Annual Report 2015





Fraunhofer CHALMERS Research Centre **Industrial Mathematics** This and other FCC reports are distributed by: FCC

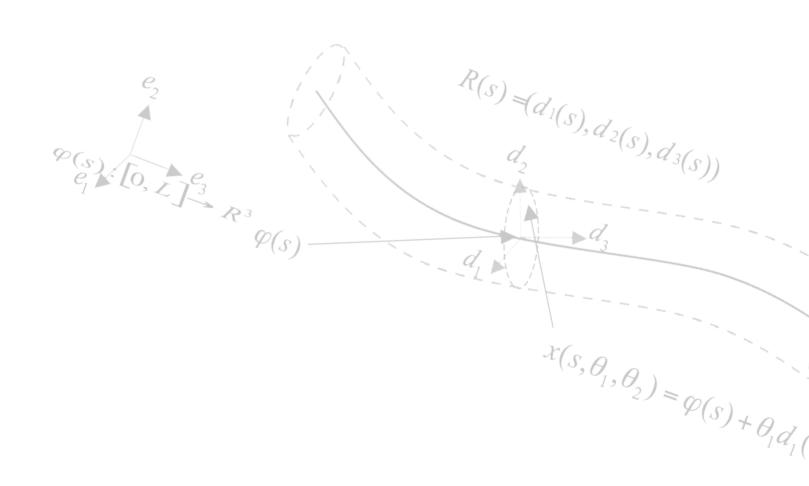
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Cover
Areas of Advance and industrial applications

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for Industrial Mathematics, FCC
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Preface and Profile

PREFACE AND PROFILE

FCC is offering contract research, services, algorithms and software based on advanced mathematics within Modeling, Simulation and Optimization (MSO). MSO provides a significant leading edge in industrial innovation of products and production systems. In 2015, we have successfully proved this together with clients from the automotive and vehicle, metrology, pharmaceutical, wood and paper, and electronics industries. Examples include simulation and optimization of robotized adhesive stations, simulation of assembly ergonomics, modeling and simulation of drug compound distribution and effect, off-line programming of robot carried inspection sensors, and solder jetting on printed circut boards.

I am proud to say that during 2015, we have performed around 40 projects for our industrial clients and 20 public projects financed by public research agencies such as SSF, VINNOVA and the EU. The revenue shows a growth of almost 5 percent since last year, an industrial income of 44 percent and a positive net result. Our work and technologies have helped clients mainly in Sweden, but also in Germany, US, Finland, Denmark, Japan, Israel, Korea, Great Britain, and China.

However, the full potential of using advanced mathematics in industry is far from reached and new technologies together with increased efforts in marketing and sales will hopefully continue our growth in 2016 and beyond.

We have been fortunate to recruit eight new coworkers. To be attractive for our clients and employees in the long run, the scientific activities of FCC are indeed important. In 2015 we have published 30 scientific papers including 16 in journals. We have recruited one new student to our Advanced Engineering Mathematics research program (AEM) and can also congratulate two of our coworkers who earned their Licentiate degree during 2015. Also, 13 students from Chalmers worked half a day a week as contracted students and six students from Chalmers did their master thesis work at FCC.

A great advantage for FCC is the possibility of long term collaboration with Fraunhofer and Chalmers. The cooperation and exchange of projects with ITWM during 2015 have involved a variety of subjects such as dynamics, biomechanics, the simulation of flexibles, virtual paint, position tracking systems, product configuration optimization, continuous production, the simulation of ultra-fast electronics, and big data analytics. We have also grown our cooperation with several other Fraunhofer units.

The well-established collaboration with Chalmers centres and departments in 2015 includes projects, grant applications, guest lectures, PhD's and master students with Wingquist Laboratory, Product and Production Development, Systems and Synthetic Biology, Fluid Dynamics, Chalmers e-Science Centre CheSC, Signals and Systems, and Mathematical Sciences. FCC is also very active in Production, Built Environment, Materials Science, and Life Science Engineering within the Areas of Advance.

I am proud and impressed by the excellent work done by my coworkers at FCC and I appreciate the fruitful collaboration with my colleagues at Chalmers and Fraunhofer ITWM. In May 2015, FCC was evaluated by an international committee selected by Fraunhofer and Chalmers. The mission was to assess the scientific and economic development and future strategy of the centre. The successful evaluation concluded that the centre has since its start in 2001 developed into an excellent research institution and that all targets have been achieved or surpassed.

Strengthened by the evaluation and the increased support and interaction with our founders, we will continue the challenging but rewarding work with FCC – a Swedish centre in industrial mathematics following the Fraunhofer model with a high level of contracted research boosted by pre-competitive research, funded by Fraunhofer and Chalmers.

Below, some of our activities are highlighted in four profile projects.

Enjoy your reading!



The department Geometry and Motion Planning works in close cooperation with the Chalmers Wingquist Laboratory and participates in the ten-year Wingquist Laboratory VINN Excellence Centre for Virtual Product Realization 2007-2016. In 2015, the department continued and extended several projects, e.g. on automatic path-planning and line-balancing, sealing, virtual paint, flexible materials, metrology, massive point clouds and intelligently moving manikins. The software platform IPS for rigid body path planning, robot station optimization and flexible cable simulation is recognized through licensing by industrial clients in Europe, United States and Japan. The department has substantial joint development with the ITWM department Mathematical Methods in Dynamics and Durability. In 2015, there has also been extensive cooperation with our two spin-off companies; Industrial Path Solutions Sweden AB and fleXstructures GmbH.

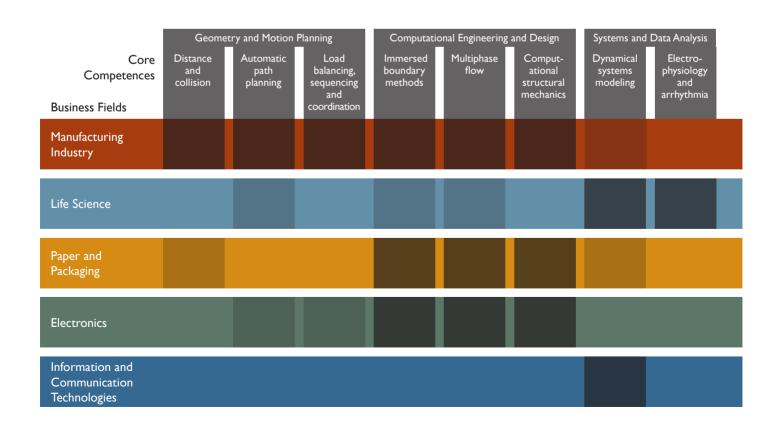
The department Computational Engineering and Design has continued and expanded its work on novel numerical methods, fast algorithms and engineering tools to support virtual product and process development. The simulation tools are applied in projects together with Swedish and international industry, and public partners, for applications in fluid dynamics, structural dynamics and electromagnetics. The department collaborates with the ITWM departments Optimization, Flow and Material Simulation, and Mathematical Methods in Dynamics and Durability, and runs several multiphysics projects involving fluid-structure, fluid-heat transfer and fluid-electromagnetics interaction including simulation of paint and surface treatment processes, cooling of electronics and the project on innovative simulation of paper with Swedish paper and packaging industry. The industrial impact of the core competences and technologies has increased through the founding of the spin-off company IPS IBOFlow AB.

The department Systems and Data Analysis offers competence in dynamical systems, prediction and control, mathematical statistics, big data analytics, and data science in both technical and biological/biomedical applications. In 2015, the department has continued its activities in model based data analysis in drug development and the development of robust and efficient computational tools for mixed effects modeling. Another key activity has been the successfully completed project Remote Data Collection and Visualization with Volvo Cars, with the aim to develop technology for data processing of remotely collected automotive data to be used for decision support for product development of new and existing functions in the car. We have also worked in close collaboration with ITWM department System Analysis, Prognosis and Control on machine learning methods such as incremental clustering and classification and subspace clustering.

FCC offers Contract Research, Software and Services for a broad range of industrial applications. The cornerstones in all activities are Modeling, Simulation, Optimization (MSO) and Visualization of products and processes. For marketing the MSO activities they are divided into the business fields Engineering Industry, Life Science, Paper and Packaging, Electronics and Information and Communication Technologies. To continue the growth, a number of new fields will be investigated during the next few years including Additive Manufacturing, Continuous Production, Built Environment,

Big Data, Robot and Human Collaboration, Scanning/3D point clouds, and Mechanical Fatigue. The activities within each business field is based on the centre's core competences. The core competences are developed by the departments and the aim is to keep-up and ahead of the state-of-the-art, and have an interaction with the scientific society, in these areas. The business fields are not linked to a specific department, and several projects in for example Engineering Industry involve researchers from two departments.

Business Fields and Core Competences



BUSINESS FIELDS

Manufacturing Industry

In the largest business field Manufacturing FCC strives to be a leading developer of advanced mathematical tools and algorithms supporting virtual product and process development for complex assembled products in the sub fields of assembly and industrial robotics, geometry assurance and metrology, and surface treatment. For Swedish economy and export the manufacturing industry is an important sector, representing half of the export value and 30% of all R&D investment in Sweden. In Industrial Robotics, we have been able to develop and implement an automatic solution for robot motion programming and optimization, supporting applications such as welding, assembly, inspection, sealing and gluing. In Geometry Assurance and Metrology, FCC has in tight collaboration with Wingquist Laboratory been developing and implementing methods and algorithms supporting the technical vision to create a closed loop from breaking down requirement to inspection features, via automatic programming and optimization of the motions of the coordinate measurement machines or robots, to advanced analysis of the inspection data. In Surface Treatment FCC's position is very strong with the only software on the market that can accurately simulate the spray painting of a car in a few hours on a desktop computer. The same software can also be used to simulate the laydown of sealing and glue material.

Life Science

In Life Science FCC strives to be a leading provider of advanced services and tools based on state-of-the-art mathematics and beyond in model based drug discovery and development, systems and synthetic biology, computational cardiology, and quantitative bioimage analysis. In these fields we have successfully acquired industrially and publicly funded projects on both the national and European level. A major part of FCC's life science activities falls within pharmacometrics, i.e., science concerned with mathematical models of biology, pharmacology, disease, and physiology used to describe and quantify interactions between drug compounds and patients. Here we have well-developed relations with AstraZeneca with a mix of projects and project types, ranging from multi-year contract research projects, long term service contracts, and jointly executed public projects.

Paper and Packaging

In Paper and Packaging FCC supports the Swedish industry with multi-scale methods, algorithms and software for simulation of the papermaking process and paperboard package quality. The focus is in particular on detailed simulations of the build-up of the paper in the forming section of the paper machine, and how the paperboard's resilience to edge penetration depend on pulp, chemical and forming fabric properties, and process conditions. The unique results have received significant attention and have contributed to new process knowledge.

Electronics

In Electronics FCC develop simulation tools for drop-on-demand solder jet printing that take the complex rheology of the solder paste into account and the strong fluid-structure interaction in the printer head. In addition, a thermal solver based on IBOFlow is developed for electronics cooling applications. A collaboration with a large software house was initiated after a benchmark study showed that IBOFlow was at least as good, or better, than available commercial tools. When the product is ready for the market in 2016 a dramatic increase in the number of IBOFlow users is expected.

Information and Communication Technologies

In the Information and Communication Technologies business field FCC has set out to be a high-end provider of tailor made methods and tools with a high mathematical content. This is a field where our customers can be found among both SMEs and large corporations. Our goal is to excel on mathematical tools and algorithms of importance for ICT applications where our engineering mathematics background and wide experience from a large number of applied projects can be exploited. Areas of particular interest are on-board and off-board data analysis of car signals and function utilization in the automotive industry and automation, control, and sensor solutions in the process industry.

Core Competences

Geometry and Motion Planning

At the Geometry and Motion Planning department the following core competences are developed: (i) Distance and Collision algorithms that fast and accurately detects collisions and calculate distances between large geometrical objects; (ii) Automatic Path Planning algorithms that fast calculates collision free motions for moving objects in cluttered environment; (iii) Load Balancing, Sequencing and Coordination algorithms that optimize cycle time and equipment utilization in multi robot stations and lines.

