 1 januari 2007 - 31 december 2007

Resultaträkning (kSEK)	070101- 071231
Intäkter Nettoomsättning	27 241
Övriga intäkter Summa intäkter	9 27 250
Kostnader Externa kostnader Personalkostnader Avskrivningar av materiella	-8 779 -18 143
anläggningstillgångar Summa kostnader	-417 -27 339
Rörelseresultat	-89
Resultat från finansiella investeringar Ränteintäkter och liknande	247
Räntekostnader och liknande	e -34
Resultat efter finansiella poster	124
Bokslutsdispositioner Årets skatt	-56 -46
ÅRETS RESULTAT	22
Balansräkning (kSEK)	071231
Anläggningstillgångar Maskiner och inventarier Summa anläggningstillgångar	939 • 939
Omsättningstillgångar Kundfordringar Förutbetalda kostnader och upplupna intäkter Övriga kortfristiga fordringar	5 954 I 203 75
Kassa och bank Summa omsättningstillgånga	4 98 r 12 213
SUMMA TILLGÅNGAR	13 152
Eget kapital Eget kapital vid årets ingång Årets resultat Summa eget kapital	2 605 22 2 627
Obeskattade reserver	819
Kortfristiga skulder Leverantörsskulder Övriga kortfristiga skulder Upplupna kostnader och	728 933
förutbetalda intäkter Summa kortfristiga skulder	7 045 9 706
SUMMA SKULDER OCH EGET KAPITAL	13 152

Styrelsen för Stiftelsen Fraunhofer-Chalmers centrum för industrimatematik, FCC, får härmed avge följande redovisning över verksamheten under tiden 1 januari 2007 – 31 december 2007, stiftelsens sjätte verksamhetsår.

Stiftelsen bildades av Chalmers och Fraunhofersällskapet i juni 2001 och registrerades av Länsstyrelsen i Västra Götalands län i oktober 2001 som en svensk näringsdrivande stiftelse. Stiftelsen skall enligt strategiplan från oktober 2005 bygga upp en verksamhet som år 2010 omsätter tre och en halv miljon euro och omfattar 35 anställda. Chalmers och Fraunhofersällskapet kommer att under denna period att stegvis öka sin finansiering från 400 000 euro 2006 till 500 000 euro 2010.

Årets omsättning har varit drygt tjugosju miljoner kronor. Medeltalet anställda har ökat från tjugosex personer (varav fem kvinnor) 2006 till tjugosju personer (varav fem kvinnor) 2007. Stiftelsen har tecknat ett femårigt hyresavtal till och med 31 mars 2011 omfattande 1 096 kvm i Chalmers Teknikpark med Fastighets KB Forskarbyn.



Styrelse och ledning den 2 april 2008. Sittande från vänster till höger Dieter Prätzel-Wolters (Fraunhofer ITWM), Peter Jagers (ordförande, Chalmers). Stående från vänster till höger Uno Nävert (föreståndare, FCC), Bo Johansson (Chalmers), Johan Carlson (biträdande föreståndare, FCC). Saknas på bilden Helmut Neunzert (vice ordförande, Fraunhofer ITWM).

FÖRVALTNINGSBERÄTTELSE

Stiftelsen Fraunhofer-Chalmers centrum för industrimatematik skall utveckla och anpassa matematiska metoder för industrin. Stiftelsen bedriver konkurrensneutral forskning och marknadsföring med finansiering från grundarna och genomför projekt definierade av företag och offentliga finansiärer på kommersiell grund.

Rörelsens intäkter har uppgått till 27 250 kSEK. Av detta utgör 50% industriprojekt, 21% offentliga projekt och 29% finansiering från grundarna. Årets resultat efter skatt är 22 kSEK. Eget kapital uppgick den 31 december 2007 till 2 627 kSEK.

Stiftelsens styrelse har under verksamhetsåret sammanträtt två gånger. Ersättning har utgått till ordföranden med 7 050 kronor per möte och till övriga ledamöter med 4 700 kronor per möte man deltagit i.

Stiftelsens ställning och resultatet av dess verksamhet framgår av efterföljande resultat- och balansräkningar, vilka utgör en integrerad del av årsredovisningen.

