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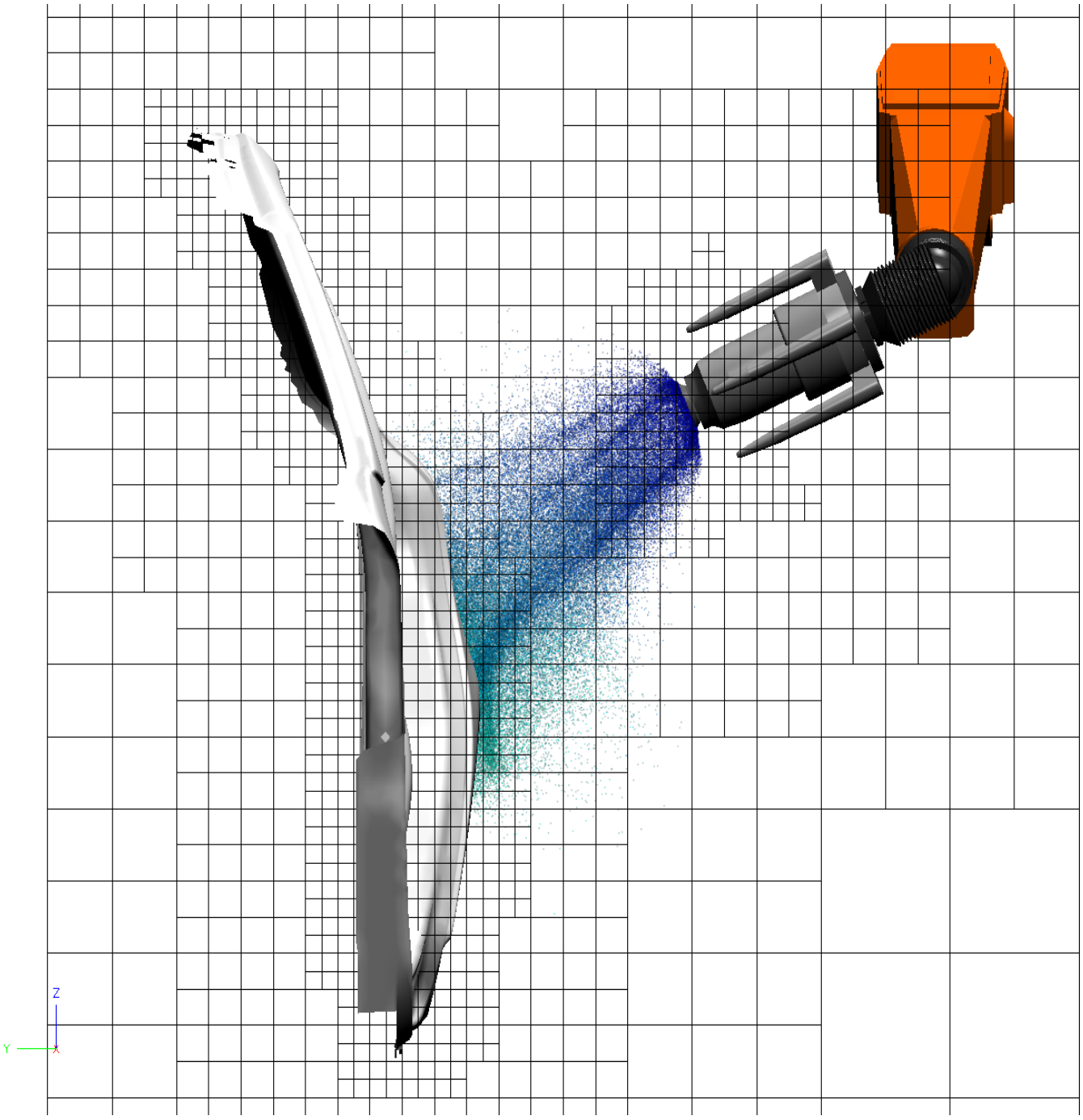
FORWARD LOOK

Mathematics and Industry
Success Stories - DRAFT



European Mathematical Society

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Foreword

This brochure shows via several success stories the crucial contribution of mathematics to the industrial creation of value and the key position of mathematics in the handling of complex systems, amplifying innovation.

Each story describes the challenge that led to the industrial cooperation, how the challenge was approached and how the solutions were achieved and implemented, and when brought together, they illustrate the versatile European landscape of projects in almost all areas of applied mathematics and across all business sectors.

> "In view of concrete economic and social challenges, Mathematics plays a central role. Mathematics enables innovations in the industrial and service sectors that lead to more jobs and an increasing competitiveness."
>
> Dr. Annette Schavan
> German Federal Minister
> of Education and Research

Today models are used everywhere to describe real world processes in the language of mathematics. The art of modelling is to focus on the important relationships to make the model as useful as possible to the user, and modelling therefore needs support from domain specialists. Indeed, close collaboration between industry experts and academia is both highly valued by all parties and highly valuable to successful projects.

The next step after creating the mathematical model is the analysis or numerical simulation, to validate the model in comparison with experimental data and to investigate the robustness and sensitivity of the model. Once a mathematical model has been validated, then this model can be used to improve, optimize or control the process described. Model based control and optimization is a crucial element of automation in all areas of industry, often reducing the cost and time of product, process and service development and innovation.

All of this is unthinkable without the existence of modern computers and information technology. However, the progress in computer technology is not alone sufficient for the future development of high technology innovation. Many of the success also rely to a large extent on the progress in the development of mathematical algorithms and tools.

Although this brochure only describes a snapshot of all the European activities in industrial mathematics, it demonstrates that the level of cooperation between academia and industry is not equally well established throughout Europe and that there exists great opportunity for more industrial challenges to be addressed with the powerful ideas and tools at the disposal of mathematicians. The impact achieved in industrial mathematics is through a wide variety of timescales and engagement mechanisms, from PhD studentships and post-doctoral research contracts to shorter-term Internships, Study Groups and consultancy contracts.

Automotive industry

Virtual Paint Shop

Executive summary

In 2006 Volvo Car Corporation initiated together with the Swedish automotive industry and Vinnova a research project on developing software for simulation of processes in automotive paint shops. The software development was done by the Fraunhofer-Chalmers Research Centre for Industrial Mathematics (FCC) and the first version of the virtual spray painting tool was released in 2009.

Challenge overview

Due to the complexity of the problem there is a lack of useful commercial software for simulation of spray painting. The current situation in the automotive industry is to rely on individuals' experience and physical validation for improving their processes.

In 2006 Volvo Car Corporation contacted FCC to discuss the possibilities of developing simulation software for spray painting in automotive paint shops. An investigation including a literature survey and initial attempts of performing simulations were made. After this pre-study it was decided necessary to proceed with a larger research project involving the major companies in the Swedish automotive industry.

Implementation of the initiative

The project is part of the MERA (Manufacturing Engineering Research Area) and FFI (Fordonsstrategisk forskning och innovation) programs that support the Swedish automotive industry and runs 2006-2012. A project group consisting of devoted researchers and engineers from all parties has been formed. The researchers at FCC are responsible for the development of new novel algorithms and the software in the project, whereas the industrial representatives are application experts and responsible for providing measurements for validation.

The problem

For the simulations a solver called IBOFlow, based on algorithms for coupled simulations of multiphase and free surface flows, electromagnetic fields, and particle tracing, was developed. In IPS Virtual Paint, the solver is included in the in-house package for robotic path planning, IPS. A major improvement of computational speed is realized through the use of grid-free methods which in addition simplifies pre-processing.

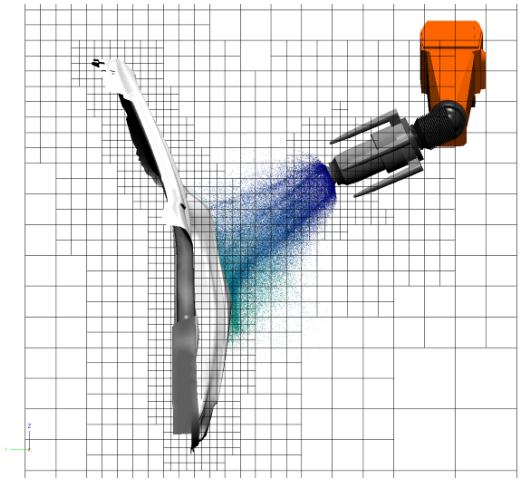

Figure 1: Painting a car side using IPS Virtual Paint.

Results and achievements

The first software version was released in 2009 and is currently used at the participating companies. The project leader at Volvo Cars predicts that positive effects will include a reduced time required for introduction of new car models, a reduced environmental impact and increased product quality.

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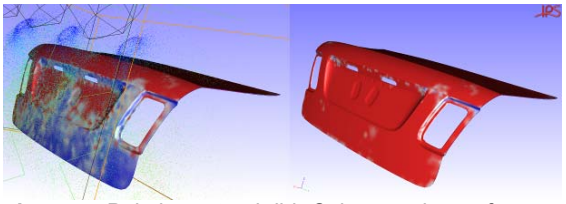


Figure 2: Painting a trunk lid. Colors on the surface show the film thickness with blue being un-painted and red a film thickness of at least 100 µm after 3 s (left) and 6 s (right). (Geometry courtesy of Saab Automobile).

CHALMERS

ITWM

Fraunhofer Institut Techno- und Wirtschaftsmathematik

Modeling and simulating the flow generated by new automotive injectors

Executive summary

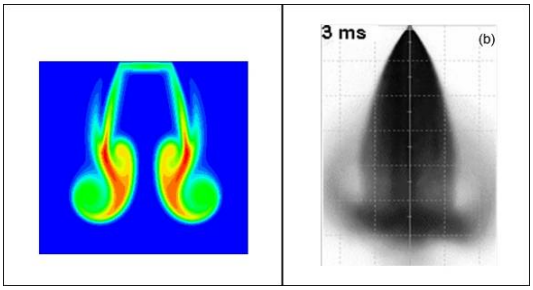
This collaboration contributed to a better fundamental understanding of physical and numerical issues appearing in the study and design of modern injectors that are currently developed to reduce fuel consumption and CO_2 emissions of automobile engines.

Challenge overview

High-pressure direct injection of the fuel in the combustion chamber is nowadays used to respond to the severe European standards for the environmental compatibility of automotive engines. The opportunity to discuss with researchers from the French Institute of Petroleum (IFP) and automotive manufacturers (Siemens Automotive, Peugeot) about these topics was offered by supervising a Master training period at IFP and participating at several industrial congresses. It appeared that new physics was involved and the industrial numerical codes had difficulties in capturing it. In particular, it was pointed out the need of a precise theoretical and numerical description of the large scale vortex structures generated at the tip of the injection flow slug (see figure). After several discussions, the industrial partners were finally convinced to state the problem on a more fundamental basis: use mathematical vortex models to characterize these structures and academic precise numerical codes to simulate the flow. Since it was the first time that an applied mathematics laboratory was involved in this research area, a precise requirement from the industrial partners was to ensure the transfer of the academic knowledge into the industrial framework. The challenge was then to study also the behaviour of main industrial codes and run them on the same test cases as the academic numerical codes. This implied a total immersion into the industrial numerical environment.

Implementation of the initiative

The first collaboration on this topic was established with the IFP, the Division of Energy and Application Techniques, and took the form of an 18 months research contract. Since the industrial aspects of this collaboration were vital to assess, an important part of the work was undertaken in company's offices because of the confidentiality of the industrial numerical tools implied. The second contract on the same topic was concluded with Siemens Automotive (now Continental Automotive France) for a 9 months period. This time, the (small) financial support was entirely devoted to fundamental research and allowed the publication of two papers in first rank journals.



Examples of vortex structures generated during the fuel injection. Numerical simulation of the gas-gas injection using an academic code (left) and experimental visualization of a Diesel injection (courtesy of IFP).

The problem

Vortex rings models are based on an elliptic partial differential equation. The difficulty comes from the fact that the boundary of the definition domain is also an unknown of the problem. Vortex models were obtained numerically and then validated by performing numerical simulations using a full Navier-Stokes academic solver.

Results and achievements

A numerical tool for computing vortex models was developed. The academic Navier-Stokes numerical code was adapted for the simulation of the flow generated by a gas-gas injection. An important effort was devoted to derive, from the obtained theoretical models and numerical data, quantities relevant for the engineer. Diagnosis based on this fundamental study were then used to assess for the performances of industrial codes in simulating the injection systems. The continuation of this theoretical and numerical fundamental study is now part of a three-year national program on the direct gasoline injection systems. We are the only applied mathematics laboratory involved in this huge program coordinated by Continental Automotive and implying several academic and industrial partners.