Computational Engineering and Design

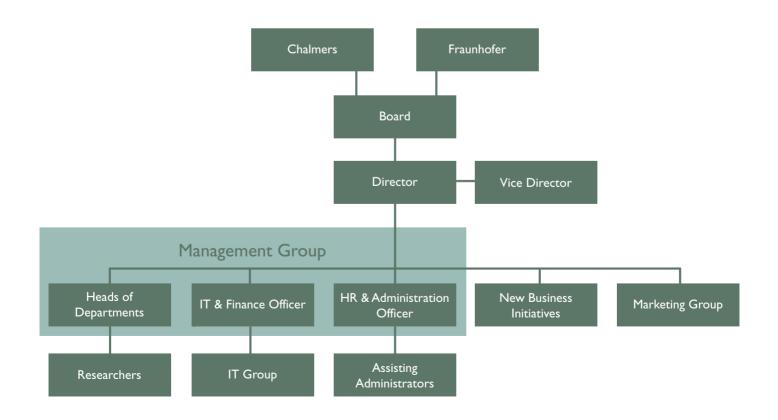
At the Computational Engineering and Design department the following core competences are developed: (i) Immersed boundary methods that greatly simplify preprocessing by avoiding the need of a body-conforming mesh, and handle fluid-structure interaction efficiently; (ii) Multiphase flow simulation using a novel robust VOF method; (iii) Computational Structure Mechanics for simulation of welding and composite materials to e.g. support our activities in geometry assurance.

Systems and Data Analysis

At the Systems and Data Analysis department the following core competences are developed: (i) Dynamical Systems Modeling for characterizing, understanding, predicting, and controlling the time evolution of physical and living systems; (ii) Electrophysiology and Arrhythmia for addressing cardiac disease and cardiac drug safety which are essential for clinical diagnosis and interventions, as well as for the development of new drugs.



ORGANIZATION





HEADS OF DEPARTMENTS



Dr. Johan S. Carlson Director Head of department Geometry and Motion Planning



Dr. Fredrik EdelvikVice Director
Head of department
Computational Engineering and Design



Head of department Systems and Data Analysis



Business Area Leader Continuous Production

CENTRAL SERVICES



Jenny Ekenberg, MSc IT & Finance Officer



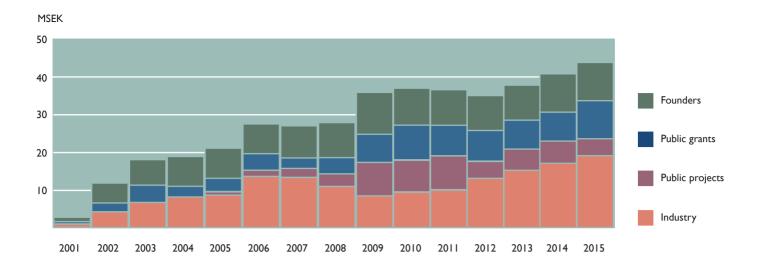
Annika Eriksson HR & Administration Officer



Lisa Torstensson Administrator



Karin Sandin Administrative assistant



TOTAL INCOME

In 2015, the total income increased to 44 million Swedish crowns or almost 5 million euros which was once again all-time-high. The result was a positive net, as has been the case every year since our start in 2001.

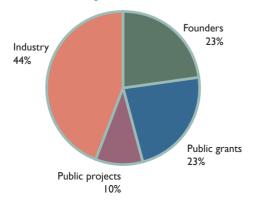
The profile of the Centre is controlled by its income structure, in 2015, 44% came from industrial projects,

33% from public funding, and 23% base funding from the founders. The public funding includes 10% from public projects under industrial command and 23% from public grants. Compared to the previous year we had an increase of industrial projects and public grants, but a decrease of public projects under industrial command.

FACTS ANI

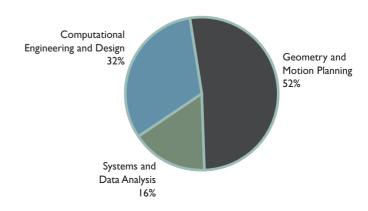
PROJECT MIX BY INCOME

The profile of the Centre is controlled by its income structure. We distinguish between four categories: industrial projects, public projects (under industrial command), public grants, and base funding. In 2015, these four were in good balance, showing a clear industrial profile.

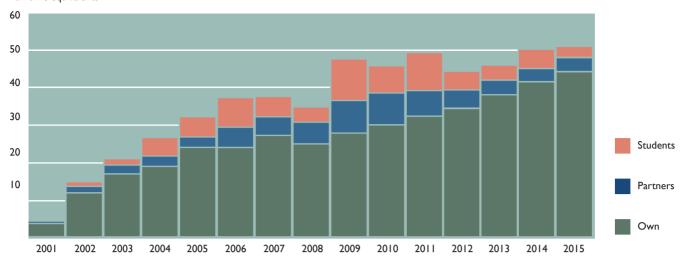


DEPARTMENTS BY INCOME

The Centre has three departments; Geometry and Motion Planning, Computational Engineering and Design, and Systems and Data Analysis, with a relative income divided as follows:



Full-time equivalents



Staff – Full-time Equivalents

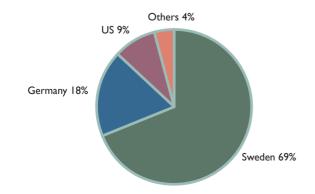
The number of staff 2015 was 51 full-time equivalents (FTE) including own staff (43 FTE), students (4 FTE), and partners (4 FTE). We were happy to recruit eight new coworkers, two of which were previously contracted students. The number of students was 19 (4 FTE) including two female students; 6 (3 FTE) doing their Master's thesis projects, and 13 (1 FTE)

students in Master's programs contracted on 10-20% for project work. Six (4 FTE) own staff-members are in the Chalmers two-year licentiate program Advanced Engineering Mathematics (AEM), two of them have earned their Licentiate degree during the year. Three (3 FTE) own staff-members are in PhD programs, in parallel with project work.

FIGURES

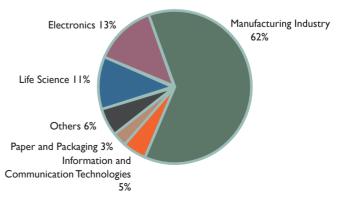
COUNTRIES BY INCOME

During the year FCC have had customers in many different countries. The total project volume was divided between:



Business Fields by Income

During 2015, we have performed around 40 projects for our industrial clients and 20 public projects financed by public research agencies such as SSF, VINNOVA and the EU. Our largest business area is manufacturing industry and in particular the vehicle industry.

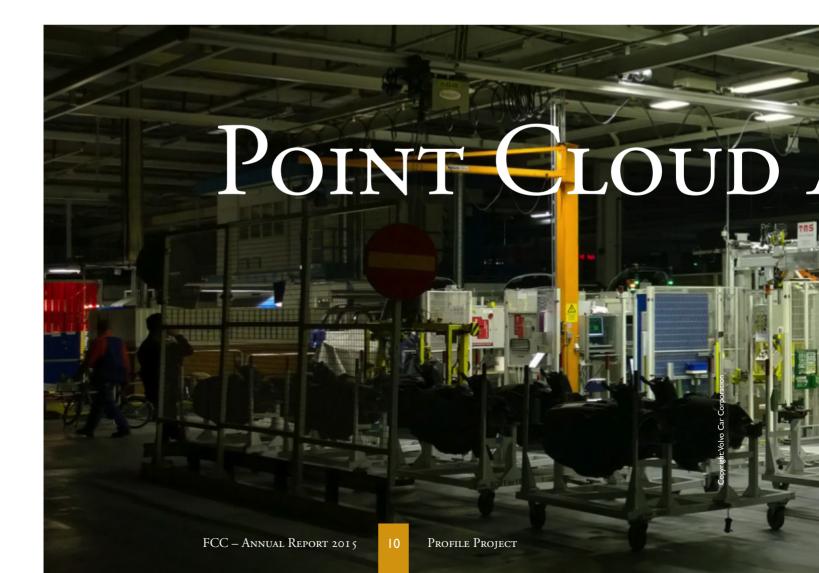


PRODUCTION

FCC has developed new algorithms and software tools for laser scanned point clouds supporting manufacturing industry to maximize equipment utilization, save time and enhance their competitiveness.

The development has been in close cooperation with Volvo Cars, Wingquist Laboratory, the Production Area of Advance at Chalmers, and ATS AB.

The researched technology will in the next step be utilized in the Building Futures Area of Advance with the goal of increased productivity and quality.



Production

The revolution is upon us but it is happening via something surprisingly small; infinitely small in fact. And in spite of their size they are now filling up terabytes of hard drives around the world. With these tiny wonders many concepts which have so far only lived in the minds of researchers and the pages of scientific journals are now entering the industrial world. The digital factory is upon us and the empowering technology is a laser-scanned point cloud.

Over the last decade laser scanners have ushered in a revolution. It has happened by the hardware and software for laser scanners becoming orders of magnitude cheaper. This has opened up new business opportunities revolving around the scanning and documenting of physical factory facilities. However, the scanning and documentation of industrial complexes is only the first step. The most important part for industry is what comes next; deriving value from their data. This means asking questions of the scanned factory layouts such as, does this new chassis fit along the assembly line? Can we rebuild this manufacturing process? Is there enough space for the new production line? It is questions such as these that new and unique tools developed at FCC are able to answer, and it all began with a piece of cardboard.

Before the advent of laser scanning, the testing of new car models at Volvo Cars was usually done with cardboard silhouettes of chassis. They were moved through an assembly line on a Sunday while nothing was being produced. In spite of this, there were sometimes problems with the verification of new car designs. During introduction, new models could crash in the manufacturing line with the result that the chassis became scrap metal, and worst of all, a stop in production since different models are assembled on the same line.

It was around 2009 when Volvo Cars saw that laser scanning had matured to the point of now being affordable and reliable. So they turned to FCC to solve one of their major bottlenecks in production; the verification of new car designs. We were able to take their point cloud data and develop new tools which could combine both traditional CAD geometry and point cloud models in one simulation tool. This tool allowed Volvo to answer one of their important design questions by being able to guarantee that new designs would pass along their assembly line collision free. This has saved Volvo Cars both money and time in their verification processes.



PRODUCTION

3D Scanning and Point Clouds

A 250 meters scanned factory section from Volvo Torslanda (courtesy of Volvo Cars).

Since our first successful foray into the point world, we have continued our development of point cloud tools. We are now able to carry out most of our usual virtual processes and computations in point clouds. Companies can now compute distances and collisions, path plan, compute largest noncolliding volumes and much more in hybrid triangle meshpoint cloud environments. We have also started exploring the concept of unlimited detail which allows users to visualise massive point clouds with billions of points and compute distances between such point clouds and other objects. Our tools leverage the latest technological advances to produce fast and accurate results. For example, when computing the largest non-colliding volume, we build a sparse hashbased octree to be able to abstract away the geometry and perform fast collision queries. Then by using the adaptive bisection method we are able to quickly determine which areas of the path do not constrain the largest non-colliding volume. Finally all computations are done in parallel to exploit the latest multi-core computer architectures.

In the meantime, we have also successfully demonstrated the academic importance of our work by publishing 6 new papers in the area. We have saved our industrial partners significant sums of money with the new tools and allowed them to do things virtually which were previously impossible. We are also noticing significant interest from other companies for the tools we have developed.

These advances will lead to a new revolution in the usage and value of virtual processes. Having a digital factory model, which can genuinely add value by allowing engineers to answer important questions with it not only saves money but can reduce lead times, make cooperative work easier and simplify work flows. Although the objects we are dealing with are infinitely small their benefits seem infinitely large.

Geometry and Motion Feasibility Study

Moving a CAD/triangulated chassis along its production path through the scanned factory (courtesy of Volvo Cars).

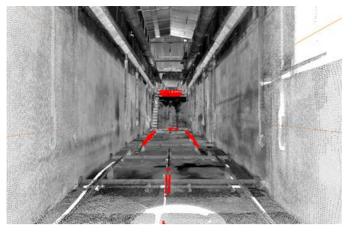


Distance Measure

Calculating the exact shortest distance between the chassis and the surrounding point clouds for the 250 meters. The distance measure is indicated by the red line (courtesy of Volvo Cars).