Göteborg den 2 april 2008

Peter Jagers, ordförande Helmut Neunzert, vice ordförande Bo Johansson Dieter Prätzel-Wolters

Räkenskaperna har granskats av Deloitte.

Result (kEUR)	070101- 071231
Income Net sales	3 027
Others Total income	ا 3 028
Cost External cost	-976
Staff	-2016 -46
Depreciations Total cost	-3 038
Result of business	-10
Result of financial investment Interest and similar income Interest and similar cost	ts 27 -4
Result including financial investments	13
Appropriations Tax	-6 -5
TOTAL RESULT	2
Balance (kEUR)	071231
Fixed assets Machinery and equipment Sum of fixed assets	104 104
Current assets Accounts receivables	662
Prepaid expenses and accrued income	134
Other current receivables Cash and bank	8 553
Sum of current assets	357
TOTAL ASSETS	46
Equity capital and debts Equity capital at	
beginning of year Result	290 2
Total equity capital	292
Untaxed reserves	91
Short-time debts Debts to suppliers	192
Other debts Accrued expense	103 783
Sum of short-time debts	I 078
SUM OF DEBTS AND EQUITY CAPITAL	46

Appendix

Presentations / Conferences

J Almquist, H Becker, C Salzig, H Schmidt: Modeling the Interplay between Neurons and Glial Cells, 2nd Workshop on Mathematical Aspects of Systems Biology Göteborg, March 21-24, 2007.

F Edelvik:

Finita Elementmetoder för elektromagnetiska vågproblem, Chalmers Kontaktdag Högskolaindustri, May 2007.

F Edelvik:

A stable hybrid FDTD-FEM solver for antenna applications, Workshop on antenna simulations for industrial applications, Kaiserslautern, September 2007.

F Edelvik:

Time domain finite element modeling of thin sheets and coatings using shell elements, EMB 07, Lund, October 2007.

F Edelvik:

Multiobjective optimization applied to antenna design, Workshop on Robust multiobjective design optimization with simulation, Göteborg, December 2007.

S Jakobsson:

Multiobjective optimization applied to antenna design, Workshop on antenna simulations for industrial applications, Kaiserslautern, September 2007.

S Jakobsson:

Time domain finite element modeling of thin sheets and coatings using shell elements, EMB 07, Lund, October 2007.

M Jirstrand:

Introduction to Computational Systems Biology. Invited lecture at Mälardalens högskola, April 2007.

M Jirstrand:

Introduction to Computational Systems Biology and Tutorial on PathwayLab. Invited lecturer for The 2nd International Course in Yeast Systems Biology, Gothenburg, June 2007.

M Jirstrand:

Systems Biology at the Fraunhofer-Chalmers Centre. Invited talk at the annual Yeast Retreat workshop at Rörbäckstrand, August 2007.

M Jirstrand:

Parameter Estimation in Biochemical Reaction Networks – Observer Based Prediction Error Minimization, 8th International Conference on Systems Biology, Long Beach, USA, October 2007.

M Jirstrand:

Parameter Estimation in Biochemical Systems Using Prediction Error Minimization, Invited lecture at RICAM Workshop on Systems Biology, Johann Radon Institute for Computational and Applied Mathematics (RICAM), Linz, November 5-9, 2007.

M Jirstrand:

Modelling and Analysis of Biochemical Systems - Systems Theory and Computational Tools, co-lecturer in the course Mathematical Modelling and Computational Tools, Int. Master's Program for Bioinformatics and Systems Biology, Chalmers University of Technology, Gothenburg, Sweden, November 2007.

P Johannesson:

Variation Mode and Effect Analysis: A Case Study of an Air Engine Component. Invited lecture at Mathematical Statistics, Lund University with Lund Institute of Technology, May 2007.

P Johannesson:

Statistical analysis of constant and different variable amplitude spectra. Presented at Fatigue 2007, Cambridge, UK, March 26-28, 2007.

P Johannesson:

Probabilistic Variation Mode and Effect Analysis, A Case Study of an Air Engine Component. Presented at the 10th international QMOD conference (Quality Management and Organisational Development) in Helsingborg, Sweden, June 18-20, 2007.