Lessons learned and replicability

Cooperations with industrial partners require supplementary efforts. Otherwise, it is difficult to maintain the balance between fundamental and industrial research.

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Designing oil filters for automotive industry

Executive summary

The development of process specific models, algorithms and software allow for virtual design and for significant improvement in the performance of the designed filters, by providing engineers with detailed information about flow and particles capturing details within a filter element

Challenge overview

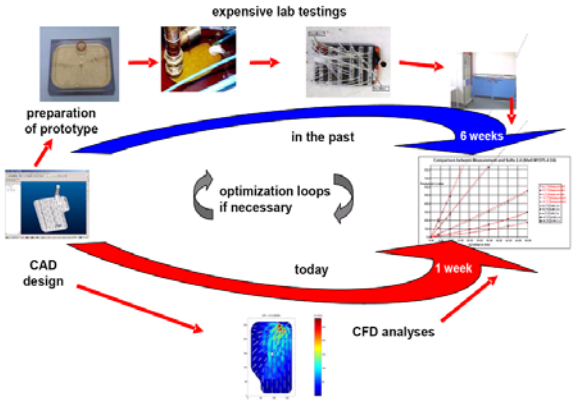
Some results we had obtained were demonstrated at a filtration exhibition, where a contact to IBS Filtran, a SME manufacturing transmission oil filters for automotive industry, was established. At that time IBS Filtran was searching for proper software tool for simulation of flows through filters. They have been already in contact with different academic groups and commercial software tools developers. However, those tools were not giving satisfactory results, especially at cold regimes, and Filtran engineers wanted to obtain a software tool reliable in all regimes. They started trying to find a solution adapting commercial software tools, before realizing that investing in specialized software could be a significant investment even for a SME, in terms of the return it can give.

Implementation of the initiative

Starting point for us was the analysis of the existing models and algorithms. We recognised that a bottleneck for our application is the explicit treatment of the term governing the flow in the porous (filtering) medium. An algorithm with implicit treatment of this term was developed, and the tests showed excellent performance. Additionally, special care was taken for proper treatment of the discontinuity of the PDE coefficients on the plain/porous interface, what allowed obtaining the desired by the company accuracy. The work on the project, especially the validation, was done in close collaboration with Filtran engineers.

Results and achievements

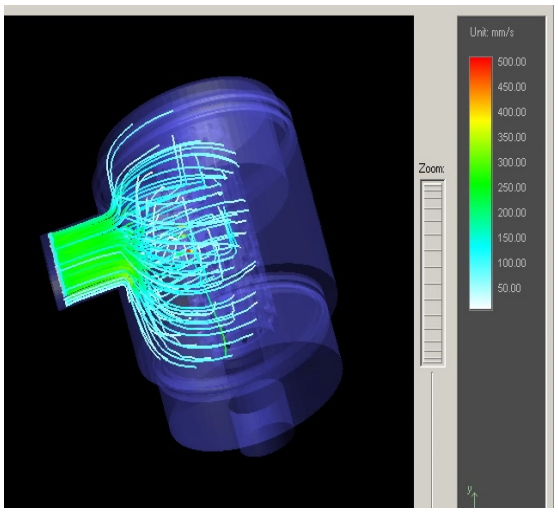
After the first project, several new challenges were posed by IBS Filtran. Sub-grid resolution approach was developed to account for complicated geometries, in particular for perforated filter media. The computer simulations allowed for design of new type of filters and resulted in patent application. Proper algorithms for coupled flow and particles transport were developed, and equipped with parameter identification procedure. These, and most of the other developments, contained essential research component. Two PhD theses were successfully defended in this area, and about ten papers were published in scientific journals and conference proceedings.



Sketch of the design process (courtesy IBS Filtran)

Lessons learned and replicability

For eight years the company invested several hundred thousands of Euro, current contract lasts till 2012. According to the company, the design time is now reduced six times (see Fig.1), and the performance of the designed filters is significantly improved. Several designs went to production line without manufacturing a prototype, relying on simulation results only. The company's philosophy is that the highly competitive market requires new innovative solutions, and they are confident that the industrial mathematics will further support them in finding such solutions



Simulation of flow trough a pleated filter

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Fraunhofer ITWM

Speeding Up Simulation for Automotive Industries

Executive summary

The numerical simulation of parts of car engines may be quite time consuming. For running hardware-in-the-loop systems, computation times must be reduced by a factor 100.

Challenge overview

AVL List, Graz, is the world's largest privately owned and independent company for the development of power-train systems with internal combustion engines as well as instrumentation and test systems. AVL is a partner in the Industrial Mathematics Competence Center (IMCC), which was established in 2002 and which is co-financed between industry and the public. By connecting automotive hardware and simulation software in a test-bed environment, the requirements on computational time get extremely high, as every engine cycle should be replicated by numerical simulation of the parts under consideration within real-time. The idea how to achieve this is to introduce surrogate models in the form of support vector machines.

Implementation of the initiative

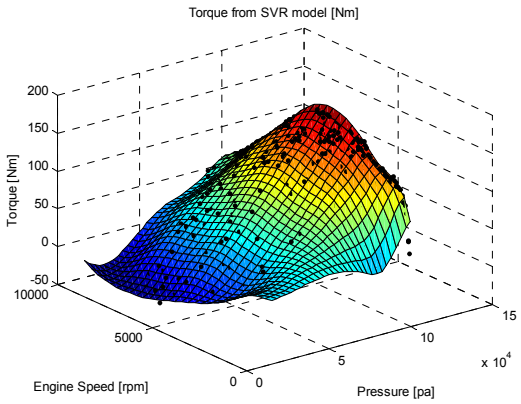
The joint research team consisted of experts in mechanical and automotive engineering and in numerical mathematics.

The problem

For the various components of a car engine, the power-train and the virtual driver system, sophisticated software tools are available to study, e.g. fuel consumption, exhaust gas after treatment or optimal gearing. If a hardware-in-the-loop-system is used, some components are realized in hardware and some of them as simulation programs to study, e.g. various designs of hybrid engines. In such a combined test-bed environment, it is essential that the simulation software runs at least as fast as the hardware meaning that every millisecond of real time must be simulated in not more than a millisecond.

Results and achievements

The approach which was realised in the project was based on surrogate models, here in the form of so-called support vector machines. These surrogate models aim to evaluate a function which is easily to calculate instead of solving numerically a partial differential equation. They require a training phase during which the shape of the ansatz function and its parameters are determined. After this training phase, which can be carried out offline, the surrogate model may achieve speed-ups of a factor 1000 and more compared to the full numerical simulation. From the academic point of view, such collaborations allow for industry-driven PhD theses, as the mathematical theory for obtaining accurate and robust training schemes is quit challenging, and to prepare young scientist for industrial problem solving. Other projects in the field of automotive simulation carried out between the project partners, were in the fields of vibration analysis or the simulation of combustion.



Torque measurements (black dots) and surface obtained from the surrogate model using a support vector machine (SVM).

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IMCC

Acoustic car design

Executive summary

In cooperation with SFE GmbH Berlin, a new solver for large scale parametric linear systems and nonlinear eigenvalue problems arising in acoustic field computations for car interiors was developed and implemented.

Challenge overview

The company SFE GmbH – Gesellschaft für Strukturanalyse in Forschung und Entwicklung mbH specialize in software developments in structural mechanics and acoustics. Their customers include many major car manufacturers. The collaboration exists since 2003, where a difficult problem in the solution of palindromic nonlinear eigenvalue problems was solved in the context of an internship and a diploma thesis. This problem with major applications in the design of high speed railtracks initiated a new mathematical theory in the treatment of structured nonlinear eigenvalue problems. Because of this successful cooperation SFE GmbH initiated the collaboration in acoustic car design and contacted the researchers of MATHEON for support in the development of further algorithmic technology.

Implementation of the initiative

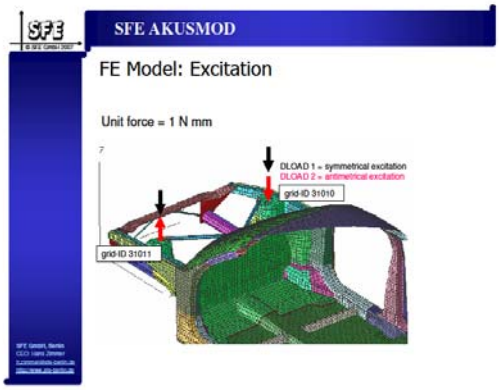
The initiative was carried out by a research and development contract. The staff came from the research group including research students which were all paid by the company. The industrial partner gave support with the modeling and implementation environment, and helped by testing the algorithms and the implemented software with real data. Difficulties arose from industrial time constraints but also due to the fact that the current research in nonlinear eigenvalue methods was insufficient in the efficient solution of the problems. So new research on algorithms for large scale parametric eigenvalue problems and linear systems was necessary.

The problem

The mathematical problems are nonlinear eigenvalue problems f(a,z)x=0 and multi righthand side linear systems M(a)Y=B with parameter vectors a, describing the material, geometry and topology properties of the car, and desired eigenvalues z, eigenvectors x and frequency responses Y. Problems sizes of several millions arise from detailed finite element modelling of the car and the air within the car, and present challenges for all currently solution techniques, in particular since the problems have to be solved for varying parameters within an optimization loop.

Results and achievements

The cooperation revealed the great need for new algorithmic developments for large scale nonlinear parametric eigenvalue problems and frequency response systems as well as new adaptive discretisation methods for the underlying systems of partial differential equations (pde). Therefore MATHEON started basic research projects about adaptive solutions of parametric pde eigenvalue problems and also for the development of new recycling techniques for frequency response systems.



Lessons learned and replicability

Many of the results from this project but also from the newly initiated research projects will be useful in other context of modeling, simulation and optimization of complex systems.

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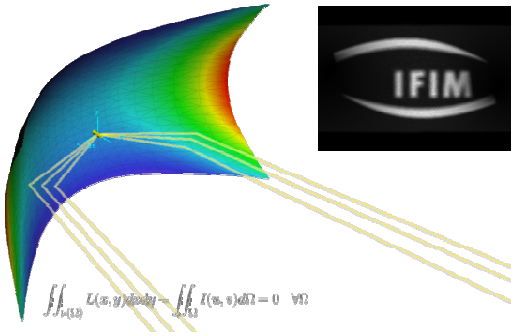
Computation of optical free-form surfaces

Executive summary

Modern automotive lighting devices make use of optical free-form surfaces (reflectors, lenses) to realise the complex light distributions needed for the different lighting functions. Within this project new mathematical techniques for the computation of such optical free-form surfaces for innovative lighting functions were developed.



Challenge overview

For the computer aided design of standard automotive lighting devices like headlamps or brake lights, the German automotive supplier Hella KGaA Hueck & Co. has well established software tools to compute the necessary optical free-form surfaces.

Due to increasing requirements e.g. from legal regulations or new design concepts of car manufacturers, these methods are pushed to their limits. In particular, for new and innovative lighting functions the existing methods often fail.

Implementation of the initiative

An initial research project was financed by the L-LAB, a Public Private Partnership between the University of Paderborn and the Hella KGaA Hueck & Co. The successful execution of this research project led to a series of specific research contracts between Hella KGaA Hueck & Co. and IFIM.

To integrate and test the newly developed mathematical methods with the existing tools, an IFIM staff member worked within Hella's software development team. Furthermore, the research was accompanied by student projects within practical courses at the University of Paderborn. A diploma thesis co-supervised by Prof. Dr. Dellnitz and the head of the above-mentioned software development group of Hella is currently in progress.

The Problem

Each point of an optical surface has an exactly defined function: to collect light, concentrate, direct and distribute it. Thus, the exact shape of the surface determines the resulting light distribution. The established method to determine the required shape of such a free-form surface for a given light distribution is based on an appropriate optimisation problem. This approach works well for standard lighting functions but for lighting functions with complex light distributions it often fails or leads to surfaces with undesired properties.

Results and achievements

A new approach for the computation of optical free-form surfaces for a prescribed light distribution based on the solution of an associated nonlinear partial differential equation was taken. A numerical algorithm for its solution was developed that has successfully been integrated into and tested with the Hella in-house software. Future developments will improve the applicability of the new method to a broader class of use cases.