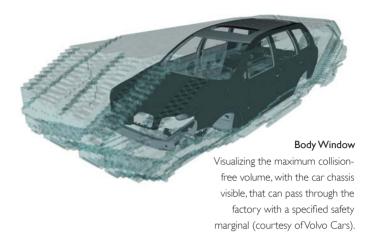


Production



Collision Indication

Computing and visualizing the set of potential colliding points for the chassis (courtesy of Volvo Cars).



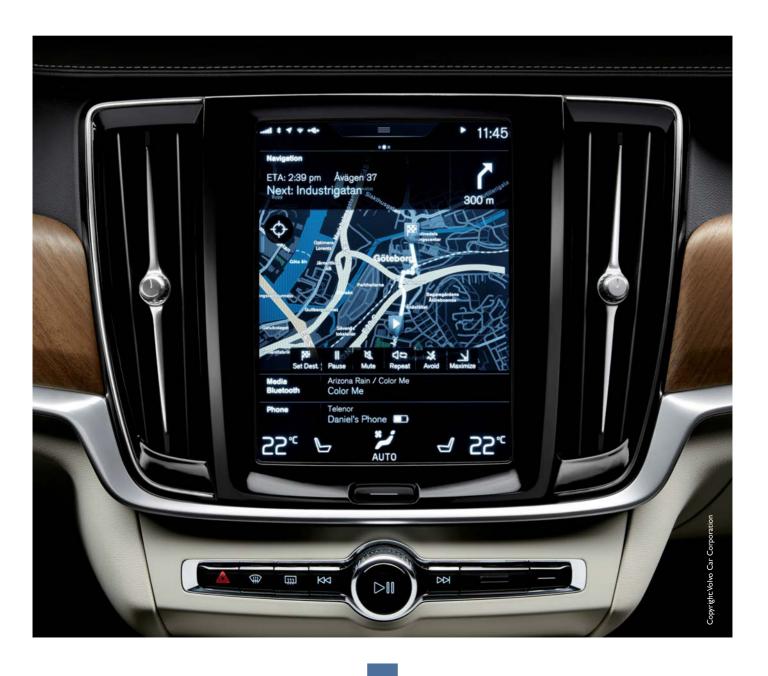


Ergonomics Factory ergonomics can be evaluated by combining point clouds with human motion simulation (courtesy of Volvo Cars).



Towards Automotive Big Data Analytics

Data Mining for Usage Patterns



Information and Communication Technologies

The data available in today's and future cars contain vast amounts of information and turning this into useful knowledge for decision support for product development of new and existing solutions in the car would provide a highly competitive edge. Volvo Cars has recognized this opportunity and launched the project Remote Data Collection and Visualization (RDCV), partly funded by the VINNOVA's FFI program.

The purpose of the project has been to study the whole chain from data collection in the vehicle to visualization and analysis in the office, where the focus has been on use cases regarding human machine interaction (HMI). An important part of the RDCV project has been to develop technology for data processing and visualization where FCC has analyzed and developed methods using tools from mathematical statistics, multivariate data analysis, classification and machine learning, regression, and clustering techniques.

The vision of the RDCV project has been that all units within project development shall have access to an anonymized tailored subset of field data to be included in their daily work process. To obtain this, tools and techniques to process and visualize big data resulting from remote data collection from Volvo cars has been investigated and developed. The knowledge mined from the processed data should eventually be used for:

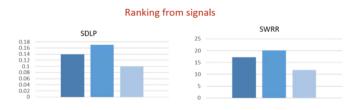
- Decision support for product development of new and existing solutions in the car
- Detection of market trends
- Detection of characteristic operational modes of individual cars on an anonymized level
- Optimized non-critical system components, like media systems and HMI Interfaces

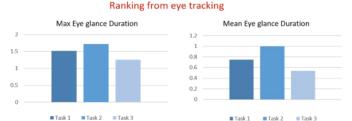
A prerequisite for allowing data collection from customer cars is to get customer's consent to sharing data and also to actively select to what level data sharing is allowed.

FCC's part of the project has evolved around two themes: (i) quantification of distraction using HMI functions and (ii) detection of characteristic operational modes of individual cars on an anonymized level.

Quantification of Distraction

A thorough understanding of how the infotainment system in a car is actually used is of outmost importance to improve the driver's experience. What functions are frequently used, how easily operated is the user interface, and under what driving modes or driving conditions are different functions used? One way to quantify how well the user interface is designed for simultaneous interaction and driving is to measure driver distraction for different functions such as dialing a telephone number, switching channel on the radio, or operating the navigator system. Distraction can be estimated by direct measurement on eye movements, and having the fraction of time when the eyes are not directed towards the road but on the user interface to be used as a measure of distraction. This requires extensive measurement equipment in the car including camera, so called eye-tracker system, and controlled conditions.





Evaluation of measure of distraction based on standard deviation lane position (SDLP) and steering wheel reversal rate (SWRR) compared to the measure of distraction based on an eye-tracker system. The bars show the ranking of three different tasks in terms of distraction for four different computed measures (task1: switch radio channel, task2: dial a phone number and hang-up, task3: maximize bass and treble of the equalizer).

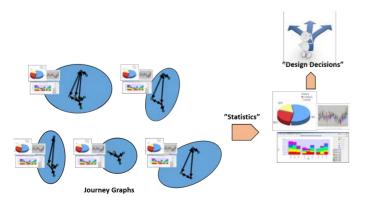


Information and Communication Technologies

In this project we investigated to what extent the information content in signals from the infotainment systems and other available signals in the car could be used to replace the eye-tracker system and controlled conditions constraints for quantification of distraction. If the level of distraction can be inferred from signals already available in the car, without any extra measurement equipment, it would facilitate direct feedback from actual use of different versions of the infotainment system from that part of the car fleet whose drivers actively have chosen to share this information. Examples of analyzed time resolved signals are lane position and steering wheel angle. The lane position standard deviation and steering wheel reversal rate were two candidates for measure of distraction. In a simulator study performed at Swedish National Road and Transport Research Institute (VTI) these two signals, as well as the corresponding eye-tracking measure, was used to rank the degree of distraction for a number of selected driving conditions and use cases of the infotainment system. The study showed that the ranking of the performed tasks with respect to distraction was preserved by computing measures of distraction, using signals already available in the car compared to distraction measured by an eye-tracker system.

Detection of Characteristic Operational Modes

Working with so called digital user experience (DUX) the understanding of the actual car usage and its context is of central importance. Traditionally, questionnaires, focus groups, interviews, and prior experience are used to investigate DUX related matters. Using signals available in regular cars, from drivers who have given their consent, cars can be categorized into different typical cases or driving modes and in this way one may deduce the actual usage of the cars. With this as a starting point the car can better be adapted to the anticipated needs of that typical case or driving mode. The adaptive design process can be implemented on different time scales, from direct adaptive user interfaces in the car that automatically change between driving modes such as highway driving and low speed/many turns trip segment to larger in between car generations design changes.

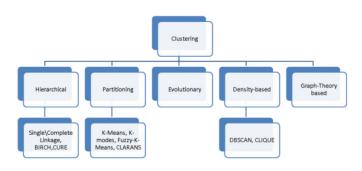


In this project the term journey graph was coined, which can be used to quantify and visualize the set of different trip types a specific vehicle is involved in over time. In the project data spanning several months from a selected set of daily used company cars were analyzed. Both hypothesis driven analysis and more explorative analysis were carried out. In the explorative data analysis different clustering methods and platforms for big data analytics were evaluated.

The knowledge gained by the statistical data analysis and data mining approach of this project can be further explored for evidence based engineering, market quantification, predictive HMIs, etc.

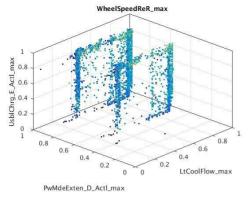
Methods

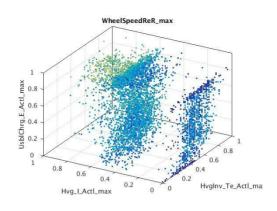
The computational tools used and developed in this project belongs to the fields of mathematical statistics and machine learning. Data of both categorical and time-series character has been analyzed using various statistical techniques ranging from simple mean and variance computations to more advanced ones such as feature extraction based on empirical histogram representations, similarity measures based on distance of distributions, and matching algorithms originally developed for DNA sequence similarity matching. An important aspect has been to apply machine learning techniques such as clustering and classification. Given the different tasks at hand, a range of different clustering approaches have been surveyed, see figure for an overview. More extensive work was spent on K-means clustering, the Markov Cluster Algorithm, and subspace clustering. The subspace clustering approach has found considerable interest in the data science community during the recent years and has been of particular interest in this project due to the high-dimensionality character of the available data.

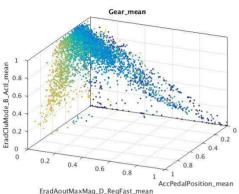


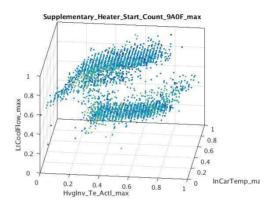
Statistical data analysis based on "Journey Graphs" for market quantification, evidence based engineering, predictive user interface, and value added sales.

Information and Communication Technologies









Examples of subspaces with clusters found using subspace clustering using all available signals in the sample data. Interpretation requires expert signal knowledge.

Overview Clustering Approaches

A particular aspect of the work has been to also address the streaming character of the data, i.e., that data is generated and accumulates over time. This calls for incremental approaches where algorithms not only work on static batches of data, but can be initialized by a previous analysis result and update such a result by only using the most recent data.

Collecting and using personal driver data must be done in a way that protects privacy of individual car owners. In this project privacy was addressed by investigating to which extent algorithms can handle mixed levels of data sharing from different users, e.g., by missing value approaches. The privacy aspect was also handled by looking into the concept of differential privacy and privacy preserving features.

RESULTS

The simulator study performed at VTI showed that for the included use cases distraction could be measured using signals available in the car without the use of advanced eye-tracking technology. With direct access to these signals and simultaneous logging of user interface operations with Volvo Cars it would be possible, in continued work involving test vehicles in regular traffic or ordinary vehicles operated by drivers who has given their consent, to quantify the level of distraction for different functions of the infotainment system. Through scale-up of the numbers of participants in studies of this kind, one can evaluate different versions of a user interface by comparing the level of distraction for drivers using the different versions

(known as "A/B-testing" in statistics, which for example is used on a regular basis to evaluate web-based user interfaces). In the classification of car usage, the journey graphs of the test vehicles were identified and hypotheses about the vehicles usage were tested. The application of clustering methods from the field of machine learning was shown to give insights about different trip types and their characterization. Clustering on smaller sets of manually selected signal types and so called subspace clustering on a large set of signal types were employed. The project showed that explorative data analysis based on clustering and other techniques from machine learning have large potential and needs to be employed with a big data perspective. Furthermore, the project identified a number of use cases for these methods such as:

Market quantification

Understanding and trends with respect to typical usage modes on different markets