K Logg, M Kvarnström,

A Diez, K Bodvard, and M Käll: Automatic image analysis of in-vivo protein localization in fluorescence microscopy: a quantitative study of GFP-tagged proteins in budding yeast. SPIE Photonics West Bios. January 2007.

M Kvarnström:

Image Analysis for Quantitative Microscopy, Workshop on Phenomics-Advancing high-resolution genome-wide phenotyping in yeast. Göteborg, March 2-4, 2007.

M Kvarnström:

Identification of 3-d gel structures from transmission electron micrographs. Uncovering Hidden Pattern, Symposium for Mats Rudemo. Göteborg, June 8, 2007.

P Lindroth (M Patriksson and

A-B Strömberg, coauthors): Approximating the Pareto optimal set using a reduced set of objective functions, presentation at the 22nd European Conference on Operational Research, Prague, July 8-11, 2007.

S Lorén:

Skattning av utmattningsgränsens fördelning under inhomogena spänningsvillkor. UTMIS nätverksmöte, Braås, January 30-31, 2007.

S Lorén:

Skattning av inklusionsfördelning med och utan direkta inklusionsmätningar. Presented at Stål 2007, Borlänge,May 9-10, 2007.

M Patriksson:

On the applicability of bilevel optimization models in transportation science – A study of the existence and robustness of solutions to SMPEC models, at the symposium Networks: Modelling and Control organised by the Royal Society, London, September 24-25, 2007.

M Patriksson, A-B Strömberg and F Edelvik: Organizers of the workshop Robust multi-objective design optimization with simulation in co-operation with GMMC , Chalmers Science Park, Göteborg, December 3-4, 2007.

M Patriksson:

On the existence and computation of robust solutions in hierarchical optimization, at the Workshop on Robust Multiobjective Design Optimization with Simulation, FCC, December 3-4, 2007.

M Saif-UI-Hasnain:

Combustion engine optimization: A multiobjective approach, Workshop on Robust multiobjective design optimization with simulation, Göteborg, December, 2007.

H Schmidt:

Systems Biology at FCC - From Theory to Application. Seminar at the Hamilton Institute, National University of Ireland, Maynooth, Ireland, 2007.

H Schmidt:

Complexity Reduction of Biochemical Reaction Networks, Talk at the opening workshop of the FUNCDYN networking programme, Haslev Udvidede, Denmark, 2007.

H Schmidt:

Complexity Reduction of Biochemical Reaction Networks, Invited talk at the 2nd Workshop on Mathematical Aspects of Systems Biology, Gothenburg, Sweden, 2007.

A-B Strömberg:

Logistikoptimering för kostnadseffektivt underhåll, presentation (in Swedish) at a seminar organized by NFFP, Volvo Aero, Trollhättan, February 7, 2007.

A-B Strömberg: Participated in NFFP:s program seminar, Volvo Aero, Trollhättan, March 21, 2007.

A-B Strömberg:

Optimering av opportunistiskt underhåll, presentation (in Swedish) at the conference STÅL 2007 in Borlänge, May 9-10, 2007.

M Sunnåker, G Cedersund, and H Schmidt: A New Method for Model Reduction Based on Time Scale Separation and Lumping, 2nd Workshop on Mathematical Aspects of Systems Biology Göteborg, March 21-24, 2007. M Sunnåker and M Jirstrand: A Nonlinear Mixed Effects Modeling Toolbox for Matlab, 3rd BioSim conference, Potsdam, October 2007.

M Sunnåker and M Jirstrand:

A Nonlinear Mixed Effects Modeling Toolbox for Matlab. EUFEPS Conference on Optimising Drug Discovery and Development, Basel, Switzerland, December 2007.

M Wallman, H Schmidt,

M Jirstrand, and I Jacobson: Simulation of Electrical Activity in Canine Atrial Tissue, 2nd Workshop on Mathematical Aspects of Systems Biology Göteborg, March 21-24, 2007.

M Wallman, M Jirstrand,

L Gan, and I Jacobson:

In Silico Simulation of Fibrillation in Canine Atrial Tissue EUFEPS Conference on Optimising Drug Discovery and Development, Basel, Switzerland, December 2007.