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Manufacturing

Modeling the instabilities in aluminum reduction cells

Executive summary

The modeling and simulation of the electrolysis cells used for the industrial production of aluminum is a problem of outstanding difficulty, related to very important environmental and economic questions.

Challenge overview

This research was initiated 14 years ago by C. Le Bris, P.-L. Lions and M. Bercovier. It has been carried out in close collaboration with the Rio Tinto - ALCAN -Pechiney company. It started with mathematical analysis of nonlinear partial differential equations and numerical analysis of problems involving magneto-hydrodynamics (MHD) and free surfaces. Then, specific numerical methods were developed, and implemented in a research software, which is currently used by the Rio Tinto - ALCAN - Pechiney engineers.

Implementation of the initiative

The collaboration between the academic research group and the engineers from the company benefited from a series of PhD thesis, and several one-year training periods of students from the Ecole des Ponts ParisTech. Several contracts were signed between the company and the academic research group to support this collaboration.

The problem

Aluminum is produced from alumina dissolved in a bath through an electrolytic process, in aluminum reduction cells. This reaction requires a very intense electric current (of the order of 10^5 A), and creates high temperatures, so that both the aluminum and the bath are liquid. Liquid aluminum, being heavier than the bath, sinks to the bottom of the cell. The array of conductors bringing electric current to the cell creates large magnetic fields (200 times larger than the Earth magnetic field), which imply some motion of the liquids and of the interface in-between. These dynamical phenomena are very important to understand the stability of the cell.

The industrial challenge is the following: in the presence of these dynamical phenomena, the distance between the anodes immersed in the bath and the aluminum should be kept small to reduce the energy loss by Joule effect, but sufficiently large to avoid short-circuits (when the interface touch the anod). This control and optimization problem is of outstanding difficulty, since the typical anod-aliminum distance is of the order of 5 cm, for horizontal dimensions of the order of 3 meters wide and 13 meters long, and height of the bath and the metal pad of the order of 20 cm. The high temperature and the corrosive nature of the bath make measurements and observation difficult. The main challenge of the research was to model the two-fluid MHD problem, and to develop appropriate numerical methods to solve this highly nonlinear problem. The originality of our approach is that we propose a direct numerical simulation of the full nonlinear two-fluid MHD equations.

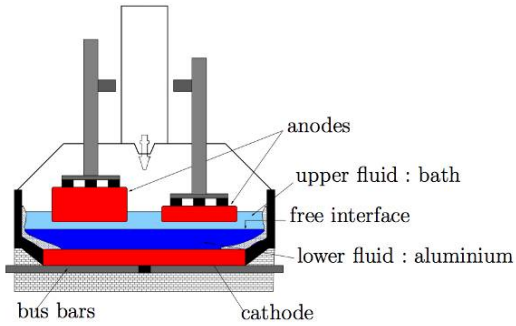


Figure 1: Vertical cut of an aluminium cell

Results and achievements

After a series of works dealing with the mathematical analysis of the two-fluid MHD equations, we developed an efficient numerical method to discretize these equations based on (i) an adequate coupling of the magnetic effects and the hydrodynamic effects, (ii) a stabilized formulation and (iii) an Arbitrary Lagrangian Eulerian (ALE) formulation for treating the motion of the interface. We have been able to reproduce and study an important source of instability in industrial cells, namely *the metal pad rolling*. Such studies can for example contribute to devise better-tuned magnetic fields for stabilizing the free interface.

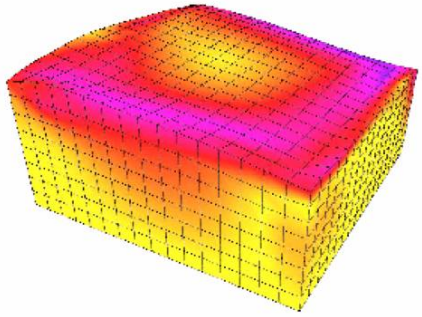


Figure 2: The rolling phenomenon in a cell.

Jean-Frédéric Gerbeau - Project-team REO, INRIA Rocquencourt - Le Chesnay
Claude Le Bris and **Tony Lelièvre**
Ecole des Ponts ParisTech, CERMICS Marne la Vallée

Numerical simulation for the aluminum industry

Executive summary

An extensive Mathematics & Industry collaboration has enabled the simulation of two essential processes in the primary aluminum production:
- The process Hall - Héroult, in which aluminum is produced by electrolytic reduction of alumina dissolved in a bath based on molten cryolite; the metal is formed around 960ºC at the melted aluminum cathode.
- The casting process in which the aluminum alloy ingots are obtained by pouring the molten metal through a molding collar onto a shallow pan or "bottom block". When the metal at the border of the ingot is solidified, the bottom block gradually descends, leaving room for more molten metal in the collar zone.

Challenge overview

In the 1990s, although the transfer from mathematics to industry in Spain was very scarce, the heads of Inespal Metal S. A., now Alcoa, decided to innovate in their metallurgical processes through collaboration with the University of Santiago de Compostela; the collaboration that lasted for about 10 years addressed the simulation of electrolysis and casting processes. For the former, the objectives were improving the energy efficiency of electrolytic cells, increasing their life and, in general, achieving a better understanding of the influence of several parameters on the process such as cathode design, bath composition, profile of the ledge, electric intensity, etc. In the casting process, the objectives were avoiding possible accidents associated with the butt curl and predicting the shape of the solidified ingot using the mold or inductor geometry, cooling conditions and casting speed as parameters.

Implementation of the initiative

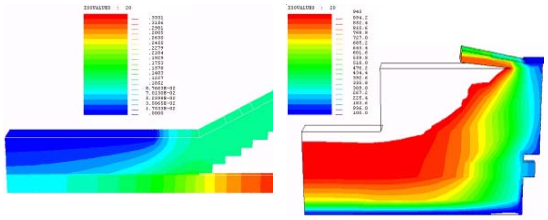
The researches were financed by fifteen successive contracts with Alcoa Inespal, the most important company of the Spanish aluminum industry; additional financial resources came from the Xunta de Galicia and the Spanish government (CICYT).

The problem

From a mathematical point of view it has been necessary to solve systems of coupled nonlinear partial differential equations involving free boundaries. A summary of keywords on their mathematical resolution are: thermal models, Joule effect, solidification, Kirchhoff transformation, enthalpy formulation, free boundary phenomena, electrical model, parameters depending on temperature, thermo-mechanical model, thermal contractions, visco-elasticity, creep effects, parameters depending on temperature, metallostatic pressure, contact, magneto-hydrodynamic model, incompressible Navier Stokes equations, Lorentz Forces, electromagnetic model, Maxwell equations, meniscus shape, surface tension effects, numerical simulation, fixed domain techniques, finite element methods, mixed finite element methods, boundary elements, multipliers, Bermudez-Moreno algorithm, generalized Newton methods, penalty methods, industrial-scale experiments, mathematical analysis, existence, uniqueness, regularity.

Results and achievements

The simulation of electrolytic cells allowed reduced testing on real tanks and designing new cathodes with a smaller potential drop.



Isopotentials in electric domains and isotherms in the cathode.

Similarly, simulating casting processes allowed analyzing the influence of the casting parameters in the solidification.
The numerical algorithms have been implemented in powerful software packages: THELSI (2D and 3D thermo-electrial simulation for electrolytic cells); CEM2D (2D magneto-hydrodynamic simulation of casting); C2D and C3D (2D and 3D thermo-mechanical simulation of casting).

Other results were the publication of original research in high impact journals, 4 PhD theses partly or totally funded through contracts with the company. On completion of the collaboration with the company, and due to the mathematical and computational challenges encountered in solving both problems, some of these research lines still remain open.

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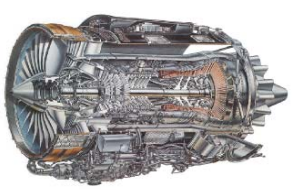
Imbalance Estimation in Rotating Machinery

Executive summary

In most cases the balancing of rotating machinery is a time consuming and expensive process. Using modern mathematical methods, the imbalances / balancing weights can be calculated from measurements of the vibration of the machine, and thus efficiency and accuracy of the balancing process can be significantly increased.

The problem

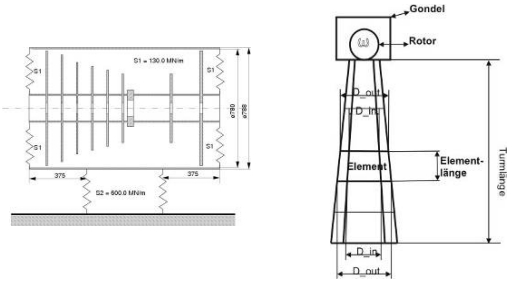
Aircraft engines, vacuum pumps, wind turbines, and generators are all types of rotating machinery which are subjected to imbalances. Imbalances are inhomogeneous mass distributions that can arise from manufacturing tolerances or develop in the course of time due to various reasons, e.g., coop damage in aircraft engines or water inclusions in wind turbine blades.
Imbalances lead to unwanted vibrations of the system which can decrease the lifespan, deteriorate the performance of the machine, or even result in dangerous failure.
Thus it is of vital importance to balance a machine before initiation and monitor imbalances during the lifetime in order to keep the vibrations smaller that a given tolerance.
The present procedure to balance a machine involves the measurement of the imbalanced induced vibrations, the successively mounting of several test weights at different positions, and the measurement of the vibrations with these additional test weights. The mounting of the test weights can be difficult depending on the machine.



Examples of rotating machinery from industrial collaboration projects with RollsRoyce Germany, Oerlikon Leybold Vacuum GmbH, BerlinWind GmbH, and Siemens AG.

Results and achievements

Our approach to avoid the costly test runs is based on Finite Element (FE) models of the machines. Those models connect the forces from imbalances and the resulting vibrations of the machine at every node of the FE model mathematically.



Simple FE models for an aircraft engine and a wind turbine.

If measurements of the vibrations are given on these nodes where sensors can be mounted, then the problem of reconstructing the imbalances is an Inverse Problem. Depending on the structure of the model, linear or nonlinear Inverse Problems have to be considered. Applying appropriate regularization methods for a stable reconstruction we obtain excellent imbalance estimations even in the presence of high noise. The developed methods have been used in several joint projects with different industrial partners, e.g., with RollsRoyce (for reconstruction of imbalances in aircraft engines), Siemens Automation and Drives (for generators), Oerlikon Leybold (for vacuum pumps) and BerlinWind GmbH (for wind power plants).

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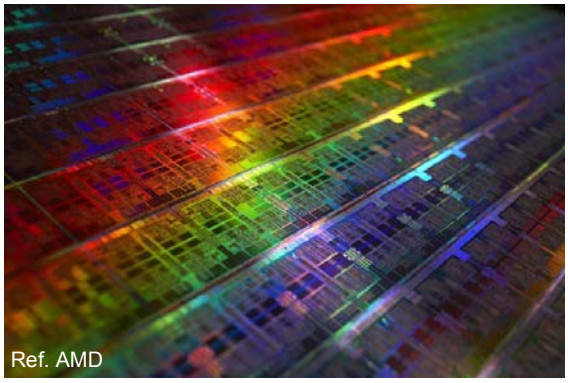
Modeling and Optimal Control of Chemical Mechanical Planarization

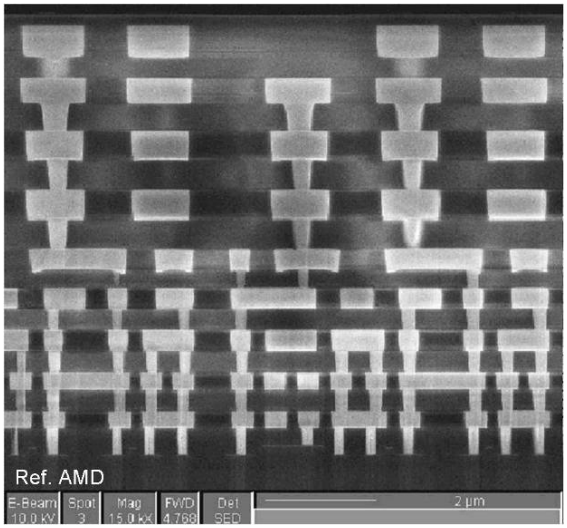
Executive summary

In 2006, the Chemnitz University of Technology and AMD Fab 36 Limited Liability Company & Co. KG (now GLOBALFOUNDRIES Dresden Module One Limited Liability Company & Co. KG) started a collaboration regarding the modeling and optimal control of chemical mechanical planarization (CMP), a polishing procedure which is a basic technology for wafer processing today.
A growing demand for functionality and speed of integrated circuits (ICs) poses a challenge for IC fabrication. This fact increasingly narrows the tolerances for all manufacturing activities involved. One parameter considered in this work is the planarity of semiconductor surfaces monitored during the chemical mechanical polish processes.
Due to a significant number of input variables and their complex interdependencies, fundamental process understanding and modeling is difficult. On this account, a process-specific model for chemical mechanical planarization was developed, which describes the material removal subject to varying pressures.
Moreover, in the framework of a diploma thesis, an appropriate cost functional and an optimal control strategy was derived, numerically implemented, and tested to optimize the removal performance and thereby improve the final removal profile.