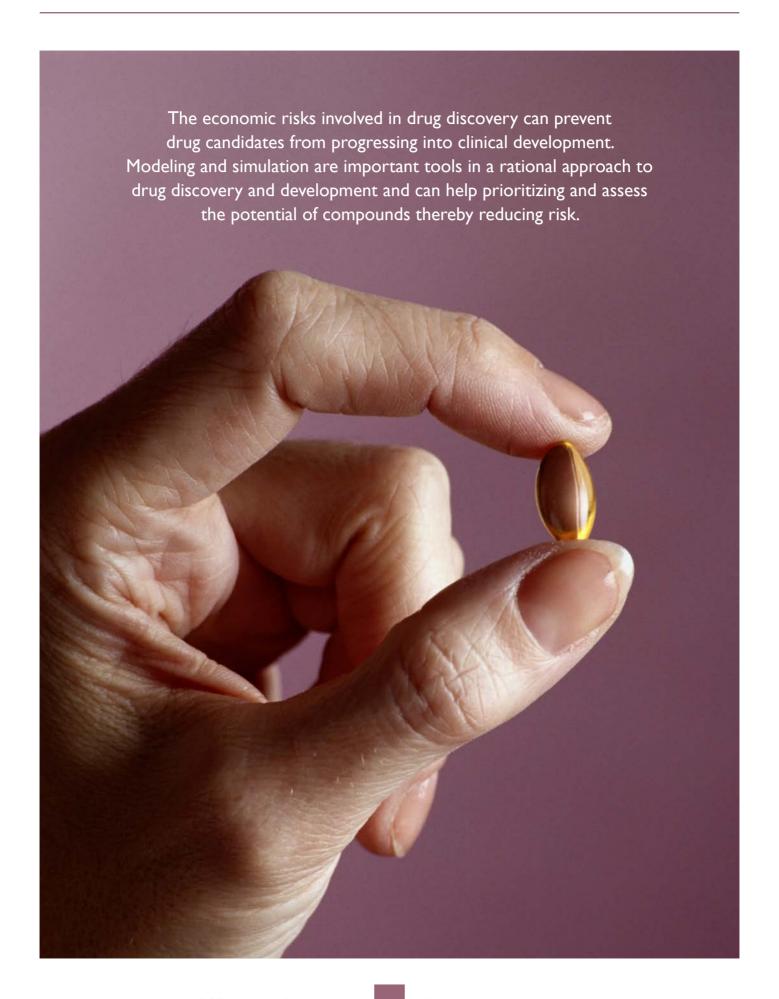
Evidence based engineering

Measuring actual usage, identification of important or novel functionality, improving the design and development process

■ Predictive user interface

Identification of car usage mode and initialized trip type, automatic adaption of user interface

LIFE SCIENCE



Modeling and Simulation for Predictive Model Based Drug Discovery and Development

The work at FCC aims at delineating and streamlining the modeling and simulation process in model based drug discovery and development to increase both the pace of model development and the predictive power of future models. FCC has worked together with AstraZeneca in a 3-year project to develop new tools and increase usage of advanced modeling and simulation within the Drug Metabolism & Pharmacokinetics and Pharmacokinetics-Pharmacodynamics (PKPD) scientific areas.

Mathematical model based analysis of experimental data on how novel compounds are taken up, distributed, and eliminated, and their pharmacological effect, are used both in preclinical studies as well as in translational science to rationally design dosage regimens for clinical studies. However, the use of already existing data and models to answer question of integrative character is often under-used. For example, to predict drug effects when scaling from healthy to diseased individuals a meta-analysis of already existing studies can be utilized. Quantification of uncertainty is another important topic where there has been a lack of proper tools and techniques. The dynamics of non-esterified fatty acids (NEFA) in response to administration of nicotinic acid in the rat have served as a test bed to address the objectives of the project.

Industrial Applications and Needs

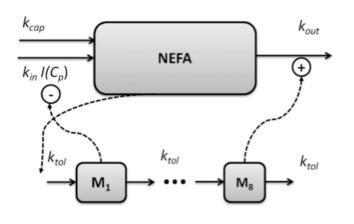
The increased use of advanced modeling and simulation in PKPD analysis provides means to address the so called 3Rs (replace, refine, reduce), rationally approach the design of biologics to target specific points in mapped out mechanisms, to help characterize pharmacodynamic effects of compounds without systemic exposure, and handle the complexity introduced by systems involving feedback resulting in tolerance and rebound phenomena. These areas are in turn described below and have to different extent been addressed during the project.

Replace, Reduce, Refine

The iterative cycle of experimental studies complemented by computer simulations are instrumental to implementing any serious 3R strategy. Here, small pilot experiments followed by modeling and simulation provides input to the design of new experiments (dosage, number of individuals, number of sample points, etc) for optimal utilization of resources. This is important since the size and cost of experimental studies increase during the course of a project when moving from pilot exploratory acute PK studies to chronic toxicokinetic studies with a large number of individuals.

Design of Biologics

Models of increasing complexity compared to today's gallery of standard PKPD models will be needed to characterize the behavior of for example novel biologics. One example is target mediated drug disposition (TMDD) models required to describe the highly nonlinear dose dependence of some ligand-receptor interactions. One may also expect this type of models, that include biological mechanisms from receptor pharmacology, could be very useful to investigate where and how a novel compound should interact to maximize its effect. This is partly what the emerging field of system pharmacology is expected to be able to deliver.



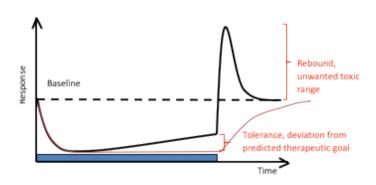
Parameter	Definition	Parameter	Definition
k _{in}	Turnover rate constant	р	Amplification factor
k_{out}	Fractional turnover rate constant	$I(C_p)$	Inhibitory drug mechanism function
k_{tol}	Turnover rate constant of moderator	M_1	Moderator in compartment 1
k_{cap}	NEFA formation in the capillaries	M_8	Moderator in compartment 8

Dose-Response-Time Analysis

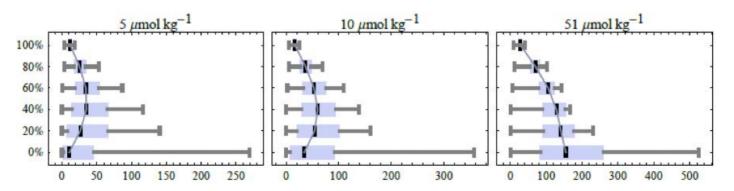
Compounds that exert their effect without entering the circulation (other than possibly as a secondary effect), such as topical delivery, lung disposition, or ocular drug delivery are all examples where models have to be built without the traditional sequential PKPD approach. Here the area of dose-response-time analysis plays an important role, where the traditional PK part is replaced by a bio-phase model feeding into the PD model.

Tolerance Build-up and Rebound

The role of feedback and how to rationally design dosing schedules, minimizing the effect of tolerance build-up and rebound, is also an important field. Mechanistic PKPD models are required to unravel the complexity, and to generate optimal steady state concentration-response relationships, response-time courses and dosing schedules.



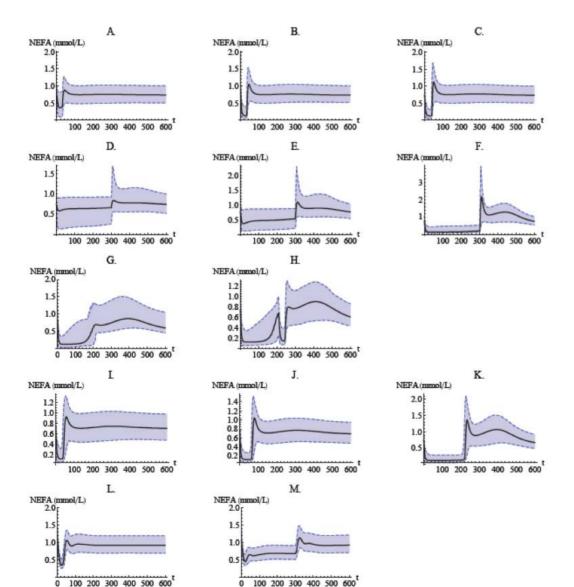
The extent of rebound following the termination of a 300 min infusion was quantified as the maximum level of NEFA reached, expressed in percentage above the baseline. The population variability of this quantity was calculated for different degrees of disease (0%, 20%, 40%, 60%, 80%, and 100%, respectively) for three different doses (5, 10, and 51 μ mol kg–1, respectively). Results are presented as box and whisker plots, showing the median values, 25% and 75% quantiles, respectively, and the minimum and maximum observations. For each dose, a trajectory is joining the medians to emphasize the changes in extent of rebound as a function of the degree of disease.



Meta-analysis Using Existing PKPD Models and Data

To provide predictions of drug effects when scaling from healthy to diseased individuals, a joint analysis of the data from normal and diseased animals is of interest. For instance, a drug that has proven effective in the normal case may not display the same effect in the disease system, which in turn can lead to underestimation of suitable dose levels. The purpose of the joint analysis carried out during this project was to determine in what way disease affects the pharmacodynamics and to quantify this effect by a combined analysis, where all data sets from both normal Sprague Dawley rats and obese Zucker rats have been used

simultaneously. Parameter estimation results from the combined analysis was then compared to a population PKPD analysis previously done separately for each group. The meta-analysis led to the identification of the pharmacodynamic parameters most affected by the disease, which turned out to be the maximum drug-induced inhibitory effect, the plasma concentration at 50 percent reduction of maximal effect (i.e., potency), and the sigmoidicity factor of the drug effect inhibitory function, respectively.



Population model simulation of NEFA plasma concentrations for normal Sprague-Dawley rats after infusion (a-h), oral administration (i-k), for obese Zucker rats after infusion (I-m). Infusion of (a) I µmol kg-1; (b) 5 μmol kg-1; (c) 20 μmol kg-I, over 30 min; (d) 5 μmol kg-I; (e) 10 µmol kg-1; (f) 51 µmol kg-1, over 300 min; (g) 5 µmol kg-l over 30 min followed by a stepwise decrease in infusion rate every 10 min for 180 min; (h) 5 µmol kg-1 over 30 min followed by a stepwise decrease in infusion rate every 10 min for 180 min, and another 5 µmol kg-1 infusion over 30 min. Oral dose of (i) 24 µmol kg-1, (j) 82.1 µmol kg-1, and (k) 812 µmol kg-1. Infusion of (I) 20 µmol kg-1 over 30 min and (m) 51 µmol kg-1 over 300 min. Shaded bands show the Monte Carlo-derived 90% population variability bands.

MODEL UNCERTAINTY

The vast majority of today's PKPD models are not able to handle uncertainty in the model dynamics. However, so called nonlinear mixed-effects (NLME) modeling, the current workhorse in PKPD data analysis, allow for variability and uncertainty both within and between subjects being modeled. In this project we have investigated how to also incorporate uncertainty in the model dynamics in NLME modeling. This turns out to provide both more robust estimation methods (modified and regularized likelihood function to be optimized) and the ability to quantify and detect model misspecification.

A formal way of specifying uncertainty is through the use of probability distributions. The most common use of concepts from statistics and probability theory in biological applications is to describe variability that stems from the stochastic nature of single reactions, variations between individuals, noise and variability introduced in the process of taking single or repeated measurements, etc. However, probability distributions can also be used to characterize uncertainty in a broader sense, in particular in combination with measurement data. Assigning probability distributions to entities such as parameters, state variables,

and system and measurement noise variables in dynamical models of biochemical networks, provides understanding of both the quantity itself and how precise or uncertain it is known. This approach becomes even more useful if one not only uses these prior probability distributions and studies their time evolution, but also updates them using time series experimental data to obtain so called posterior distributions. This more elaborate way of representing the system under study naturally comes with the cost of more complex computations and requires more advanced mathematics but the gain of obtaining not only single numerical values for quantities but also some measure of quality or quantified uncertainty is a tremendous advantage. To fully exploit the described methodology there is a need to abandon systems of Ordinary Differential Equations (ODEs), in favor of systems of stochastic differential equations (SDEs). These are more complex mathematical objects than ODEs since they represent not only a single solution trajectory but a family of solutions, so called realizations, whose statistical properties can be captured in terms of time varying distributions for the state variables.