Publications

K Wärmefjord, J S Carlson, R Söderberg: 10th CIRP Conference on Computer Aided Tolerancing, Specification and Verification for Assemblies, March 21-23, Erlangen, Germany, 2007.

M Anguelova, G Cedersund, M Johansson, C-J Franzen and B Wennberg: Conservation laws and unidentifiability of rate expressions in biochemical models, IET Systems Biology, 2007, I, (4), pp. 230–237.

G Cedersund, P Strålfors and M Jirstrand: Core-box modeling for biosimulation of drug action, In Eds. Bertau et al. Biosimulation in Drug Development. Wiley-VCH, Weinheim, 2007.

F Edelvik, E. Abenius:

Time domain finite element modeling of thin sheets and coatings using shell elements, In EMB07, Lund, Sweden, pp. 35-41, October 2007.

F Edelvik:

Virtuelle Blitzeinschläge - Blitze Abblitzen Lassen, Innovisions - Das Zukunftsmagazin des Fraunhofer-IuK-Verbunds, pp. 68-70, no 4, 2007.

S Jakobsson, F Edelvik, B Andersson: Multiobjective optimization in computational electromagnetics, In EMB07, Gothenburg, Sweden, pp. 99-104, October 2007.

S Jakobsson:

Evaluation of Integral equation formulations of Maxwell equations for dielectric bodies, In EMB07, Lund Sweden, pp 233-237.

M Benson, L-O Cardell, S Hohmann, M Jirstrand, M Langston, R Mobini, O Nerman: Systems Biology May Radically Change Healthcare – Individually Based Prediction, Prevention, and Treatment, Läkartidningen, 104(42): 3037-3041, 2007.

P Johannesson, B Johannesson, T Svensson and M Karlsson: Statistical analysis of constant and different variable amplitude spectra. Proceedings of Fatigue 2007, Cambridge, UK, March 26-28, 2007.

P Johannesson, T Svensson and L Samuelsson: Probabilistic Variation Mode and Effect Analysis: A Case of an Air Engine Component. 10th QMOD Conference (Quality Management and Organizational Development), Helsingborg, Sweden, June 18-20, 2007.

P Johannesson, T Svensson,

L Samuelsson, B Bergman, J de Maré: Variation Mode and Effect Analysis: an application to fatigue life prediction (submitted for publication).

M Kvarnström, C Glasbey: Estimating Centers and Radial Intensity Profiles of Spherical Nano-Particles in Digital Microscopy. Biometrical Journal (49), 300-311, 2007. R Nisslert, M Kvarnström, N Lorén, M Nydén and M Rudemo: Identification of the Three-Dimensional Gel Microstructure from Transmission Electron Micrographs. Journal of Microscopy (225), 10-21, 2007.

M Kvarnström, K Logg, A Diez, K Bodvard, and M Käll: Image analysis algorithms for cell contour recognition in budding yeast, submitted.

M Kvarnström, A Westergård, N Lorén, and M Nydén: An adaptive time stepping algorithm for Brownian dynamics simulations, submitted.

M Kvarnström, A Westergård, N Lorén, and M Nydén: Brownian dynamics simulations in hydrogels using an adaptive time stepping algorithm, submitted.

B Bergman, J de Maré, T Svensson (eds): Robust Design Methodology for Reliability, A collection of essays. The different approaches for reliability assessment represented by the groups in the project have been discussed to be merged into a common framework. The result of this discussion will be a number of essays collected in a book. The book proposal has been accepted by Wiley.

T Almgren, N Andréasson, D Anevski, M Patriksson, A-B Strömberg, and J Svensson: Optimization of opportunistic replacement activities: A case study in the aircraft industry. Submitted to European Journal of Operational Research.

M Josefsson and M Patriksson: Sensitivity analysis of separable traffic equilibria, with application to bilevel optimization in network design, Transportation Research, B, vol 41 (2007), pp. 4-31.

M Patriksson:

A survey on the continuous nonlinear resource allocation problem, European Journal of Operational Research, vol. 185 (2008), pp. 1-46 (to appear). T Larsson, J Marklund,

C Olsson, and M Patriksson:

Convergent Lagrangian heuristics for nonlinear minimum cost network flows, European Journal of Operational Research (to appear).