Challenge overview

A major use of CMP is the fabrication of inlaid trenches filled with metal, particularly copper, the so-called damascene process. In this process, the underlying silicon oxide insulating layer is patterned with open trenches where the metal lines will be. Following, copper is electrochemically plated so that it significantly overfills the trenches. Then CMP is used to remove the excessive copper to the level of the top of the insulating layer. The copper filling the trenches of the insulating layer is not removed and becomes the patterned conductor. Therefore, CMP realizes patterning and planarization simultaneously. With successive layers of insulator and copper, a multilayer interconnection structure is created. Without the ability of CMP to remove the copper coating in a planar and uniform fashion, and without the ability of the CMP process to stop repeatably and reliably at the copper-insulator interface, this technology would not be realizable.



The problem

Due to a large number of variables and a complex interaction amongst them, the CMP process is complicated. Hence, an experimental model was developed, which is capable of mirroring the process. On the basis of this model, an optimal control strategy was developed. A linear-quadratic optimal control problem can be treated with purely algebraic methods – by solving the differential Riccati equation. Due to this significant advantage over solving an optimization problem, a study of the Riccati approach applied to the CMP problem was made and promising solutions were obtained.

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CHEMNITZ UNIVERSITY OF TECHNOLOGY

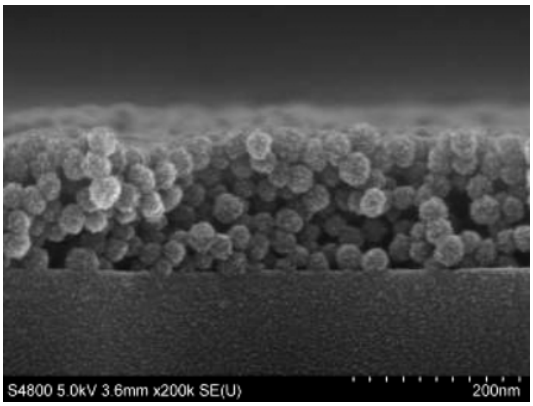
Anti-reflection coatings

Executive summary

The purpose of this consultancy project was to investigate the inverse determination of a spacewise dependent index of refraction of a dielectric obstacle. Such a dielectric specimen could be an optical anti-reflection coating (ARC) structure as is used in various optical instruments.

Challenge overview

In recent years, ARC's have become a key and vital feature for high-efficiency solar cell design. They are also widely used to increase transmission and reduce glare resulting from window coatings in a diverse range of industries such as photovoltaics, buildings, displays and opthalmics. ARC's currently in use enhance the transparency of certain surfaces by the introduction of a smooth and gradual change in effective refractive index between two media, see figure. This results in improved efficiency of some commercial architectural glazing and solar collectors.



Implementation of the initiative

Last year, J. Ockendon from the Oxford Centre for Industrial & Applied Mathematics (OCIAM) heard people from Oxford Advanced Surfaces Group Plc talking about the determination of the index of refraction of anti-reflection coatings and he suggested that at Leeds University there are researchers specializing in industrial inverse problems which may help with professional advice. The initiative was further supplemented by meetings at OCIAM and the problem was also exposed at the University of Leeds within the *4th Industrial Inverse Problems Sandpit* supported by the Leeds EKT and the KTN.

The problem

The problem is formulated as an inverse coefficient identification of the index of refraction of the optical coating, for the Helmholtz equation in one dimension. The additional data necessary for the inversion can be the full complex reflection coefficient or its absolute value only, measured for many wavenumbers. The numerical method was based on a finite-difference direct solver combined with a nonlinear Tikhonov regularization procedure. The choice of the regularization parameter was based on the discrepancy principle or the L-curve criterion.

Results and achievements

The results of this project resulted in a paper being accepted for publication in the journal *Mathematics-in-Industry Case Studies*. It was shown that, in general, the knowledge of the full complex reflection coefficient is necessary to determine uniquely a spacewise continuous index of refraction. When only the absolute value of the reflection coefficient is used as input data, constraints need to be imposed, e.g., the knowledge of the full integrated refraction index, additional smoothness assumptions on the index of refraction, or more reflectance data measured for many wavelengths. Also, the use of additional reflectance data at non-normal incidence, the finite-dimensional parameterisation of the unknown coefficient using cubic splines or the piecewise constant layered material assumption could be useful ideas to reduce the non-uniqueness of solution of the inverse problem. Apart from this insight, overall it can be concluded that a better fit of the reflectance measured data is obtained by using a continuously varying index of refraction than when this coefficient is sought as piecewise constant function, as in previous studies.

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Modeling plasma PVD

Executive summary

This project involved the modeling of glow discharge in low pressure plasma PVD (physical vapour deposition) for industrial application. The researchers of I^2T^3 (Industrial Innovation Through Technological Transfer) in collaboration with the Department of Mathematics of the University of Firenze, developed a model to describe the plasma atmosphere induced by a low pressure glow discharge in an industrial plant.

Challenge overview

Galileo Vacuum Systems srl (GVS) is a leading company in the production of industrial plants for PVD applications such as metallization of plastic films, alumination of headlamps for automotive etc. GVS had already established collaboration with I^2T^3 and a dialogue on a new scientific approach to the product innovation was already in place. In this particular case, the input for the project came from the request, made by some of the main international clients of GVS, of a description of the effects of the main control parameters (such as pressure of the plasma atmosphere or shape of production chamber) on the quality of the final products. Such a description needed a more systematic and scientific approach on the process of the design of new plants, involving, possibly, the development of a mathematical simplified model of the industrial process and some experimental analysis.

Implementation of the initiative

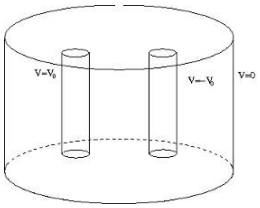
The 12-month project involved the development of mathematical modeling and simulations. The initiative was partly co-funded by the Toscan Regional administration in the framework of funding projects aimed at introducing new and innovative products and processes in industrial companies.

The problem

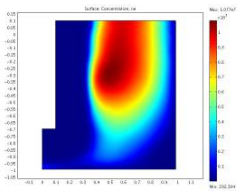
The model focused on the prediction of the main features of the plasma atmosphere induced within an industrial plant by a strong (~2000kv) electric field.
The industrial process described (PVD) proceeds in three main steps as follows

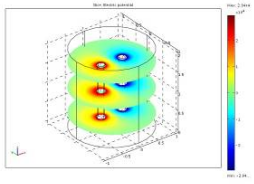
1. vacuum (10^{-3} mbar) is made into a chamber
2. a strong (~2000kv) electric field is applied to the electrodes within the chamber and a glow-discharge is produced; the residual atmosphere is turned into a plasma
3. a monomer flows throughout the chamber; the monomer polymerises in the plasma atmosphere and a polymer film covers the plastic substrates lying in the chamber

This project concerned in particular the modeling and simulations of the second step.



The mathematical model involved in particular the mass conservation equation coupled with a drift diffusion model for the conservation of momentum. All the effects of transient electric were neglected and a stationary state solution was found. The boundary conditions needed for the set of equations turn out to be rather complex as, even neglecting second order terms, they depend on the solution itself. The set of equations, otherwise rather straight forward, therefore couple with each other in a strongly non-linear way. Furthermore, some parameters would need an experimental evaluation. However, such parameters are usually estimated in the literature for very simple and ideal composition of the atmosphere.





Results and achievements

With this project, the company began a new path of innovation aimed at a renewal of the whole production and concept of industrial plants. I^2T^3 developed a new and powerful know-how on PVD and mathematical modeling.

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Crystal growth in travelling magnetic fields

Executive summary

Mathematical simulation and optimisation within the innovation award-winning project KRIST*MAG* for improvements in semiconductor crystal production

Challenge overview

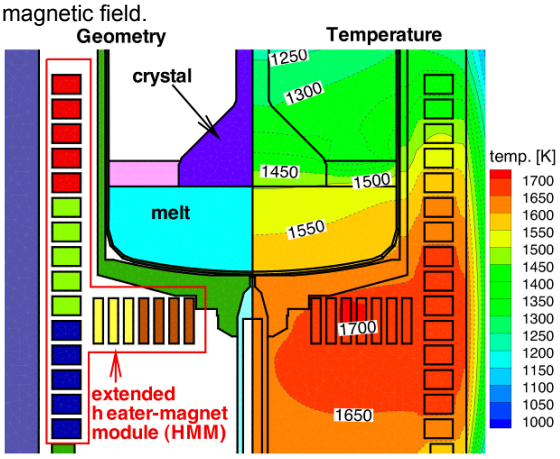
WIAS successfully cooperates with both, industrial companies and academic partners from applied sciences and economics. Long-lasting and widely recognised expertise in the mathematical description of phase transitions, in particular in crystal growth problems, and successful co-operation with the coordinating Leibniz Institute for Crystal Growth (IKZ) made WIAS participate in this project.

Implementation of the initiative

The consortium consisted of four partners: IKZ (crystal growth experiments; device development), WIAS (mathematical simulation and optimisation), AUTEAM Industrie-Elektronik GmbH and Steremat Elektrowärme GmbH (end-users). It was funded for a period of three years by the federal states of Berlin and Brandenburg, as well as by the European Regional Development Fund (ERDF). The WIAS team consisted of two scientists from the permanent staff and one additional scientist funded by the project.

The problem

The most important production methods for semiconductor bulk crystals start at high temperature with a melt, and then the crystal is obtained on controlled cooling. During the so-called Czochralski process and its variants, the crystal is pulled from a rotating melt. In order to achieve a homogeneous crystal, three requirements must be met: one needs, preferably, a spatially and temporally homogeneous temperature, a controlled flow within the crucible, and a convex interface between melt and crystal. The desired process up-scaling (increase of the production device in order to achieve larger crystals) leads to serious complications. This new requirement calls for major changes of the growth device, and new experiments to determine the new optimal parameters become necessary. To be able to produce larger crystals with the same quality, one may even need some additional technical equipment. For example, travelling magnetic fields are successfully used to control the melt flow during Si growth. But the application of this new technology to the growth of III-V compounds leads to an unfavourable high power consumption, since the magnetic fields are typically generated by induction coils placed outside of the growth apparatus so that the thick walls of the pressure chamber significantly diminish the applied magnetic field.



Left: Growth configuration with a heater-magnet module extended by two additional coils below the crucible. Right: simulated global temperature distribution

For the reliable and efficient mathematical simulation and optimisation, a coupled system of partial differential equations on a complicated, non-smooth cylindrical domain had to be solved. The scientific software tools WIAS-HiTNIHS and NAVIER were extended and applied for the numerical treatment.

Results and achievements

Within the KRIST*MAG* project, the partners could show that an internal heater-magnet module can generate travelling magnetic fields that are able to control temperature, flow, and interface boundary in the favoured sense. Several pilot devices have been manufactured; a couple of patents were filed and awarded (two of them with the participation of mathematicians). The groundbreaking nature of these developments was recognized by the Innovation Award Berlin-Branden-burg 2008. Presently, there is a cooperation of the same partners and another company in a new project, which deals with controlling the growth of silicon for solar cells from the melt by using travelling magnetic fields. On the academic side, a mathematical breakthrough could be achieved by proving existence and uniqueness of the solution to the coupled system of partial differential equations modelling the growth process.

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steremat elektrowärme

IKZ

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WIAS

Polysilicon Fuses

Executive summary

Developing a mathematical model of the physics of blowing polysilicon fuses.