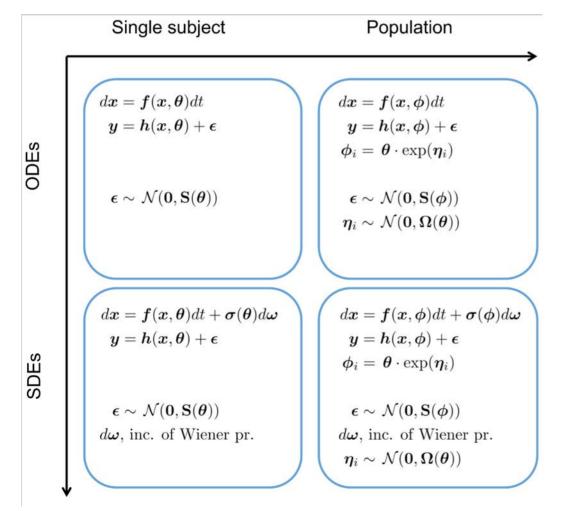
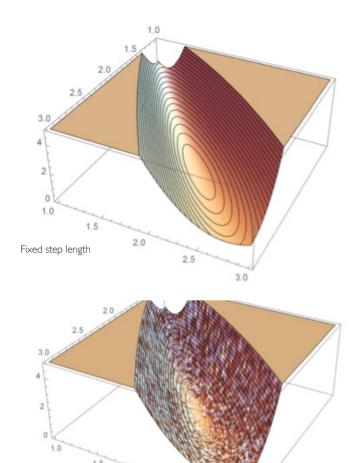


Illustration of different modeling frameworks. The approaches range from a single subject explained by a set of ordinary differential equations to a population of subjects where the underlying dynamics is described by a set of stochastic differential equations (SDE). Note that the differential equations are written on differential form, which is the standard notation for SDEs.



Adaptive methods for numerical integration cause non-smooth behavior of the negative log-likelihood (at small scales).

Fixed step length

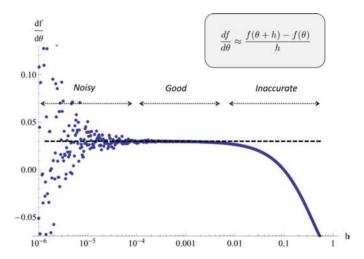
IMPROVED ESTIMATION ALGORITHMS

One of the most used methods for parameter estimation in NLME models are maximization of the approximate population likelihood function resulting from the first order conditional expectation approximation. The optimization is performed using efficient gradient-based optimization methods such as the Broyden-Fletcher-Goldfarb-Shanno (BFGS) algorithm. The gradient of the objective function needed by methods such as BFGS is typically computed by finite difference approximations. However, finite difference approximations might become an unreliable description of the gradient due to the numerical solutions of the model equations. Numerical ODE solvers using adaptive step length are known to introduce quantification errors to the objective function, making it non-smooth on small scale. Instead, to overcome such problems, the gradient can be determined by formally differentiating the objective function. To calculate the components of the likelihood gradient with respect to the parameters, one typically needs to solve the so called sensitivity equations of the parameterized differential equations. These equations are obtained by differentiating the

system equations with respect to the parameters to be estimated. Not only is the approach of using sensitivity equations more accurate, but it is also generally faster since a lot of likelihood function evaluations are avoided.

We have implemented a sensitivity-equation-based parameter estimation algorithm, which uses sensitivity equations for determining gradients for both the optimization of individual random effect parameters, and for the optimization of the fixed effect population parameters. Information provided by the sensitivity equations can also be exploited to obtain better initial values for the individual optimization of the random parameters. The algorithm is applicable to models based on ODEs as well as on SDEs. Because of its high accuracy in determining the gradients, the new algorithm shows more robustness to pre-optimum termination and to converge in situations where current industry-standard software such as NONMEM fails.

A finite difference approximation to a component of the likelihood gradient may be both noisy and inaccurate depending on the choice of perturbation scale. In worst case different perturbations may be needed for different components. Sensitivity based gradient computations can resolve the problem.



A finite difference approximation to a component of the likelihood gradient may be both noisy and inaccurate depending on the choice of perturbation scale. In worst case different perturbations may be needed for different components. Sensitivity based gradient computations can resolve the problem.

Software

The developed methods have been implemented, verified, and benchmarked in Mathematica. FCC is collecting methods and tools for advanced modeling and simulation for drug discovery and development in a software platform with the aim to provide easy access to efficient and robust methods for dynamical mixed effects modeling.

Collaborating partners: Prof. Johan Gabrielsson, Swedish University of Agricultural Sciences, Prof. Bert Peletier, Leiden University, Christine Ahlström, AstraZeneca

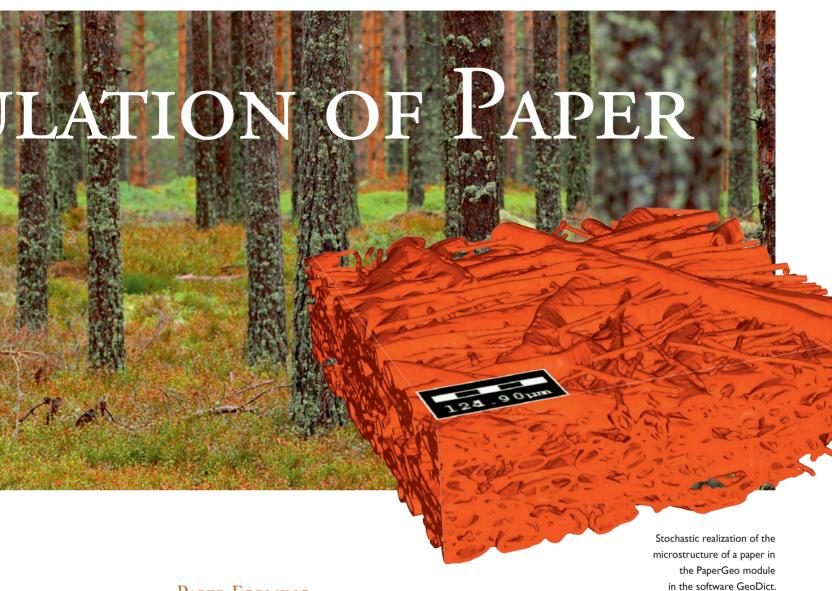


The aim of the ISOP project is to develop novel tools for simulation of papermaking and paperboard package quality that are based on microstructure models of the fiber web. The project is performed together with a consortium of companies from the Swedish paper and packaging industry.

The main innovation in the ISOP project is to perform simulations on the fiber microstructure to predict macroscopic paperboard properties with industrially relevant accuracy. Substantial progress in the fundamental understanding of the papermaking process is achieved, and is particularly important to be able to develop products with increased functionality but with less material and energy input. This is crucial for the competitiveness of renewable packaging materials in order to meet the increasing threat from fossil packaging materials such as plastics.

The main goal of the second three-year phase, 2012-2014, was to further develop and extensively validate the software such that it can contribute to a faster, cheaper and more

efficient process and product development at the companies. Our efforts focused on the simulation tools used for investigation of how the build-up of the paper in the forming section and the paperboard's resilience to edge penetration depend on pulp, chemical and forming fabric properties, and process conditions. In the long term this means that paperboard packages with better functional properties can be developed. The software is based on an object-oriented C++ framework and consists of the following tightly coupled modules: PaperGeo for virtual structure generation, IBOFlow for fluid dynamics simulation, and LastFEM for structural dynamics. The IPS platform is used for pre- and post-processing.



Paper Forming

In the paper forming section of the paper machine a fiber suspension in the form of a free jet leaves the headbox and impinges on a permeable belt called a forming fabric. The initial forming influences the properties of the fiber web and the subsequent dewatering, and depends on fiber characteristics, chemical additives, forming fabrics and other process conditions. Since the effective paper properties depend on the micro-structure a continuum model is inadequate. The fluid-structure interaction of flow and moving fibers and flocs needs to be accurately modeled in this application. The fact that the fibers are buoyant with the same density as the surrounding water makes this a very challenging problem.

Our in-house Navier-Stokes software, IBOFlow, is perfectly suited for this application. The flow around the moving fibers is resolved by the adaptive octree grid and immersed boundary methods are used to model the presence of fibers in the flow. The fibers are approximated as slender bodies represented by hollow elliptical segments. The fluid force on each fiber segment is calculated by integrating the

pressure and the viscous stress tensor around the segment surface. To be able to calculate the deformation, rotation and translation of the fibers, finite-strain beam theory, including shearing is utilized and discretized in a FEM framework. The chemical and physical interactions in the fiber suspension and with the forming fabric are modeled by DLVO theory that takes electrostatic and van der Waals forces, and Born repulsion, into account. In the simulation software, individual fibers, filler and fines are generated and visualized in the process of laying down onto the forming fabric. The buildup of surface density of paper material across the forming fabric as well as fiber orientations are computed and used as a measure for comparison with experiments. In the ongoing third three-year phase, 2015-2017, the paper forming module is further developed, and the effect of pressing and drying of the sheet structure are taken into account. The resulting sheets are validated by simulation of air permeability and mechanical properties.



MATERIALS SCIENCE

An outline of the Tetra Brik Aseptic filling machine.

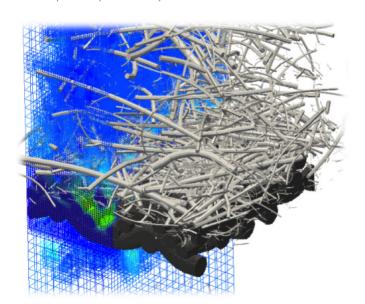
The paperboard material enters the peroxide bath localized to the top right before the tube forming and filling take place in the machine.

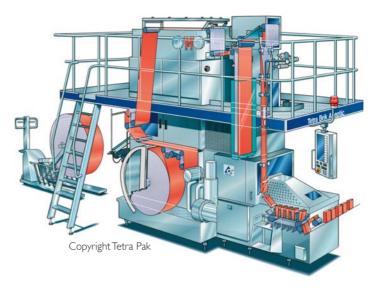
Product Quality – Edge Wicking

During startup of the Tetra Brik Aseptic (TBA) filling machine after a short stop the bath is filled with a liquid mixture of water and peroxide, and the liquid starts to penetrate the open edge of the paperboard. Only a few millimeters penetration can be allowed, otherwise a tube break might occur that destroys the aseptic environment in the filling machine. The resulting penetration depends on fiber properties, chemical additives, sheet structure and other process parameters.

To simulate the edge penetration, a multi-scale framework has been developed. The macro-scale model requires the relative permeabilities and capillary pressure curves for each ply from the micro-scale as an input. Small pieces of 3D paper microstructure are therefore generated using PaperGeo. For these microstructures a pore-morphology model generates active pore radius and saturation levels for different pressure drops. Using a model for the contact angle that depends on time, saturation and local chemical additive concentration, the capillary pressure curves can then be calculated. One-phase

A fluid-structure interaction simulation of the initial laydown of fibers on a forming fabric. The dynamic adaptive octree grid is shown and colored by the velocity (forming fabric courtesy of Albany International).



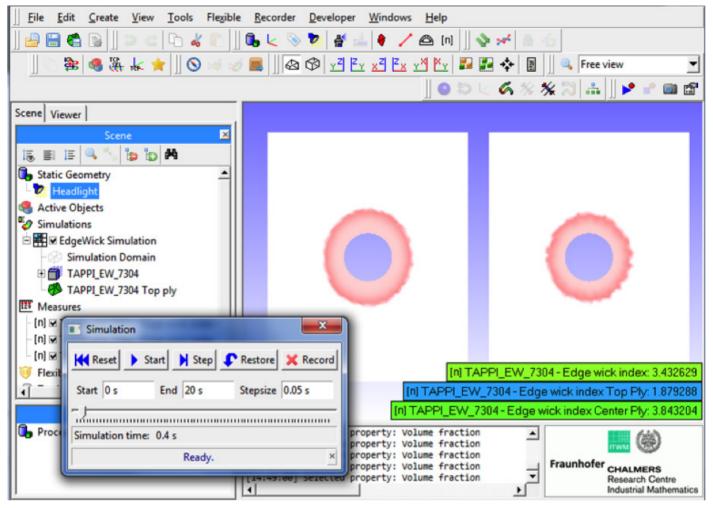


flow simulations are performed on active pores to calculate the relative permeabilities. A virtual macro board (2D distribution of surface weight and anisotropy for each ply) is then generated based on the micro properties. Two-phase porous media flow simulations on the macro board give the liquid front as a function of time in each ply. This unique multi-scale framework has been validated with stationary and transient edge wicking experiments with excellent agreement, as can be seen in the picture. These simulations have led to new insights of the process, e.g., that the diffusive meniscus must be taken into account to accurately predict the transient wicking behavior and that a random distribution of chemical additives yields a less uniform wicking.