M Patriksson:

Robust bilevel optimization models in transportation science, Philosophical Transactions of the Royal Society, A: Mathematical, Physical & Engineering Sciences (to appear).

P Marcotte and M Patriksson:

Traffic Equilibrium, in Transportation, volume 14 in the series Handbooks in Operations Research and Management Science, C Barnhart and G Laporte (eds), North-Holland, Amsterdam, 2007, pp. 623-713.

T Larsson, A Migdalas, and M Patriksson: A generic column generation scheme, submitted to Optimization Methods and Software.

M Daneva, M Göthe-Lundgren,

T Larsson, M Patriksson, and C Rydergren: A sequential linear programming algorithm with multi-dimensional search - Derivation and convergence, revised for Computational Optimization and Applications.

M Patriksson:

On the applicability and solution of bilevel optimization models in transportation science: A study on the existence, stability and computation of solutions to SMPEC models'' submitted to Transportation Research, B.

I Rychlik, M R Leadbetter: Estimating capsize risk for a vessel in a following sea. ISI 2007 meeting in Lisbon, pp. 1-4.

A Baxevani, I Rychlik:

Fatigue Life Prediction for a Vessel Sailing the North Atlantic Route, Probabilistic Engineering Mechanics, 22, pp. 159-169.

S Gupta, I Rychlik:

Rain-flow Fatigue Damage due to Nonlinear Combination of Vector Gaussian Loads, Probabilistic Engineering Mechanics, 22, pp. 231-249. S Åberg, I Rychlik:

Doppler-shift approximations of encountered wave statistics, to appear in Ocean Engineering.

A Baxevani, S Caires and I Rychlik: Spatio-temporal statistical modelling of significant wave heigth, to appear in Environmetrics.

A Baxevani, C Borget and I Rychlik: Spatial Models for the Variability of the Significant Wave Height on the World Oceans. Proceedings of the 17th ISOPE conference

K Podgorski, I Rychlik:

Envelope Crossing Distributions for Gaussian Fields, under revision for Probabilistic Engineering Mechanics (submitted for publication).

K Bogsjö, I Rychlik: Vehicle fatigue damage caused by road irregularities, (submitted for publication).

A Bengtsson, I Rychlik:

Uncertainty in fatigue life prediction of structures subject to Gaussian loads (submitted for publication).

H Schmidt:

SBaddon - High Performance Simulation for the Systems Biology Toolbox for MATLAB, Bioinformatics, 23(5), 646-647.

H Schmidt, G Drews, J Vera, Wolkenhauer: SBML Export Interface for the Systems BiologyToolbox for MATLAB, Bioinformatics, 23(10), 1297-1298.

H Schmidt, M Madsen, S Danø, G Cedersund: Complexity Reduction of Biochemical Rate Expressions, Bioinformatics, accepted.

A Ericsson, D Mojzita, H Schmidt, S Hohmann: Case study in systematic modelling: Thiamine uptake in Yeast S. cerevisiae, Essays in Biochemistry - Systems Biology. Portland Press, accepted.

D Dell'Orco, H Schmidt:

Mesoscopic Monte Carlo simulations of stochastic encounters between photoactivated rhodopsin and transducin in the ROS-disc membrane, Journal of Physical Chemistry, accepted.

L Nedbal, J Cervený, U Rascher, H Schmidt: A modeling approach to understand chlorophyll fluorescence transients and complex dynamic features of photosynthesis in fluctuating light, Photosynthesis Research, accepted.

M Madsen, S Danø, H Schmidt, B Quistorff: A Constrained, Top-Down Strategy for Modelling of Whole-Body Metabolism, submitted.

N Nedbal, J Cerveny, H Schmidt: Scaling and Integration of Kinetic Models of C3 Photosynthesis:Towards Comprehensive E-Photosynthesis (book chapter), submitted.

J Segeborn, J S Carlson, R Bohlin, and R Söderberg: Proceedings of the fourth International Conference on Intelligent Robotics and Manufacturing Automation, 2007, Venice 23-25 November:

T Svensson, J de Maré: On the choice of differential quotients for evaluating prediction intervals, to appear in Measurement.

M Hedelind, M Jackson, P Funk, J Stahre, R Söderberg, J S Carlson, M Björkman, M Winroth: I proceedings av 1st Swedish Production

Symposium, 28-30 August, Göteborg, Sverige, 2007.