Challenge overview

Polysilicon fuses are components of silicon chips which are blown as an irreversible programming step. Currently the ideal blowing voltage must be re-determined experimentally for every new chip design. These experiments are time consuming and delay the introduction of new products. Analog Devices contacted MACSI to ask if a mathematical model could be developed to model the fuse blowing process. This was a very challenging problem since the physical basis of fuse blowing was very poorly understood and only limited experimental evidence was available: namely the current-time transient of the blowing fuse and electron micrographs of blown fuses.

Implementation of the initiative

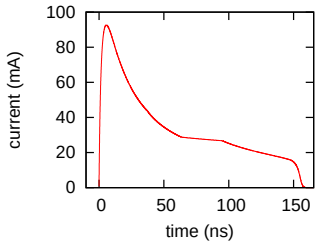
After initial analysis of the problem MACSI decided that the problem would benefit from an intensive brainstorming session involving using experts from a wide range of mathematical disciplines. Therefore the problem was included in the 62nd European Study Group with Industry: the first ever industrial study group held in Ireland, organised by MACSI at the University of Limerick. The study group format also simplified the consideration of intellectual property and confidentiality issues since results obtained by study groups are released into the public domain.

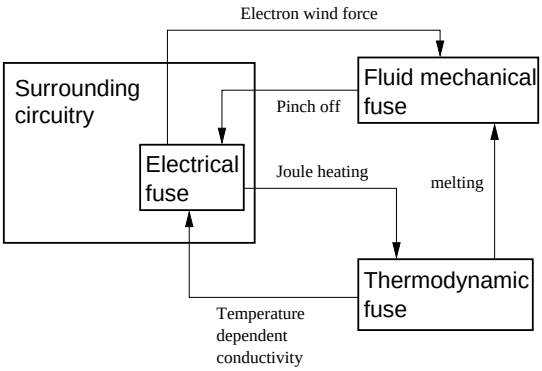
The problem

There were two challenges to this problem. The first was to determine the physics behind the blowing of the fuse; the second was to implement that understanding in a mathematical model. The first objective was achieved by considering a great number of fuse blowing scenarios and by order of magnitude estimates determine whether they were consistent with the observed phenomena. The final conclusion was that fuse blowing was the result of a complex combination of electronic, thermodynamic and fluid mechanical phenomena. To fulfil the second objective a 'multiphysics compartment model' was constructed, reducing the complexity of the blowing process to several ordinary differential equations.

Results and achievements

Remarkably, given the extreme simplicity of the model its results show good agreement with experimental observations. This strongly suggests that the model has captured the underlying physics of the fuse blowing process. MACSI continue to collaborate with Analog Devices on fuse simulations with the aim of turning the mathematical model into a tool that can replace the experimental characterisation of fuses. Analog Devices also submitted a problem to the 70th European Study Group with Industry which was organised by MACSI at the University of Limerick.





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Numerical simulation of metallurgical processes in silicon production

Executive summary

The collaboration between the company Ferroatlantica I+D and the Department of Applied Mathematics of the University of Santiago de Compostela (Spain) on the numerical simulation of several metallurgical processes is described below.

Challenge overview

This company, which belongs to the Ferroatlantica Group, is devoted to the production of ferroalloys and, in particular, of silicon. The main purpose of Ferroatlantica I+D is to develop and coordinate the research activities of the group. In 1996, the manager, Javier Bullón, contacted the team at the Department of Applied Mathematics because he knew about the collaboration between this team and other companies, such as INESPAL. The first problem proposed by the company was the numerical simulation of a metallurgical compound electrode, the so-called ELSA electrode, patented in those years by the company and used nowadays in a great part of the world's silicon production. They had little experience in the working of this electrode and the numerical simulation was a useful tool to improve its design and the operation conditions.

Implementation of the initiative

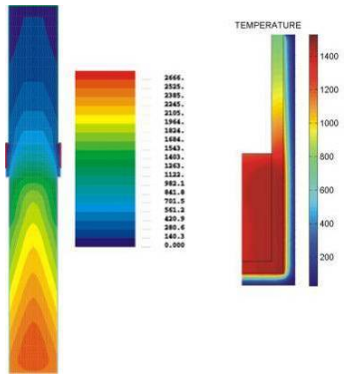
The research activity was financed by the company under annual contracts. It also had support from public funds. In particular, the company invested more than €100,000 to simulate the thermo-electrical and thermo-mechanical behaviour of the ELSA electrode during the period 1996-2000. The university group was directed by Professor Alfredo Bermúdez and the methodology they used can be summarized in three main steps: to understand the physical phenomena involved in the metallurgical process by developing suitable mathematical models; analyzing efficient numerical techniques to approximate its solution; and providing a bespoke software package to simulate the full process. Thus, the group developed the package ELSATE which allows knowing the distribution of the temperature, the electric current and the mechanical stress in a radial section of the electrode, under different operational & geometric conditions. The meetings with the company have been very frequent. The main difficulties encountered were to translate all the information collected by the engineers from the plant to the mathematical model, validate the numerical results by using experimental measures and characterize the physical properties of the materials.

The problem

The mathematical model involves the coupling between the eddy current problem, the transient heat equation and the mechanical problem. The finite element method has been the common tool to solve the different models by using iterative methods to deal with the coupling. From a theoretical point of view, the definition of suitable boundary conditions in the electromagnetic model and the well-posedness of the thermo-electrical problem have been the most relevant topics.

Results and achievements

The numerical results provided relevant information about the working of the compound electrode and were used for specific industrial purposes (to improve the baking process or reduce breakages in the plant). Some of these results have been presented in metallurgical conferences in collaboration with staff members of the company. From an academic point of view, the collaboration opened interesting research fields; two members of the university group developed their respective Ph. D. thesis in this framework and the theoretical research was also funded by the Galician and Spanish Administrations. After the successful experience on this first problem, the collaboration continued in order to optimize other technologies also developed by Ferroatlantica I+D. Indeed, in 2001, they designed a new casting system, a copper plate cast machine, and requested its numerical simulation. Now, they are interested in the production of silicon of high quality.



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Optimal utilization of colored gemstones

Executive summary

New mathematical optimization methods based on semi-infinite programming and physical models resulted in the first fully automated gemstone cutting machine worldwide.

Challenge overview

In autumn 2003 the Fraunhofer ITWM was contacted by Paul Wild OHG, one of the largest gemstone manufacturers in Europe. Markus Wild, CEO, had the idea to develop an automated scanning, planning and production system for the gemstone industry, which should increase the volume yield and improve the product quality at the same time. Considering that the gemstone industry is has been characterized by century-old traditions and manual processes, this was a truly visionary idea. An automated cutting machine did not exist, and the mathematics behind the practical problem are surprisingly complex. Thousands of different cutting models have to be considered, each being flexible in size and proportions. Taking into account the huge data sets coming from a precise measurement of the rough stone and the desired computation time restrictions of 15 minutes, the problem was not solvable in at that time.

Implementation of the initiative

In order to minimize the risks and to explore the potential of the idea, several studies were carried out during 2004 and 2005. Ways to automatically control the cutting and polishing process have been investigated, leading to new physical models. Also, a software prototype was implemented and tested on reduced-size examples to demonstrate the expected gain in volume. After the studies were successfully finished, a contract for two years was signed in spring 2005. The goals of this project were to develop algorithms, the software and the hardware to the stage of a fully functional prototype. The work was carried out by several scientists at Fraunhofer ITWM, supported by research assistants. Important contributions to the problem of handling the huge dimensions of the real-world problems were developed in a dissertation. Since most of the models for gemstone cutting had to be developed ‘from scratch’, an intense communication with the customer was necessary. Formalizing the customer’s requirements, implementing solution strategies, presenting the results and adapting the models and methods according to the feedback was the only way to make progress.

The problem

The method used to tackle the gemstone optimization problem comes from the young research field of generalized semi-infinite programming. While being very flexible in terms of modeling geometrical packing and cutting problems, generalized semi-infinite programs are difficult to handle numerically. In 2003, a new numerical approach for a special class of semi-infinite programs was published, and it turned out that this approach can be applied to solve the gemstone optimization problem. However, drastic improvements in running time and stability were necessary before this method could be used in practice. The main ideas that finally led to success include an adaptive discretization scheme operating on the rough stone data and the usage of non-linear models in order to reduce the combinatorial complexity of all possible cut shapes.

Results and achievements

The result of the project is the first automated gemstone production system worldwide. All customer requirements could be fully satisfied. In particular, the solutions computed by the optimization software yield up to 30 per cent more volume than human experts. Also, the automated cutting is around 10 times more precise than the industry standards. Motivated by this success, Fraunhofer ITWM and Paul Wild OHG have started several follow-up projects dealing with further problems arising in gemstone industry, such as finding optimal compromises between volume and beauty, dealing with inclusions and simultaneously embedding several faceted gems in one rough stone. Also, continued research and application of the results to new areas, such as medicine or molding industry, are taking place in several dissertations at Fraunhofer ITWM.

Figure: Optimal embedding of a Round Portuguese Cut

Figure: Automatic cutting

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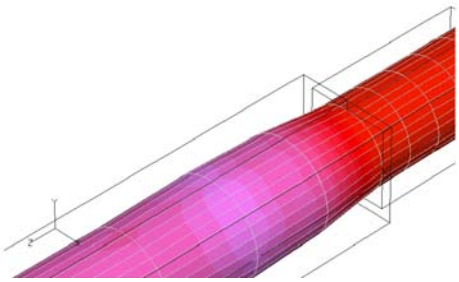
Simulation of Polymeric Textile Products

Executive summary

Technological innovation in textile industries is nowadays a mandatory challenge. The aim of this project was to develop a mathematical model and effective numerical tools for the prediction of polymeric textiles behavior both at microscopic and macroscopic level, in order to drive and support technological innovation in textile industries.



Challenge overview

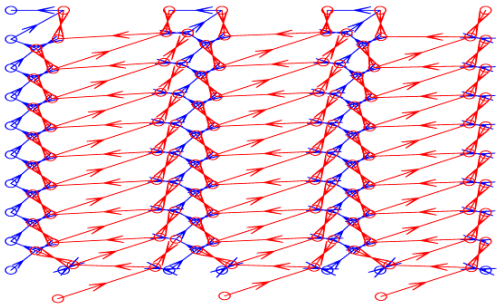
A three year project (2008/2011) has been set up as a collaboration among MOX, Department of Mathematics of Politecnico di Milano, Carvico S.p.A., a global leader in the manufacturing of warp-knitted fabrics, and RadiciYarn S.p.A., a leading Italian chemicals multinational specialized in the production of polyamide yarns. The motivation behind the project is to develop strong mathematical expertise within the context of high technology textiles. The goals were twofold. First, the analysis of the yarn extrusion process and the optimization of die lips allowing the production of hollow fibers. Secondly, the development of mathematical models and numerical algorithms that can predict how the (micro) texture topology influences the (macro) mechanical properties of warp-knitted fabrics.

Implementation of the initiative

The project is coordinated by two permanent MOX staff, P. Antonietti and M. Verani, who supervise a post-doc fellow, A. Tavakoli and a post-grad fellow, N. Fadel, who have been hired for the project. The development of mathematical models for the description of the mechanical properties of warp-knitted fabrics takes also advantage of the collaboration with other researchers of the Dapartment of Mathematics, namely P. Biscari and M. Vianello. In the project implementation process, the industrial partners are validating through experimental results the models that have been developed.

The problem

For the first goal, we considered a three dimensional numerical method for the analysis of the yarn extrusion process, together with a preliminary technique towards the optimization of die lips allowing the production of hollow fibers with a prescribed hollow volume vs total volume ratio. The material has been modeled as an incompressible non-Newtonian isothermal steady fluid. The simulations have been carried out with a constitutive model well suited for describing the Polyamide rheological behavior. For the second goal, a new model was developed based on the (micro) properties of the yarns for the prediction of mechanical behavior of warp-knitted fabrics. The approach relies on the selection of a suitable topological model for the patch of the fabric, coupled with constitutive models for the yarn behavior. The structural configuration of the fabric is related to the deformation through a global energy functional.



Results and achievements

The project is in progress, and will end in 2011. At the time of publication, we have designed preliminary geometries of the hollow yarn die which are now being validated by means of experimental results, and a mathematical model for the prediction of the structural properties of warp-knitted fabrics which is currently being tuned according to the available experimental data.