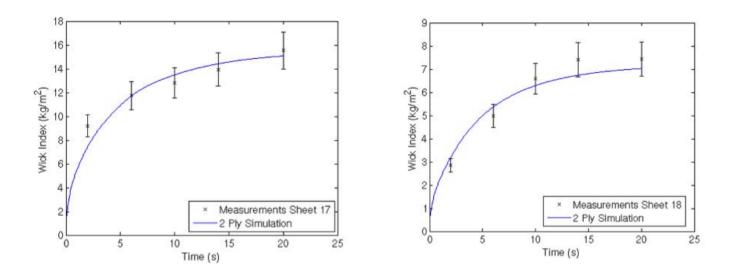
A paper machine located at the Stora Enso Kvarnsveden paper mill. The three main steps in papermaking are forming, pressing and drying. In the forming section a fiber suspension leaves the headbox and impinges on a forming fabric. Here the fiber web starts to form and the initial dewatering occurs. In the pressing section additional water is squeezed out of the web under high pressure. The remaining water is evaporated as the web runs through heated dryer rollers in the drying section.



MATERIALS SCIENCE

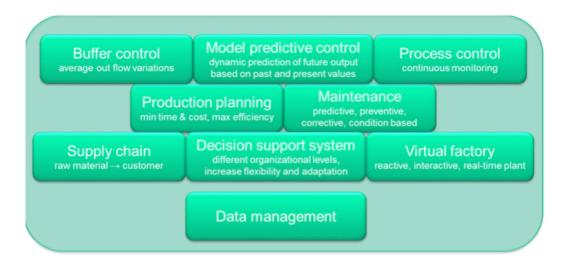


A snapshot from the software IPS ISOP Edge Wicking. The simulation shows the penetration of liquid through the hole in a paperboard.



Validation of the transient edge wicking index for a two-ply board, without chemical additives (left), including chemical additives (right). The lower levels of edge wicking in the right figure shows the effect of adding additives to prevent liquid from penetrating into the paperboard.

Continuous Production



Important areas that have been identified are, e.g., maintenance strategies, production planning and utility optimization. Modeling, simulation and optimization can successfully be used to solve such issues. MSO can be a good foundation to provide more trustworthy information enhancing the decision-making process. Besides MSO, high-quality data management and information handling are critical for decision support system to be implemented successfully.

The business area shall be a provider of high-quality decision support systems based on modeling, simulation and multiobjective optimization for continuous production systems. Such decision support tools can be used at different levels in an organization (e.g., strategic or operational), in on-line or off-line mode. The functionality can be aimed at supply chain, maintenance, or production and the main goal may vary between departments, such as route optimization, control/ monitoring or planning and process design. Besides the obvious important areas, modeling, simulation and optimization (MSO), data handling and information management are core areas for effective use of these kinds of decision support tools. The available data stored at company level in different formats have to be handled and processed in a structured way to be effectively used in MSO. The combination of MSO and data analysis will be the main focus for the business area continuous production.

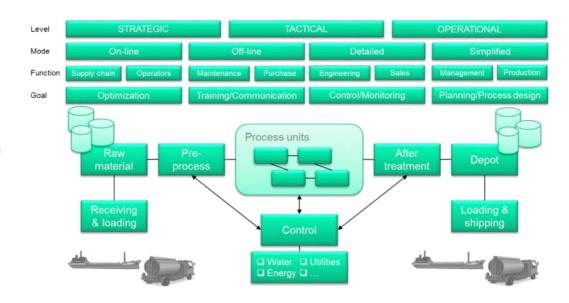
At Fraunhofer ITWM in Kaiserslautern a well-established group within MSO for continuous production is providing the German industry with decision support solutions together with the Technical University of Kaiserslautern. The business area has together with Fraunhofer ITWM initialized cooperation and the long-term goal is to have a bilateral cooperation, exchanging knowledge and competence. Chalmers has identified continuous production as a focus area for the near future, pursued by the Production area of advance with whom we cooperate closely in an effort to focus and accumulate strength by gathering separate actions within continuous production at Chalmers. A collaboration with Production area of advance and

Modeling, Simulation



CONTINUOUS PRODUCTION

To incorporate the identified areas a holistic model of the entire facility is the foremost goal. The objective of the modeling, simulation and optimization can vary on several aspects in the organization. The decision support system can be on different levels and modes, where the functionality and its goal with the tool may also be diverse.



N AND OPTIMIZATION IN



AstraZeneca has recently been initiated, with the aim to explore the opportunities and challenges going from mass production of drugs to mass-customized pharmaceuticals, personalized medicine and precision medicine.

The short-term goal is to identify companies in continuous production with the ambition to start up cooperation in the area of MSO. To quickly gain momentum the strategy is to leverage on current competences and industrial network at FCC and Fraunhofer ITWM and combine this with decision support tools for multi-objective optimization and data mining techniques. The business area will target public funding calls, while seeking industrial and academic cooperation. There are several initiatives to exploit, such as the Swedish strategic innovations program Process industrial IT and Automation (PiiA), the Swedish Foundation for Strategic Research, the Swedish energy agency, and selected topics in EU's H2020 programme. Catarina Dudas, the area leader at FCC has also been appointed as the node for the PiiA program in the western region of Sweden, to reconnoitre the area, start up a network

and be the contact person to PiiA. A mapping of the current status in the area of process industrial IT and automation in the western part of Sweden has been conducted on the behalf of PiiA. This resulted in a report written in collaboration with Chalmers Industriteknik, and a seminar together with a workshop.



Dr. Catarina Dudas
Business Area Leader
Continuous Production

GEOMETRY AND N

Many products such as car and truck bodies, engines, medical prosthesis, mobile phones, and lumbering equipment depend visually and functionally on their geometry. Since variation is inherent in all production, consistent improvements in styling, design, verification and production, aiming at less geometrical variation in assembled products, is necessary to achieve easy-to-build high-quality products. Also, the demand on short ramp up time, throughput, and equipment utilization in the manufacturing industry increases the need to effectively generate and visualize collision-free and optimized motions in the assembly plant.

During 2015, the department of Geometry and Motion Planning has successfully developed methods, algorithms and tools supporting these activities within the main subjects:

- Packing and Assembly Path Planning
- Robotics and Discrete Optimization
- Geometry Assurance and Metrology
- Massive Point Clouds, and
- Computer Graphics

In particular, the FCC software tool Industrial Path Solutions for automatic path planning of collision-free motions has been

COOPERATION

The department works in close cooperation with Wingquist Laboratory Vinn Excellence Centre for Virtual Product Realization 2007–2016 with Geometry and Motion Planning as one of its four research groups. The department has a substantial joint development with the ITWM department Mathematical Methods in Dynamics and Durability and the related two spin-off companies: Industrial Path Solutions and fleXstructures. The cooperation also includes the Industrial Research and Development Corporation and the Virtual Ergonomics Centre. The department is an active member in Chalmers' areas of advance Production and Built Environment.



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Rikard Söderberg Professor, Product and Production Development, Chalmers, Director, Wingquist Laboratory, Scientific Adviser at FCC



Robert Bohlin PhD, Deputy Head



Tobias ForsbergMSc, Marketing & Sales



Fredrik Andersson MSc



Daniel Gleeson MSc



Staffan Björkenstam



Tomas Hermansson



Niclas Delfs MSc



Jonas Kressin MSc



Fredrik Ekstedt



Peter Mårdberg



Klas Engström



Johan Nyström PhD

IOTION PLANNING

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 also part of the Master's degree program 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. The development of new algorithms, integrating line balancing, sequencing and coordination of operations with our path planning technology has been implemented at Volvo Cars and showing a 25% better equipment utilization and improvement in commission from 3 months to 3 weeks.

Today, many assembly problems are detected too late in product and production processes, involving 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 module in the IPS software. IPS is now used in Sweden, Germany, US, Korea, and Japan.



Ida-Märta Rhén PhD

Poland Poll

Roland Roll Marketing and sales



Raad Salman MSc, AEM Graduate Program



Daniel Segerdahl



Evan Shellshear PhD, Affiliated Expert



Domenico Spensieri



Sebastian Tafuri



Carl Toft MSc



 $\begin{array}{l} \textbf{Johan Torstensson} \\ \textbf{MSc} \end{array}$



Simon Vajedi MSc



Yu Yan PhD, Guest researcher



Robin Ytterlid MSc



Andreas Björklund BSc student



Pontus Eljas BSc student



Shastry Ananthram Narasimha MSc student



Jeanna Fahlin Strömberg Contracted student



Tobias Johansson Contracted student



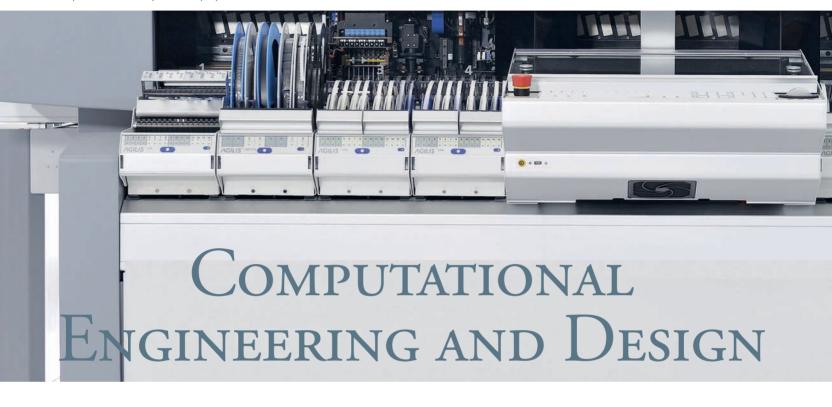
Edvin Åblad Contracted student

Cooperation

The department has a successful cooperation with the departments of Mathematical Methods in Dynamics and Durability, Optimization, and Flow and Material Simulation at Fraunhofer ITVM that has grown the past years by working on joint projects. Other strategic cooperations include Swerea IVF, Fraunhofer IPA and Chalmers divisions of Fluid Dynamics, and Nuclear Engineering. The department is an active member in Chalmers' areas of advance Production and Built Environment. The software tools are commercialized in cooperation with the spin-off company IPS IBOFlow AB.

Acknowledgement

In 2015 the department received substantial funding from Vinnova through the FFI Sustainable Production Technology and Produktion2030 programs, from the Sustainable Production Initiative and the Production Area of Advance at Chalmers, and from the Swedish Research Council (VR) for participation in a project on novel methods for safety analyses of future and existing reactors.



The rapid increase in computational power has made simulations an integrated part of the development of products and processes. Virtual prototyping stimulates industrial innovation and simulations offer an alternative to measurements, when these are too expensive or even impossible to perform. Furthermore, the risk for unforeseen costs and quality problems is reduced by offering the possibility to perform analyses and optimization in the early phases of product and process development. The department of computational engineering and design supports these activities by developing novel numerical methods, fast algorithms and engineering tools, in particular for application in the areas:

- Fluid Dynamics
- Electromagnetics
- Structural Dynamics
- Optimization

The research in fluid dynamics is focused on immersed boundary techniques and the development of methods and algorithms for multiphase flows, complex rheologies and fluid-structure interaction. The department strives to provide an innovative software that integrates state-of-the-art research on meshless techniques and offers unique possibilities for efficient simulation of complex industrial flow applications.

The IBOFlow (Immersed Boundary Octree Flow Solver) software is tailored for applications involving moving objects interacting with the flow and sets a new standard for CFD software by avoiding the cumbersome generation of body-fitted 3D volume meshes. In an ongoing collaboration with a large software house the focus is on electronics cooling applications. The capabilities of IBOFlow have been boosted in many ways. The octree grid is more flexible, the immersed boundary techniques handle heat transfer inside solid objects, the turbulence models have been improved, and fan models have been added. In another electronics project together with Mycronic AB we simulate solder jetting on a printed circuit board including multi-phase flow, complex rheologies and strong fluid-structure interaction. Furthermore, the efforts on simulation of paint and surface treatment processes in automotive paint shops have continued with successful validation campaigns and commercial releases of the spray and sealing modules in IPS. We also actively work in several research projects on laydown of glue and adhesive material, as well as on simulation of the hemming process which requires modeling of the complex fluid-structure interaction, where the glue interacts with the folded structure. Another major activity is the project on simulation of papermaking and paperboard package quality with industrial partners from Swedish paper industry that has successfully completed its second threeyear phase and started the third phase.