L Lindkvist, R Söderberg, and J S Carlson: Proceedings of IMECE2007 ASME International Mechanical Engineering Congress and Exposition November 11-15, 2007, Seattle, Washington, USA.

PhD students

M Karlsson (Volvo 3P and Chalmers); advisors J de Maré, T Svensson, P Johannesson. Load Analysis for Fatigue Assessment of Vehicles – a Statistical Approach, Doctoral thesis, Department of Mathematical Sciences, Division of Mathematical Statistics, Chalmers University of Technology and Göteborg University, February 23, 2007.

P Lindroth (Volvo 3P and Chalmers): advisors M Patriksson and A-B Strömberg. Product configuration with respect to multiple criteria in a heterogeneous and dynamic environment (in progress).

J Segeborn (Volvo Cars and Chalmers): advisors J Carlson, R Söderberg, A Carlsson. Cost Effective Manufacturing Engineering by Automatic Path Planning & Line Balancing, Integrated with Tolerance Analysis and Control Logic (in progress).

J Svensson (Volvo Aero and Chalmers); advisors D Anevski, J de Maré, T Svensson. Survival Estimation for Opportunistic Maintenance, Doctoral thesis, Department of Mathematical Sciences, Division of Mathematical Statistics, Chalmers University of Technology and Göteborg University, June 1, 2007.

Master students

J Almquist and N Lämås (Chalmers); supervisor H Schmidt, examiners K Lindgren and C Breitholtz. Mathematical Modeling of a Xenopus laevis Oocyte Expressing the NBC and MCT Membrane Transporters - Towards a Better Understanding of the Neuron-Glial Interplay, Master Thesis, February 2007.

M Eckerljung and T Nordlund (Chalmers); supervisor J Johansson, examiner S A Andréasson. Framtagande av utvecklingsmiljö för matematiskt simuleringsspråk. Master Thesis, March 2007. J Johansson (Chalmers); supervisors M Jirstrand and H Schmidt, examiner Bernhard Mehlig. Model Reduction of Nonlinear Biochemical Systems (in progress).

A Kirsch (Technical University of Munich); supervisor M Jirstrand. Two Optimization Methods Implemented in Matlab – BFGS vs Brent, Internship, March 2007.

J Rudholm and A Wojciechowski (Chalmers); supervisor S Jakobsson, examiner M Patriksson. A Method for Simulation Based Optimisation Using Radial Basis Functions, Master Thesis, August 2007.

N Skaar (Chalmers); supervisor M Jirstrand, examiner Bernhard Mehlig. Parameter Estimation Methods for Continuous Time Dynamical Systems given Discrete Time Measurements (in progress).

KViltersten and KViltersten (University of Gothenburg), GMMC Master thesis, supervisor M Kvarnström, examiner M Rudemo. New methods for simulating diffusion in biological gels (in progress).

P Zarrineh (Chalmers); supervisor M Jirstrand, examiner O Nerman. Development of Parameter Estimation Methods for Biochemical Reaction Systems, Master Thesis, February 2007.

Bachelor students

G Eek and M Olvegård (University of Gothenburg); supervisor F Ekstedt, examiner M Karlsteen. Beräkningseffektiv dilatation i 3D. Bachelor report, December 2007.

Other assignments

F Edelvik: Reviewer for IEEE Transaction on Antennas

and Propagation. F Edelvik:

Reviewer for IEEE Transaction on Electromagnetic Compatibility.

F Edelvik: Reviewer for Journal of Computational Physics.

M Jirstrand:

Reviewer for the Computational Life Science programme 2007, Dutch National Science Foundation.

M Jirstrand: Reviewer for EURASIP Journal on Bioinformatics and Systems Biology.

M Jirstrand:

Opponent for Licentiate Thesis by Henrik Tidefelt: Structural Algorithms and Perturbations in Differential-Algebraic Equations, Division of Automatic Control, Department of Electrical Engineering, Linköping University, June 2007.

P Johannesson:

Member of the board of UTMIS (the Swedish Fatigue Network).