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Dipartimento di Matematica,
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http://mox.polimi.it/it/progetti/tessile/

Contractors: Carvico S.p.A. and RadiciYarn S.p.A

Modeling and analysis of Rotary Fiber Spinning

Executive summary

Using mathematical modeling, theoretical and numerical analysis of the resulting model, and experimental verification, we have described the process characteristics of the *rotary spinning process.* The mathematical model provides a general insight in the spinning process, and suggests a way to produce arbitrarily long fibers.

Challenge overview

Rotary spinning is a process for the production of strong and temperature-resistant aramid fibers. These fibers have a wide range of applications in the automotive industry, protective gear and clothes, composites, and linear-tension products. However, in the current state of the technology only short fibers can be obtained, while the ability to manufacture arbitrary long fibers would substantially improve the processability of the product resulting in an increase of the equipment efficiency of the total production unit.

The scope for experimental investigation of the process is both limited and extremely expensive. Hence there is a case for mathematical analysis of this problem.

Implementation of the initiative

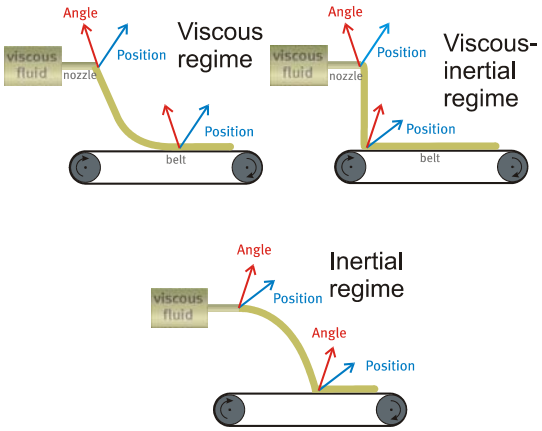
The company Teijin Aramid brought the problem of rotary spinning to the mathematical community at the 48th European Study Group Mathematics with Industry in 2004 at Delft, The Netherlands. Only partial progress was made during the Study Group itself, and the rotary spinning problem became the subject of the PhD project of Andriy Hlod at Eindhoven University of Technology. The company was involved with the research throughout the project, and provided not only comments and feedback but also experimental facilities.

Mathematical modeling and analysis

The rotary spinning process is modeled by a jet of viscous fluid subjected to centrifugal and Coriolis forces and hitting a moving wall. The jet is described by a string model (analogous to elastic strings), which incorporates the effects of inertia and extensional viscosity. The steady-flow jet, which is the operationally preferred state, is described by a system of ODEs with a free boundary.

As a simplified problem we investigated the jet model in the non-rotary situation where the jet falls under gravity onto a moving surface. A central problem was the choice of boundary condition at the surface; the key insight was that the dynamic problem is of mixed hyperbolic-parabolic type, and that the boundary condition should be chosen according to the behavior of the characteristic directions of the hyperbolic part. Physically, the choice of boundary conditions reflects the dominant effect in the momentum transfer through a cross-section. This analysis showed the existence of three flow regimes with counter-intuitive dependence on process parameters. Importantly, experiments performed by Dr. Hlod with help of Teijin Aramid confirmed this non-trivial dependence, providing independent support for the choice of boundary conditions.

We subsequently applied the jet theory to the rotary spinning model. This allowed us to characterize the parameter space and obtain the parameter regions where spinning was possible. Furthermore we have developed a numerical scheme for the dynamic problem.



The three flow regimes of the jet falling onto the moving surface are characterized by the dominant effect in the momentum transfer: viscous, viscous-inertial, or inertial. Each inward-pointing characteristic (indicated by the arrows) gives rise to one boundary condition for position or angle

Results and achievements

The industrial partner received recommendations about causes of the fiber breakage in the rotary spinning which triggered further experimental investigation. The PhD thesis of Andriy Hlod was awarded the Anile-ECMI Prize for Mathematics in Industry at ECMI 2010.

Contact

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Industrial partner

Teijin Aramid

Aerospace and electronics

Modeling and Simulation of Spacecraft Charging

Executive summary

This research project is concerned with the modeling of the electric charge phenomena that spacecrafts are subject to. These phenomena are sources of in-orbit failures since high potential differences induce the formation of electric arcing which can produce irreversible failures on on-board devices. The numerical simulation of such phenomena, taking into account the specificities of the space environment, is part of the conception of new spacecrafts.

Challenge overview

The first objective is to write a relevant model that consists of a system of non linear Partial Differential Equations. Next, these equations involve several physical parameters, and, discussing the relative order of these parameters, a hierarchy of further models can be elaborated. Finally, we design numerical schemes for these problems, up to the effective implementation of a code usable at the industrial scale.

Implementation of the initiative

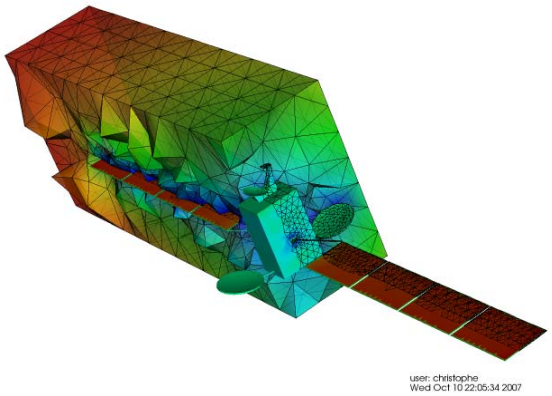
The collaboration between Thales (formerly Alcatel) and INRIA on this subject started some time ago through the project CAIMAN at Sophia Antipolis. The program is now led by the team SIMPAF in Lille. It has permitted the realization of several PhD thesis (O. Chanrion, M. Chane-Yook, S. Borghol) and post-doctoral internships (N. Vauchelet). The success of the program is based on a strong investment of the partners, in particular with the commitment of Thales' engineers (S. Clerc, J.-P. Dudon). It allows a permanent and stimulating dialogue with researchers from academics, still focused on very clear objectives.

The problem

The problem is modeled by Vlasov-Poisson or Euler-Poisson equations, endowed with non-standard boundary conditions for the electric potential. These boundary conditions, which involve time derivatives, are precisely intended to describe the charge phenomena. The derivation of the model relies on asymptiotic analysis arguments, the scaling parameter depending on the conditions of the flight (LEO, PEO or GEO atmospheres). Real-life simulations are highly demanding on numerical resources and requires a high-performance code including parellelization procedures.

Results and achievements

A key achievement stemming from this partnership is a significant contribution to the development of the code SPARCS which is currently used to prepare new aerospace missions. It allows computation of the charge of satellites with complex geometries and environments. On-going progress is devoted to speeding up the computations and to incorporating more complex physical phenomena. Part of the work is also oriented towards the design of prospective devices.



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Flow control of an air duct

Executive summary

An innovative optimization method, the topological gradient, has been used to design the duct supplying air to an aircraft engine.

Challenge overview

The Center of Applied Mathematics (CMAP) at Ecole Polytechnique has a long tradition of collaboration with the industry. Similarly Dassault Aviation has always worked at the forefront of research with university partners. Optimization is an essential tool in the design of innovative aircrafts. The CMAP has a strong research group on shape and topology optimization. The new design challenge imposed by stealth constraints on aircraft was a perfect opportunity to transfer the CMAP knowledge on topology optimization to industry through a PhD thesis. In order to get a uniform air flow in the curved air duct feeding the engine, small mechanical vortex generators (VG) can be placed at critical points on the duct boundary. Traditional optimization methods start from an initial guess of the VG location and move it to an optimal position. However, the occurrence of many local minima usually prevents a global optimization. Topology optimization is one way of providing a good initial guess, close to the global optimum.

Implementation of the initiative

The framework of this research is a collaborative contract and a PhD thesis. The PhD student is fully integrated into the advanced aerodynamics department of Dassault Aviation. He interacts with several research engineers while remaining under the supervision of the CMAP. The CMAP is responsible for the adaptation of topology optimization methods to the framework of flow control, while Dassault Aviation helps the PhD student on the implementation of the method into the in-house computational fluid dynamic (CFD) code. Dassault Aviation also provides various industrial test cases which are used to evaluate and improve the method.

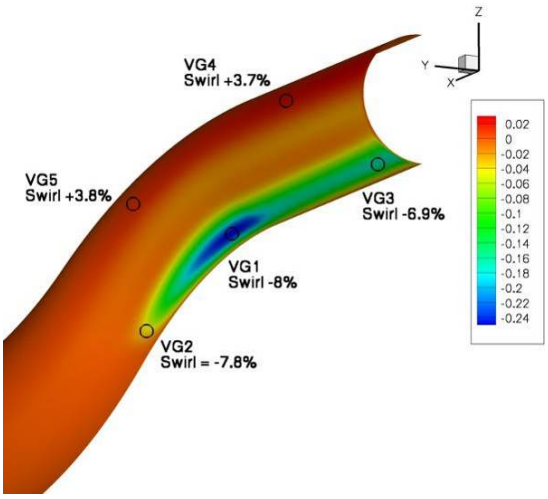
The problem

The goal is to determine where it is relevant to create a mechanical vortex generator (VG) into an air duct in order to optimize the flow feeding the engine. To this end, the idea of topological gradient, first introduced in the framework of structural optimum design is used. The computation of the topological gradient requires solving the compressible Navier-Stokes equations inside the duct and an additional system of equations, the adjoint system. One then obtains the expression of the topological gradient on the duct boundary. In order to optimize the flow inside the duct, it is relevant to introduce a new VG at the points where the topological gradient is as negative as possible.

Results and achievements

The topological gradient was successfully implemented into the CFD industrial code developed at Dassault Aviation. It has been applied to the design of several air duct configurations. Coupled to a classical procedure of parametric optimization, it yields much more improved duct designs than in a “hand-crafted” optimization, the usual process for engineers. This method can also be applied to other cases where flow control is needed, like for example the design of innovative high-lift devices. More generally, other industries can be interested in the method, such as the automotive industry.

Generic u-shaped air duct for unmanned aircraft



Map of the topological gradient in an s-shaped air duct. The area in blue is the one where it is optimal to place a mechanical vortex generator

Contact Jonathan Chetboun, Dassault Aviation and CMAP, Ecole Polytechnique - Michel Mallet, Dassault Aviation - Grégoire Allaire, CMAP, Ecole Polytechnique, France

Aero-engine Nacelle acoustic treatments

Executive summary

An original domain decomposition technique is used to model the impedance property of current and innovative acoustic liners used in the nacelle ducts in order to reduce the Engine noise.

Challenge overview

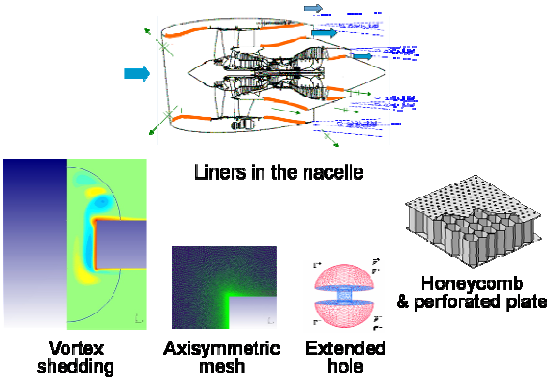
The Centre of Applied Mathematics at Ecole Polytechnique has a long tradition of addressing cutting edge modeling problems interesting the industry. That led to the creation of several successful spin-offs like IMACS. Up to seven PhDs from CMAP have been hired by the company. Corporate Research Centre of EADS (now EADS Innovation Works) has a dedicated team in Applied Mathematics for more than fifteen years. Their strong relations with academic community facilitate first contacts, and after several successful research projects, EADS and IMACS signed a cooperation agreement on the research, development and industrialization of several numerical tools for electromagnetic applications. In the same time, Airbus Operations SAS is deeply involved in the development of low noise technologies and especially acoustic liners able to reduce the overall Aircraft perceived noise level by 4-5EPNdB at take-off and 2EPNdB in approach. Thanks to the mathematical similarities, a Fast Multipole solver has been transferred from Electromagnetism to Acoustics, which is used by Airbus Operations SAS to predict noise propagation and radiation from engine inlet and exhaust ducts. Noise reduction is achieved by passive liners, which are characterized by an equivalent impedance Boundary Condition. Airbus Operations SAS has developed analytical models and measurement techniques that help to characterize and optimize the acoustic treatments in some standard situations. In order to further optimize these treatments and study innovative concepts, a precise numerical modeling was needed.