Fredrik Edelvik PhD, Associate Professor, Vice Director Head of Department Phone +46 31 772 42 46 fredrik.edelvik@fcc.chalmers.se

CORE COMPETENCES

Complex Rheologies Multiphysics Simulation High Performance Computing

Multiphase Flow

electronics.

efficiently simulated.

Immersed Boundary Methods

Computational Structural Mechanics Computational Electromagnetics

In electromagnetics research is performed on models, numerical methods and algorithms for multi species negative corona discharge simulations. The in-house software has for example been used for simulation of externally charged paint applicators and electrostatic precipitators. Furthermore, in the Fraunhofer project OptoScope we developed methods and tools for simulation of electro-optical modulators for ultra-fast





Andreas Mark

Tommy Andersson PhD, Deputy Head MSc



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Christoffer Cromvik PhD



Simon Ingelsten



Stefan Jakobsson PhD



Tomas Johnson PhD



Niklas Karlsson MSc



Gustav Kettil MSc, AEM Graduate Program



Samuel Lorin PhD



Pekka Röytää



Elin Solberg



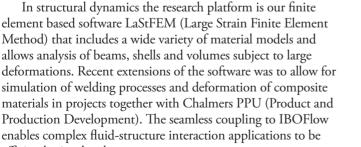
Frida Svelander MSc, AEM Graduate Program



Martin Svensson MSc



Anders Ålund



In optimization the research is focused on simulation-based optimal design and multiple criteria optimization. This includes novel optimization algorithms, coupling of simulation and optimization software and development of decision support systems that integrate multiple criteria optimization and simulation. In 2014, the spin-off company IPS IBOFlow AB was founded to focus on professional service, sales and support of the software tools developed by the department.



Cornelia Jareteg Lic. PhD Student. Chalmers PPU



Dani Irawan Contracted student



Paul Lange Contracted student



Benjamin Wettervik MSc student



Christoffer Zakrisson MSc student



Anders Logg Professor, Mathematics, Chalmers, Scientific Adviser FCC

Computational tools and techniques for systems and data analysis are key to gaining better understanding of processes and products as well as to optimize their performance. This holds true regardless of the applications being of technical or biological character since on a systems level they can be modeled and analyzed using general mathematical techniques. The department conducts research, application and development of computational methods, software tools, data analysis, and dynamical systems modeling on different levels of abstraction utilizing time and spatially resolved measurement data. In particular, within the areas:

- Estimation, Prediction, and Control
- Industrial Statistics and Machine Learning
- Systems Pharmacology and Systems Biology
- Electrophysiology and Arrhythmia

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 and systems pharmacology partly address these things and aim at elucidating the properties and function of biochemical, biological, and pharmacological processes on a systems level, e.g., how biomolecules interact and implement various functions which cannot be understood by studying the system components in isolation. Quantitative and systems harmacology combine computational and experimental methods to elucidate, validate, and apply new pharmacological concepts to the development and use of small molecule and biologic drugs. A successful systems pharmacology approach requires efficient and reliable computational methods for model based data analysis. We successfully develop and apply mathematical methods in both systems biology and systems pharmacology.

Dynamic processes play a key role in many industrial applications such as in the automotive, aerospace, pharmaceutical, and chemical process industry. Knowledge about how to build, simulate, and analyze mathematical models of such processes is crucial to be able to optimize performance, design control systems, or make highly reliable predictions about process behavior. The department provides key competence throughout the whole chain of modeling, simulation, analysis, and control of dynamical processes covering a wide range of application areas. We apply and develop tools for system identification, i.e., building mathematical models using measurement data, model based signal processing, and prediction of physical quantities from indirect measurements. Example applications include robust regression on acoustic transmission spectra for fluid property estimation with Acosense and pharmacokinetic and pharmacodynamic modeling in projects with AstraZeneca.

Recently, we successfully completed a long-term project with AstraZeneca on advanced mathematical pharmacokinetic/pharmacodynamic modeling and simulation for predictive model based drug discovery and development. The project results include improved estimations algorithms, a large model based meta-analysis of free fatty acid levels in normal and obese rats in response to nicotinic acid via

different routes and administrations, and methods and recommendations on how to incorporate and visualize uncertainty in analysis results given uncertainty in both model specification and measurements.

In industrial statistics we have carried out statistical modeling and analysis of ductility of cast iron inserts in a project commissioned by the Swedish Nuclear Fuel and Waste Management Company, SKB AB.

An important activity for the department in 2015 has been the continued long term effort together with Volvo Cars to develop technology for data processing and visualization of remotely collected automotive data. The analysis and presentation of processed data is to be used for decision support for product development of new and existing functions in the car.

Together with researchers at Mathematical Sciences at Chalmers we have been granted a 20 MSEK synergy grant from the Swedish Foundation for Strategic Research on Hierarchical Mixed Effects Modeling of Dynamical System. In this five-year project the objectives are to scale-up and increase the applicability of nonlinear mixed effects modeling to challenges in biological and biomedical applications as well as disseminate easy to use computational tools.

Mats Jirstrand PhD, Associate Professor, Head of Department Phone +46 31 7724250 mats.jirstrand@fcc.chalmers.se



Acknowledgement

In 2015, the Systems and Data Analysis department has received funding for the IMPACT project from the European Commission. We have also participated in projects funded by VINNOVA from Innovationskontor Väst (Cardiotox-Predictor, verifications grant) and the Strategic Innovation Program Process Industrial IT and Automation, PiiA (Acosense, Preventor and Acocheese). The department has received funding from the Swedish Research Council and the Swedish Foundation for Strategic Research. department also takes part in the management of Chalmers' Life Science Engineering area of advance.

COOPERATION

The department successfully cooperates with the department of System Analysis, Prognosis and Control at Fraunhofer ITWM and has close collaboration with the Swedish company InNetics. Other strategic cooperations include joint work with Systems and Synthetic Biology and Mathematical Sciences at Chalmers University of Technology; Cell- and Molecular Biology at Gothenburg University; the Systems Biology Research Centre at University of Skövde; General Zoology at Kaiserslautern University; and partners in the IMPACT EU-project. The department also takes part in the management of Chalmers' Life Science Engineering area of advance.



Joachim Almquist



Tim CardilinAEM Graduate Program



Emil Gustavsson PhD



Johan Karlsson PhD



Viktor Nilsson MSc



Mikael Wallman PhD



Robert Andersson MSc, Marie Curie, PhD student



David Janzén MSc, Marie Curie, PhD student



Magnus Gyllenhammar Contracted student



Emilio Jorge Contracted student



Ulrik Källblad Contracted student



Måns Larsson Contracted student



Helga Kristín Ólafsdóttir Contracted student



Emil Staf
Contracted student



Gregor UlmContracted student



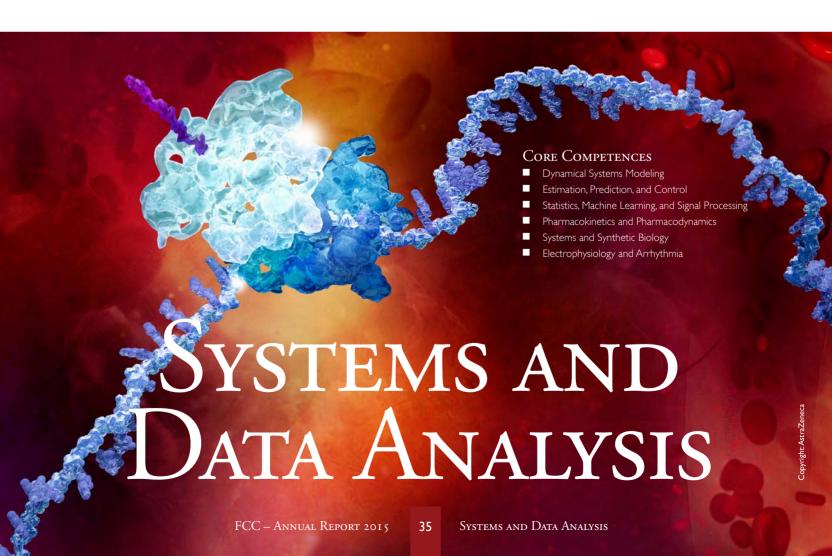
Igor RychlikProfessor, Mathematical
Statistics Chalmers,
Affiliated expert FCC



Johan Gabrielsson Professor, Pharmacology and Toxicology, SLU Affiliated expert FCC



Ingemar Jacobsson PhD Affiliated expert FCC



ÅRSREDOVISNING

Styrelse och ledning 2015



Styrelsen för Stiftelsen Fraunhofer-Chalmers centrum för industrimatematik, FCC, får härmed avge följande redovisning över verksamheten under tiden 1 januari 2015 – 31 december 2015, stiftelsens fjortonde verksamhetsår.

Stiftelsen bildades av Chalmers och Fraunhofer i juni 2001 och registrerades av Länsstyrelsen i Västra Götalands län i oktober 2001 som en svensk näringsdrivande stiftelse. Stiftelsen har till ändamål att främja och genomföra vetenskaplig forskning, utveckling och utbildning inom området tillämpad matematik i nära samarbete med universitet och andra vetenskapliga och industriella organ samt verka för användning av matematiska modeller, metoder och resultat i industriell verksamhet. Stiftelsens verksamhet skall bedrivas utan vinstsyfte.

I maj 2015 blev FCC utvärderat av en internationell kommitté som utsetts av Fraunhofer och Chalmers. Uppdraget var att bedöma den vetenskapliga och ekonomiska utvecklingen och framtida strategi för centret. Utvärderingen kom fram till att centret sedan starten 2001 har utvecklats till en utmärkt forskningsinstitution och att alla mål har uppnåtts eller överträffats.

Chalmers och Fraunhofer har under året finansierat Stiftelsen med 10 208 kSEK.

Årets omsättning har varit 44 MSEK. Antalet anställda och studenter har motsvarat 47 heltidsekvivalenter (FTE) varav 6 kvinnor. Antalet studenter utgörs av 6 (3 FTE) examensarbetare, 13 (1 FTE) studenter anställda på 10-20% för arbete i projekt, totalt 4 FTE. Härutöver har arbete motsvarande cirka 4 FTE lagts ut på partners.

Rörelsens intäkter har uppgått till 44 024 kSEK (41 957 kSEK föregående år). Av detta utgör 44% (41%) industriprojekt, 23% (22%) offentliga anslag, 10% (15%) offentliga projekt och 23% (22%) finansiering från stiftarna. Årets resultat efter skatt är 237 kSEK (1 262 kSEK). Eget kapital uppgick den 31 december 2015 till 7 646 kSEK (7 288 kSEK) inkluderat kapitalandelen i obeskattade reserver.

Stiftelsens styrelse har under verksamhetsåret sammanträtt en gång. Ersättning har utgått till ordföranden med 37 500 kronor och till övriga ledamöter med 18 750 kronor per person och år.

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

Göteborg den 16 mars 2015

Rikard Söderberg, ordförande Dieter Prätzel-Wolters, vice ordförande Frank Treppe Bernt Wennberg

Räkenskaperna har granskats av Auktoriserad revisor Gunnar Andersson

Resultaträkning

150101 - 151231, (kSEK)

Intäkter	
Nettoomsättning	44 024
Summa intäkter	44 024
Kostnader	
Externa kostnader	9 976
Personalkostnader	
Avskrivningar av materiella anläggningstillgångar	
Summa kostnader	43 377
Rörelseresultat	647
Tool clock could be a second c	
Resultat från finansiella investeringar	
Ränteintäkter och liknande resultatposter	2
Räntekostnader och liknande resultatposter	
·	
Resultat efter finansiella poster	583
Bokslutsdispositioner	
Årets skatt	191
Årets resultat	237
Arets resultat	237
Balansräkning	
151231, (kSEK)	
Anläggningstillgångar	
Maskiner och inventarier	
Maskiner och inventarier	
Maskiner och inventarier Summa anläggningstillgångar Omsättningstillgångar	412
Maskiner och inventarier	8 998
Maskiner och inventarier	8 998 7 591
Maskiner och inventarier	8 998 7 591 361
Maskiner och inventarier	8 998 7 591 361 3 081
Maskiner och inventarier	8 998 7 591 361 3 081
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Maskiner och inventarier	8 998 7 591 361 3 081
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Maskiner och inventarier	
Maskiner och inventarier Summa anläggningstillgångar Omsättningstillgångar Kundfordringar Förutbetalda kostnader och upplupna intäkter Övriga kortfristiga fordringar Kassa och bank Summa omsättningstillgångar Summa tillgångar Eget kapital Eget kapital Eget kapital vid årets ingång Årets resultat Summa eget kapital Obeskattade reserver Kortfristiga skulder Leverantörsskulder Övriga kortfristiga skulder	
Maskiner och inventarier	
Maskiner och inventarier	
Maskiner och inventarier	

Summa skulder och eget kapital.....