A-B Strömberg and M Patriksson: Advisers of the PhD student Elin Göransson (Heat and Power Technology, Department of Energy and Environment, Chalmers). Project title: Process integration – multiparameter optimization.

A-B Strömberg:

Co-adviser of the PhD student Birgit Grohe (Department of Computer Science and Engineering, Chalmers). Cost propagation – numerical propagation for optimization problems, Licentiate thesis, June, 2007.

A-B Strömberg:

Member of the external committee for the PhD thesis Feasible direction methods for constrained nonlinear optimization – suggestions for improvements by Maria Daneva, Department of Mathematics, Linköping University, May, 2007.

Courses

P Johannesson and J de Maré: A reliability course for industry was given at Volvo Trucks. The course consists of four half-days that were driven by problems from the industry.

M Patriksson and P Lindroth: Optimization, Basic course, Chalmers and Göteborg University.

M Patriksson: Optimization, project course, Chalmers and Göteborg University.

Flyers

SimIns - An ALM/DFA modelling platform, March 2007.

Robust Portfolio Optimization, March 2007.



FCC staff on December 21, 2007.

First row from left to right: Joachim Almquist, Mats Jirstrand, Domenico Spensieri, Fredrik Edelvik, Staffan Björkenstam. Second row from left to right: Johan Carlson, Sara Lorén, Robert Rundqvist, Jenny Ekenberg, Annika Eriksson, Björn Andersson, Uno Nävert. Third row from left to right: Pär Johannesson, Jonas Hagmar, Fredrik Ekstedt, Bo Johansson, Rikard Söderberg. Fourth row from left to right: Johan Segeborn, Peter Lindroth, Mikael Wallman, Stefan Jakobsson, Sebastian Tafuri, Muhammad Saif-Ul-Hasnain. Fifth row from left to right: Mikael Karlsson, Mikael Sunnåker, Tomas Hermansson, Daniel Segerdahl, Anders Ålund, Robert Bolin.

Illustrations

The year 2007 marked the Tercentenary of the birth of the Swedish Naturalist Carl Linnaeus – from 1757 Carl von Linné – world famous for his plant systematics. This has inspired us to illustrate our departments and research with pictures of flowers from fourteen Linnean classes:

Linnear	n class	Department / research area	Page
IV	Tetrándria	Computational Engineering and Design	12
Х	Decándria	Electromagnetics	4
VIII	Octandria	Fluid Dynamics	16
\vee	Pentándria	Optimization	18
XIX	Syngenésia	Reliability and Risk Management	20
IX	Enneándria	Fatigue Life	22
III	Triándria	Finance and Insurance	26
I	Monándria	Geometry and Motion Planning	28
XXI	Monoecia	Geometry Assurance	30
XIV	Didynámia	Path Planning	32
XII	Icosándria	Surface Inspection	36
XVIII	Polyadélphia	Systems Biology and Bioimaging	38
VI	Hexándria	Systems Biology	40
XXIV	Cryptogámia	Bioimaging	46

Linnaeus and his dream of order in nature are magnificently painted in the book "A Passion for Systems" (Swedish title: "System och Passion") by H Schmitz, N Uddenberg, P Östensson, Natur och Kultur 2007, ISBN 978-91-27-11522-4 (Swedish title: ISBN 978-91-27-11387-9).

We are most grateful to Ms Helene Schmitz for her courtesy and kind permission to let us use her magnificent photos of flowers, and to Ms Pia Östensson for allowing us to cite her textual descriptions, to illustrate the structure and beauty of nature – and of mathematics!

www.heleneschmitz.se www.naturochkultur.se

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The Fraunhofer-Chalmers Research Centre for Industrial Mathematics, FCC, has been founded by Chalmers and the Fraunhofer-Gesellschaft as a business making, non-profit Swedish foundation.

The purpose of FCC is to promote the application of mathematical methods in industry. To do so the Centre will undertake pre-competitive scientific research in the field of applied mathematics and work on projects defined by companies or public institutes.

The Centre, in close co-operation with Chalmers in Göteborg and Fraunhofer ITWM in Kaiserslautern, shall be a leading partner for international industry and academia to mathematically model, analyse, simulate, optimize, and visualize phenomena and complex systems in industry and science, to make development of products and processes more efficient and secure their technological and financial quality.