Implementation of the initiative

A research project has been therefore launched in 2004 by Airbus in close collaboration with EADS Innovation Works and IMACS with the aim of building an accurate and robust numerical simulation tool for liner impedance predictions. This project was funded by Airbus and EADS. A multidisciplinary team was the key factor of the success: numerical results were compared iteratively to previous analytical and experimental ones, and thus the model was improved and enriched, showing that all difficulties were not forecast at the beginning of the project.

The problem

The impedance of the liners is reached by computing the reflection coefficients of an infinite bi-periodic grating consisting of a honeycomb layer and a perforated-plate resistive sheet. Our aim is to characterize the liner in the linear and non-linear regimes, with and without grazing flow. The solution is achieved by a domain decomposition technique with a multi-physics, multi-scale and multi-method approach. In the cavity of the honeycomb and in the exterior domain, the problem is modeled by linearized Euler equations. Non-linear Navier-Stokes equations are solved in a generic extended hole in order to construct a database of impedance operators that can be reduced for the coupling between domains with a good approximation. Direct 3D computations of the Navier-Stokes problem appeared to be prohibitive which led to the introduction of an innovative axisymmetric finite element method.



Results and achievements

A new original numerical method has been developed, able to predict the impedance of honeycomb –perforated plate liners in the linear domain without flow, accounting for real geometry. The developed numerical solver has been validated by comparisons with analytical method and measurements in the linear regime and is already being used by Airbus. The validation in the non linear regime is in progress. The project has been extended in partnership with ONERA Toulouse (Laser Doppler Velocimetry measurements for the tool validation) with financial support from the French Civil Aviation Authorities.

Contact

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More Simulation – Less Testing

Executive summary

A major part of the development costs of an aircraft is incurred by wind-tunnel testing and actual flight tests which are needed in order to obtain aircraft certification. In case a problem is detected at this stage of the development it is extremely expensive to modify the design of the aircraft in order to deal with the problem. Hence it is of interest to complement the wind tunnel and flight tests by increased use of numerical simulations.

Challenge overview

The numerical simulation of aircraft aerodynamics requires the solution of a suitable mathematical model taking all relevant physical effects into account. For an industrial aircraft configuration, each simulation may take several hours on a parallel computer using hundreds of cores. In order to fully simulate the behavior of an aircraft it is estimated that up to 20,000,000 such simulations are required (using engineering experience for current configurations and technologies, still about 100,000 simulations are necessary). In order to be able to achieve this in feasible time one can make use of model reduction techniques. Model reduction seeks to replace the large-scale mathematical model with a small-scale one which is much faster to simulate (in a few seconds or minutes), but still captures the relevant characteristic behavior of the aircraft.

Relevant aerodynamic information for computational flight testing: forces and moments (left), and surface pressure distribution (right)

Implementation of the initiative

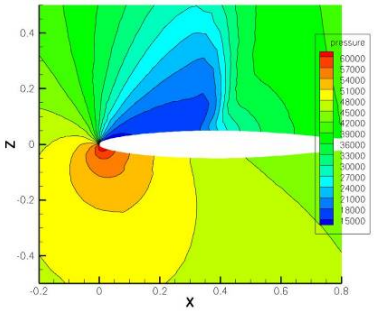
The DLR has a long tradition of cooperation with universities. The initial contact for this cooperation was made when model reduction emerged as a new research topic for the DLR. A master's thesis on model reduction performed at the AG Numerik raised DLR's interest as it appeared to be a promising approach for the simulation of aerodynamic problems looked at by the DLR. The discussions on this topic led to a joint project within the larger ComFlite (Computational Flight Testing) project funded by the national aeronautics research program (LuFo IV) of the German Federal Ministry of Economics and Technology. As part of this collaborative project, a number of researchers from both institutions teamed up to meet about once a month to plan and coordinate the project. To further the cooperation, the DLR granted the AG Numerik access to their flow solver TAU, which is also used by industry, and a subversion system was set up to easily exchange the latest code developments.

The problem

In this cooperation we concentrated solely on the model reduction aspect assuming that a suitable full order model describing the proper flow physics is available. Using the DLR-in-house computational fluid dynamics (CFD) solver TAU, flow solutions can be computed for certain parameter settings (describing certain flight conditions). Using these so-called snapshots, low dimensional models can be generated using the proper orthogonal decomposition (POD) ansatz. These reduced-order models suffer from a number of problems; in particular, they are only valid for parameter settings very close to those used to compute the snapshots.

Results and achievements

The so-called Gappy POD was implemented to be used with the DLR-in-house CFD solver TAU for the purpose of data fusion. This approach allows combining data obtained from numerical simulations with partial experimental data to reconstruct an entire flow field. The approach has been demonstrated for fusing gappy wind tunnel data of an industrial aircraft configuration with CFD data. It can also be used for design purposes such as inverse airfoil design.



Computed pressure distribution around an airfoil

Contact

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Low cost Airborne Laser Fly

Summary

A more efficient obtention of LiDAR Altimeter datasets for the construction of Digital Elevation Models in urban areas was achieved .

Challenge overview

This problem was proposed by the Spanish company Stererocarto S.L. for the III Modelling Week celebrated in 2009 in the Complutense University of Madrid (UCM). Since 2007, UCM yearly organized these modelling weeks as a part of the Master in Mathematical Engineering offered in the Faculty of Mathematics of the UCM. The company was invited to participate without previous contacts. *Tomás Fernández de Sevilla* exposed the problem.

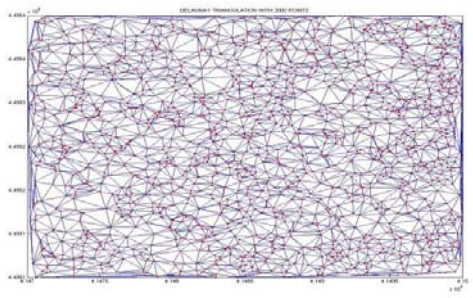
The Airborne Laser Scanning (ALS) technology is based on the ground survey from an airborne laser telemeter which measures the distance between the instrument and the echoing surface. An integrated sensor GPS/INS provides the airplane position and attitude at each instant. The principal aim is to develop a Digital Elevation Model (DEM) by filtering points which represent terrain objects by interpolation.

The problem proposal was to study how points density, thus flight height, affects to digital models precision/ resolution. And then, to answer the following question: Is there a way to reduce the data density so that this data loss does not have influence in the final digital models?

The problem

During this week, we work with 210418 data points collected by an aircraft equipped with a LIDAR system that had fly in an urban area of 300x300 m at an altitude of 800 m. Our main objective was to reduce the density of measured data but maintaining DEM precision. First, the LIDAR data set was randomly split into a prediction data set and a validation data set. To select subsequent subset of observations we used a series of uniformly distributed random numbers for obtaining data scattered in the same manner as the original data. A Delaunay Triangulation was used as computational structure to allow an optimal data triangulation in order to apply interpolation algorithms. Then, a series of DEMs were generated at spatial resolutions of 1 m and 1.5 m. Several statistical tests based on the tolerance given for the problem were also established.

We developed a software tool using MATLAB to solve the points above mentioned.



Results and achievements

Initially, the altitude of the plane was 800m and it was shown how using a grid of 1m, we could increase fly altitude until 2700m; and for a grid of 1.5m until 2250m. Consequently, these results imply a more efficient flight in terms of height and time of survey and less data to be processed and therefore a less expensive project. An agreement contract is now to be signed with the company.

STEREOCARTO

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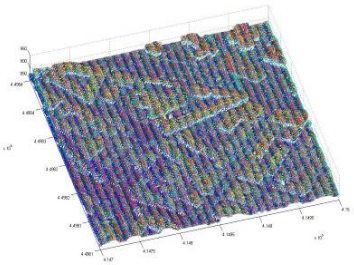

Simulation of stochastic radar signals

Executive summary

We modeled, designed and implemented a novel simulator of a stochastic radar environment.

Challenge overview

In the framework of a wide research effort, the company, «SELEX Sistemi Integrati» was looking for an effective simulation tool for the radar environment. Hence they contacted and funded our lab as one of the leading groups in stochastic algorithms in Italy for carrying out the fore above research.

Implementation of the initiative

The initiative has been carried out in a one-year contract. During the implementation, regular meetings have been held between our group and the industrial partner. In the early stage of the project, these meetings have been the way to acquire the necessary background information about radar systems and to understand the technical requirements asked by the partner. In later developments, meetings had the goal of tuning the theoretical developments and the subsequent implementation to the company's needs. Our work has been carried out by internal resources, both full-time tenured researchers and post-docs.

The problem

The problem consisted in giving a suitable representation of the objects populating the radar environment (targets, clutter, disturbances), considering their properties as the realizations of stochastic processes. Quite a lot of modeling literature has been developed in the past decades about various aspects of radar objects. Hence the main modeling issues in the work were about creating a general stochastic framework, which included some of the most suitable available algorithms, together with novel ones.
The interaction with the experienced company's staff has been very useful for the determination of the modeling parameters, as well as for making effective the computer implementation of the algorithms.

Results and achievements

After a thorough study, we have been able to propose, in an integrated view, a wide range of algorithms and mathematical models for objects in the radar environment. Moreover, a few selected algorithms have been implemented in a simulation tool, which has been delivered to the company. The quality of algorithms has been assessed in terms of their ability to mimic real-world radar signals, with a concentration on some critical issues for current radar detection, e.g., the effect of rolling blades in extensive wind-power fields. The impact of the initiative is expected to take place in the following months, when our tool will be integrated in a novel testbed for radar systems.

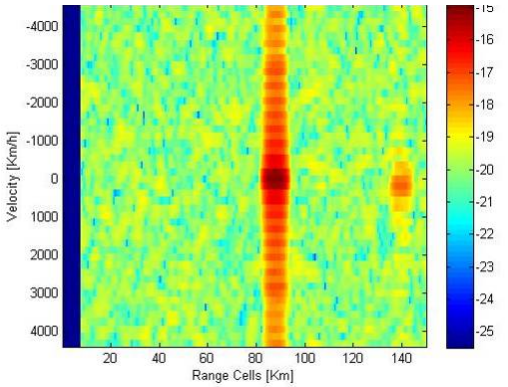

Fig. 1: The transform of the simulated return signal, identifying two targets.

Lessons learned and replicability

The initiative has been a fruitful example of how academic and industrial know-how can effectively merge into a novel product. While future interactions with the same industrial partner are expected on other topics, the collaboration experience came from a specific technological need for a simulation tool by the company. However, we might be open to work on other environment simulators, besides the field of radar systems.

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contact: Ing. Mario Teglia

Name of the Laboratory:
Istituto per le Applicazioni del Calcolo, CNR

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Optimization of Satellite Coverage

Executive summary

For effective monitoring of environmental activities by a satellite, it is the main goal to achieve maximum coverage throughout a short period of time. Due to technical restrictions of the satellite hardware, it is only possible to use the camera for a limited time period per orbit, while rotating around the Earth. The main goal is to determine the time intervals for which the coverage with respect to given target areas is maximized and the restrictions such as contact to ground stations are satisfied. To achieve a continuous objective function for the nonlinear optimization method, the coverage is modeled by polygons integrated on a sphere. For acceptable computing times, special investigations had to be made in order to achieve fast gradient computations and optimal satellite trajectories.

Challenge overview

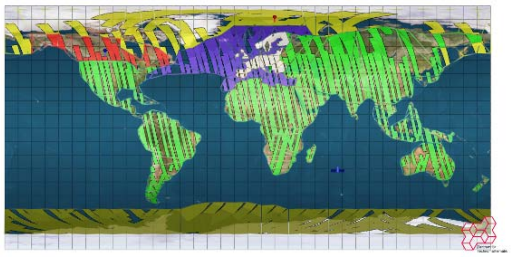
Earth observing technologies from space have become a key role in various fields of engineering and metrology. There is a rising need for global monitoring where satellites have to deliver valuable data about our planet from which we get a better understanding and an improved management of the earth and its environment. Demands for these data are increasing on a daily basis as decision-makers are faced with responding to environmental change, managing sustainable development and responding to natural disasters. In this project sensors are mounted on a satellite which rotates around the earth at a fixed orbital position taking pictures of the earth's surface. The opening angles of the left or right looking sensors are fixed. The increasing requirements for those orbital observations due to limited resources, a demand for high accuracy and various technical restrictions have become the major motivation to this project. The main technical restriction, in this project, caused that the cameras of the satellites can only be switched on for a limited time amount, while rotating around the earth. The goal is now to maximize the coverage of the satellites footprint according to the assigned target areas.