APPENDIX

Journals

| Almquist, | Leander, M | Irstrand:

Using sensitivity equations for computing gradients of the FOCE and FOCEI approximations to the population likelihood, Journal of Pharmacokinetics and Pharmacodynamics, 42:3, p. 191-209, February 23, 2015.

J Almquist, L Bendrioua, C Beck Adiels, M Goksör, S Hohmann, M Jirstrand:

A Nonlinear Mixed Effects Approach for Modeling the Cell-To-Cell Variability of Mig1 Dynamics in Yeast, PLOS ONE, April 20, 2015.

T Johnson, A Mark, J Nyström, S Rief, M Fredlund, M Rentzhog, U Nyman, J Tryding, R Lai, L Martinsson, K Wester, F Edelvik:

A multi-scale simulation method for the prediction of edge wicking in multi-ply paperboard, Nordic Pulp & Paper Research Journal, 30(4), p. 640-650, September 3, 2015.

D Gaidashev, T Johnson, M Martens:

Rigidity for infinitely renormalizable area-preserving maps, Duke Mathematical Journal, Volume 165, Number 1 (2016), p. 129-159, November 11, 2015.

T Johnson, S Jakobsson, B Wettervik, B Andersson, A Mark, F Edelvik:

A finite volume method for electrostatic three species negative corona discharge simulations with application to externally charged powder bells, Journal of Electrostatics, 74, p. 27–36, January 6, 2015.

R Reif, J Karlsson, G Günther, L Beattie, D Wrangborg, S Hammad, B Begher-Tibbe, A Vartak, S Melega, P M Kaye, J G Hengstler, M Jirstrand:

Bile canalicular dynamics in hepatocyte sandwich cultures, Archives of Toxicology, Journal no. 204, August 18, 2015.

J Karlsson, K Podgórski, I Rychlik:

The Laplace multi-axial response model for fatigue analysis, International Journal of Fatigue, In Press, December 2015.

J Leander, J Almquist, C Ahlström, J Gabrielsson, M Jirstrand:

Mixed Effects Modeling Using Stochastic Differential Equations: Illustrated by Pharmacokinetic Data of Nicotinic Acid in Obese Zucker Rats, The AAPS Journal, Volume 17, Issue 3, pp 586-596, May 2015.

S Lorin, C Cromvik, F Edelvik, R Söderberg:

Welding Simulation of Non-Nominal Structures With Clamps, Journal of Computing and Information Science in Engineering, 15(2), April 8, 2015.

B Lindau, S Lorin, L Lindkvist, R Söderberg:

Efficient Contact Modeling in Non-Rigid Variation Simulation, Efficient Contact Modeling in Non-Rigid Variation Simulation. ASME. Journal of Computing and Information Science in Engineering, November 26, 2015.

M Polikarpova, P Ponomarev, P Röyttä, R S Semken, Y Alexandrova, J Pyrhönen:

Direct Liquid Cooling for an Outer-Rotor Direct-Drive Permanent-Magnet Synchronous Generator for Wind Farm Applications, IET Electric Power Applications, Volume 9, Issue 8, p. 523 – 532, September 2015.

D Spensieri, J S Carlson, F Ekstedt, R Bohlin:

An Iterative Approach for Collision Free Routing and Scheduling in Multirobot Stations, IEEE Transactions on Automation Science and Engineering, pp (99), 1-13, June 1, 2015.

B Wettervik, T Johnson, S Jakobsson, A Mark, F Edelvik:

A domain decomposition method for three species modeling of multi-electrode negative corona discharge – With applications to electrostatic precipitators, Journal of Electrostatics, 77, p. 139-146, August 28, 2015.

R Ytterlid, E Shellshear:

BVH Split Strategies for Fast Distance Queries, Journal of Computer Graphics Techniques (JCGT), vol. 4, no. 1, p. 1-25, January 27, 2015.

Conference Proceedings

| Almquist, | Leander, M | irstrand:

Sensitivity Equations Provide More Robust Gradients and Faster Computation of the FOCE Approximation to the Population Likelihood, Proceedings of the 24th Annual meeting of the Population Approach Group in Europe, Crete, Greece, June 2-5, 2015.

S Björkenstam, J S Carlson, B Lennartson:

Exploiting sparsity in the discrete mechanics and optimal control method with application to human motion planning, Automation Science and Engineering (CASE), 2015 IEEE International Conference, 769 – 774, August 24-28, 2015.

T Cardilin, A Sostelly, J Gabrielsson, S El Bawab, C Amendt, M Jirstrand:

Modeling and Analysis of Tumor Growth Inhibition for Combination Therapy using Tumor Static Concentration Curves, Proceedings of the 24th Annual meeting of the Population Approach Group in Europe, Crete, Greece, June 2-5, 2015.

D Gleeson, S Björkenstam, R Bohlin, J S Carlson, B Lennartson:

Optimizing robot trajectories for automatic robot code generation, Automation Science and Engineering (CASE), 2015 IEEE International Conference, 495 – 500, August 24-28, 2015.

D Janzén, M Jirstrand, M J Chappell, N D Evans:

Two approaches to study structural identifiability analysis in mixed-effects models, Proceedings of Pharmacokinetics UK (PKUK) 2015, Chester, UK, November 2015.

D Janzén, M Jirstrand, N D Evans, M Chappell:

Structural Identifiability in Mixed-Effects Models:Two different approaches, In proceedings of the 9th IFAC Symposium on Biological and Medical Systems, Berlin, Germany, August 2015.

R Andersson, M Jirstrand, L Peletier, M J Chappell, N D Evans, J Gabrielsson:

Dose-response-time modelling: Second generation turnover model with integral feedback control, Proceedings of the 24th Annual meeting of the Population Approach Group in Europe, Crete, Greece, June 2-5, 2015.

G Kettil, A Mark, F Svelander, R Lai, K Wester, M Fredlund, M Rentzhog, F Edelvik:

Detailed Simulations of Early Paper Forming, COST FP1005 Fibre Suspension Flow Modelling Final Conference Trondheim 2015, June 9-11, 2015.

G Kettil, A Mark, F Svelander, R Lai, L Martinsson, K Wester, M Fredlund, M Rentzhog, U Nyman, J Tryding, F Edelvik:

Novel Contact Forces for Immersed Boundary, Paper Forming Simulations PF2 - The Past, Present and Future of CFD Papermaking; PaperCon 2015 Atlanta (Online proceeding), April 19-22, 2015.

E Shellshear, J S Carlson, R Bohlin, S Tafuri:

A multi-threaded memetic packing algorithm for the ISO luggage packing problem, Automation Science and Engineering (CASE), 2015 IEEE International Conference, 1509 – 1514, August 24-28, 2015.

E Shellshear, R Ytterlid:

Fast Distance Queries for Triangles, Lines, and Points using SSE Instructions, Proceedings of the 19th meeting of the ACM SIGGRAPH Symposium on Interactive 3D Graphics and Games, 2015.

M Wallman, F Sandberg:

Characterization of AV-nodal Properties during Atrial Fibrillation using a Multilevel Modelling Approach, Proceedings of Computing in Cardiology Conference (CinC) 2015, Nice, France, September 7-9, 2015.

THESES

A Björklund, P Eljas:

Flexible surface of air bellow simulated in IPS, Bachelor thesis, Chalmers University of Technology, supervisor J Nyström, September 2015.

C Jareteg:

Variation Simulation Customized for Composites by Including FEM Simulations of Orthotropic Lamina, Licentiate thesis, Chalmers University of Technology and University of Gothenburg, supervisors S Larsson and F Edelvik, June 2015.

R Salman:

Algorithms for the Precedence Constrained Generalized Travelling Salesperson Problem, Master thesis, Chalmers University of Technology, supervisor F Ekstedt, August 27, 2015

E Solberg:

Simulation of Electro-Optic Modulators by a Time-Domain Beam-Propagation Method, Licentiate thesis, Chalmers University of Technology and University of Gothenburg, supervisors S Larsson and F Edelvik, April 2015.

B Svedung Wettervik:

Three-species negative corona discharge simulations using domain decomposition, Master thesis, Chalmers University of Technology, supervisor T Johnson, May 2015.

Courses

R Bohlin:

Path Planning Software, Advanced Simulation and Optimization. Guest lecture in Robotics and Manufacturing Automation, Department of Product and Production Development, Chalmers, April 2015.

F Edelvik:

Optimization of sealing stations by material laydown simulations and automatic path planning, invited speaker, European Automotive Coating workshop, Nürtingen, June 2015.

S Lorin:

Reverse Engineering and Redesign Methodology, Project Supervision and Course Administration, Undergraduate Program, Chalmers University of Technology, November-December 2015.

D Gleeson:

Teaching Assistant, Control Theory, Automation and Mechatronics Program, Chalmers University of Technology, August-October 2015.

OTHER ASSIGNMENTS

R Bohlin:

Member of grading committee at Sahar Mohajerani's PhD defence of the thesis On Compositional Approaches for Discrete Event Systems Verification and Synthesis. Department of Signals and Systems, Chalmers, February 2015.

J S Carlson:

Member of the Wingquist Laboratory Board. Reviewer for CIRP CAT & CATS 2016. Reviewer of book chapter for "Math for the Digital Factory".

F Edelvik:

Reviewer for CIRP CAT 2016. Reviewer of book chapter for "Math for the Digital Factory".

C Dudas

Organizing the Initiative Seminar on Modeling, Simulation and Optimization in Continuous Production, Chalmers University of Technology, Göteborg, February 2015.

Member of the program committee for Swedish Study Group "Mathematics in Industry", spring 2015.

Team leader for the Scania case study at the workshop Swedish Study Group "Mathematics in Industry", Institut Mittag-Leffler, Stockholm, August 2015.

M Jirstrand:

Member of Chalmers Area of Advance Life Science Management Group.

Member of Steering group for the Gothenburg Centre for Systems Biology.

FCC Representative in Vehicle ICT Arena. Reviewer for Mathematical Biosciences. Reviewer for PLoS Computational Biology.

T Johnson:

Reviewer for Topological Methods in Nonlinear Analysis. Reviewer for International Journal of Bifurcation and Chaos.

| Karlsson:

Team member for the Scania case study at the workshop Swedish Study Group "Mathematics in Industry", Institut Mittag-Leffler, Stockholm, August 2015.

Press

www.chalmers.se 2015-03-03



effektiviseras



www.techviz.net



www.chalmers.se 2015-05-21



Frida Svelander was awarded best lecturer on Bachelor's level.

GP ekonomi – Advertisement 2015-09-07



Wingquist Laboratory Annual Seminar 2015-12-01



Process Nordic April 2015



www.konstruktionspraxis.vogel.se 2015-04-20



embree.github.io



hexagonmetrology.us



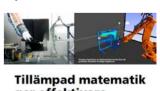
Hexagon Automation Forum, Wetzlar 2015-09-30



FCC Paper on the Cover of Nordic Pulp and Paper Research Journal 2015-12-01



Ytforum, May 2015



ger effektivare lackeringsprocesser

41

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 and undertake scientific research, development, and education in the field of applied mathematics, in close cooperation with universities and other scientific and industrial agencies, and promote the use of mathematical models, methods, and results in industrial activities.

The Centre, in close cooperation with Chalmers in Gothenburg 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.

Our vision is "Mathematics as Technology".







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