Implementation of the initiative

In partnership with the OHB-System AG a software program which uses innovative mathematical techniques to analyze and optimize satellite constellations used in global monitoring was developed. The new software is the first to automatically determine optimal satellite trajectories and the precise maximum observable area within seconds and minutes. Previous methods often took weeks or even months to arrive at an acceptable solution.

The problem

So far the covered area could only be calculated over a discrete grid by considering if a grid point is covered or not. The disadvantages are low accuracy and lack of differentiability because there is no information if the region between grid points has been observed or not. A different approach to calculating the coverage is obtained by using convex disjoint polygons as a framework to come up with a differentiable coverage calculation. Here the covered area of the satellite is expressed by convex polygons which can be integrated on the unit sphere analytically.



Results and achievements

The main achievement of this project was the development of a software tool to automatically optimize satellite trajectories and sensor operating time schedules for global observation. An easy to use graphical interface was developed to operate the software. The technical restrictions were formulated into mathematical constraints and a nonlinear optimization method was used to find a solution to the arising problem. Both partners were honored with the Löhn Award 2008 for the project. The Löhn Award recognizes outstanding transfer projects in fields using competitive technology along with knowledge transfer between science and business.

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Simulating rowing boats

Executive summary

Rowing is a sport with old traditions. Yet it is also a tough competition where new technologies and materials are experimented with to obtain the best from the athletes. The dynamics of a rowing boat is complex due to the strong interaction between the movement of the rowers and that of the boat, and that between the boat and the water free surface. Studying this complex system has been a beautiful mathematical task, proposed to the MOX Laboratory of the Department of Mathematics of Politecnico di Milano by an important Italan manufacturer of rowing boats, Filippi Lido S.r.L.

Challenge overview

The contact between MOX and the Filippi company was rather accidental. A engineer of the company was presenting some aspects of rowing at a school and one of the MOX researcher attending the school contacted him. Often, long standing collaborations start by chance! The idea behind the collaboration is the observation that standard methods to optimize a boat aim to minimize the viscous drag at the mean motion. Boats experience complex accelerations & decelerations during a race, which in turn dissipate energy by generating waves on the water surface. Thus, to obtain the best results one has to account for the full dynamics of the boat.
The mass of the rowers is usually greater than that of the boat itself: it is evident that their motion, not just their action at the scull, plays a predominant role in the boat dynamics. Finally, the interaction with the free surface is a complex mathematical task, which may lead to complex and computationally costly numerical algorithms. Therefore, we decided to develop a range of different hydrodymic models. A rather simplified model, based on potential theory, to have a quick tool for preliminary analysis, up to the most complex which requires to solve the full-fledged Navier-Stokes equations.

Implementation of the initiative

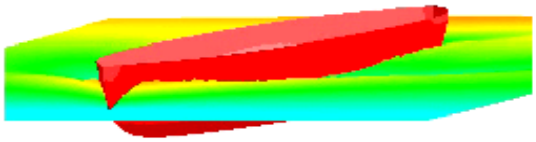
The company funded a PhD student at MOX and contributed to the extra costs. Two researchers supervised the activity of the PhD student, who was also flanked by several undergraduate students carrying out their final year project on this topic. A person with programming skills was hired for six month to help with the set up of the user interface. Collaboration with other universities were also set up to obtain experimental data.

The problem

The reference mathematical model is based on the Navier-Stokes equations with free surface coupled with a mechanical model for the boat-rower system. The boat is considered as a rigid body, the rowers as masses moving with a prescribed motion. Thus, the forces acting on the boat are the hydrodynamic forces, the inertial forces of the rowers and the thrust at the oarlocks. This general setting has been tackled using models of different complexity. In the simplest one the hydrodynamic action is reduced to added mass and damping effects on the boat dynamical system. These are computed off-line by solving a potential problem for the radiated waves and integrated by empirical formulae for the viscous drag. An intermediate model considers a quasi-2D formulation where the boat is accounted by imposing an inequality constraint on the water surface. Finally, the more complex model adopts a Reynolds Averaged Navier-Stokes formulation and a Volume-of-Fluid method to treat the free surface.
The main difficulties are linked to the proper acquisition of the rower motion, and by the fact that the boat is intrinsically unstable. Therefore, a control mechanism, which mimics the actual action of the rowers, had to be implemented as well.

Results and achievements

The code is currently installed at the company site. The collaboration is still on-going and is focusing on calibrating the model and validating it against experiments.



A snapshot of the boat with the surface waves generated by the boat motion.

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Waves for Ship-simulation

Executive summary

Real-time computation of waves for ship simulation.

Challenge overview

Our group contacts MARIN (http://www.marin.nl/) to explain the expertise we have in fast solvers for simulators. In the company there are a number of mathematicians (PhD alumni of the TU Delft), so the communication went smoothly. After a first discussion we decided that the best strategy is to define a Master Student project.

Implementation of the initiative

The implementation went well. An excellent master student located for 4 days a week at MARIN and 1 day at the TU Delft. MARIN paid 400 euro per month and housing for the student. The supervision at MARIN had a high quality.

As usual part of the project was confidential but that does not lead to problems for the master thesis. It is on the web:

http://ta.twi.tudelft.nl/nw/users/vuik/numanal/wout_eng.html

The problem

The waves should be computed in a wide region. Since they should be refreshed every millisecond, the computing time should be very small. At the start of the project it is only possible to simulate a small region of 50m x 50m. This is insufficient for a realistic wave pattern. For instance the waves does not interfere with the ship or the banks of the river. The problem boils down to a fast iterative method for a Poisson type problem.

Results and achievements

We proposed to use a fast Conjugate Gradient with a parallel preconditioner. It appears that the speedup was not good enough. After combining it with a second level preconditioner (coarse grid acceleration) the speedup was good enough to use a 200m x 200m area. The next step is to accelerate the method further by using video cards (GPU). After this it should be possible to simulate a 2km x 2km area.

The project was ended by implementing a subroutine in the C++ package used by MARIN. A master thesis was written (the grade leads to a "cum laude" distinction). And the results are to be presented at the International Conference on Computational Science 2010 (ICCS 2010), May 31 - June 2, 2010.

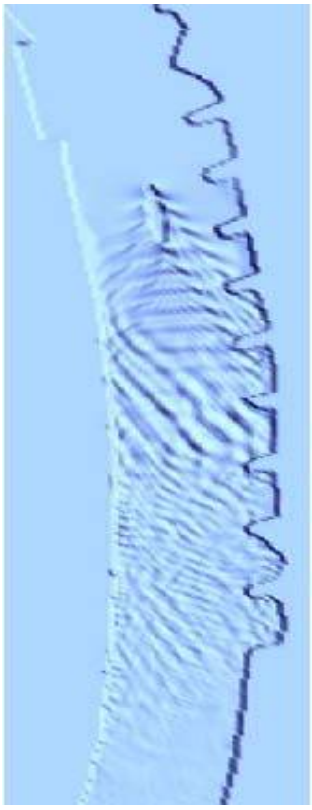

Figure. Wave pattern around a ship sailing through the river Ijssel.

Lessons learned and replicability

Good mathematical knowledge, communication skills, hard work are crucial ingredients for success.

Company details:

MARIN
http://www.marin.nl/
Haagsteeg 2
6708 PM Wageningen

Danger: rogue waves

Executive summary

Sailors have always told tales of rogue waves, describing encounters with gigantic walls of water that appear without warning and drag ships to the depths below. Until recently, oceanographers dismissed these accounts as nonsense because mathematical models predicted that such an immense wave was almost impossible. That all changed on New Year's Day 1995, when measuring instruments aboard the Draupner oil platform in the North Sea detected a wave nearly 26 metres high: the first verifiable rogue wave.

Challenge overview

Mathematicians have studied waves for centuries but this incident made them realise that more research was needed, as it demonstrated that rogue waves can occur more often than the existing linear models would predict. Now, the development of new nonlinear models has given a greater understanding of what causes rogue waves and how to avoid them.

Rogue waves appear suddenly in the middle of the ocean, seemingly without cause, and disappear just as quickly. To understand this constantly changing environment a commonly used statistic is the significant wave height, or the average height of the highest one-third of waves. The significant wave height already corresponds to a larger-than-normal wave, but a rogue wave is twice as high as this or more. At the time of the Draupner incident, the significant wave height was around 11 metres, far below the level of the 26 metre rogue wave.

In the 1960s, Benjamin and Feir found that waves of constant height would become unstable over time, with one wave “borrowing” energy from the others to become up to five times larger. A rogue wave works in much the same way, and both kinds of wave can only be explained by the nonlinear Schrödinger (NLS) equation.

Implementation and results

The system of using wave statistics over regions of the ocean has been in place for the last 20 years or so, but a recent development was the Benjamin-Feir index (BFI), which was introduced in 2003 by Peter Janssen, a mathematician at the European Centre for Medium-Range Weather Forecasts (ECMWF) in Reading. The BFI measures the level of nonlinearity in a given sea region, with higher levels of nonlinearity indicating a greater chance of rogue waves. Janssen showed how to calculate the BFI from observational data and the NLS equation, allowing for a more accurate prediction of rogue waves than previous methods.

Mathematicians have also worked with oceanographers to lower the average error in predicted wave heights from 30% to 10%, reducing uncertainty and allowing shipping companies to handle unexpected events more easily. Extending the NLS equation to cover waves travelling in multiple directions is now an active area of mathematical research.

The BFI is equal to the ratio of the steepness of the waves and the width of the frequency spectrum, and determines the kurtosis, or deviation from the normal, of the wave height distribution. If the spectrum of a particular sea state is narrow and the waves are steep, the BFI is large and deviations from the normal distribution are more likely. Conversely, if the spectrum is wide and the waves are shallow, the BFI is small and rogue waves are unlikely to occur.

Loughborough University

ECMWF

EPSRC Pioneering research and skills

Institute of mathematics & its applications

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http://www.ecmwf.int/

Modeling of sails

Executive summary

We modelled, designed and tested sails for the most worldwide known match-racing regattas.

Challenge overview

Yachts racing conduct to different kinds of competition between research centres and sail manufacturers. A challenge concerns the best sail modelling. During 80's and 90's several numerical models were investigated in Australia, USA, and Europe (Germany, France, and United-Kingdom). It uses triangular element or quadrangular element, implicit scheme or explicit one. The objective was to provide better patterns for sail construction made of novelty materials as high performance aramid fibbers.

Implementation of the initiative

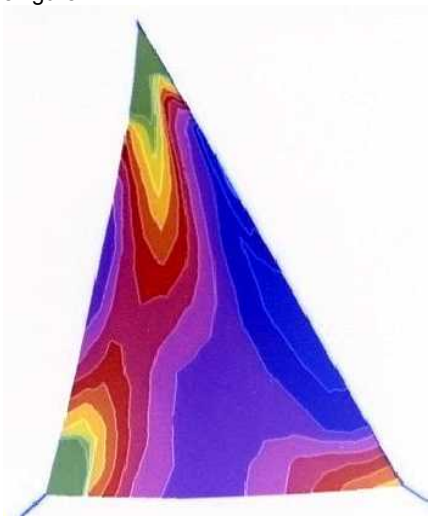
The problem clearly starts at the beginning of the racing challenge by using the points of view of the yacht-syndicate design team, the manufacturers as well as the crew abilities. The competition between national yacht syndicates will result in more efficiency in mechanical and numerical modelling. Confidentiality issue is a main challenge. Sail analysis research has provided many innovations in conception and fabrication.

The problem

The industrial competition between the manufacturers (fabric, sail) set the problem objectives. The numerical model concerns the thin shell theory and the non-linear finite-element method. The mathematical challenge is the justification of both continuous and discrete models. It used equally pre-stress material and contact method between flexible structures. The problem is situated in the theory of elasticity and is solved by a membrane finite-element method. The numerical solution must be justified mathematically and understood by the end-users.

Results and achievements

Computation results were available and their accuracy was proved in both mathematical and sport senses. Several innovations concern sails themselves (fabric pattern), battens, masts and rigs. The pattern of sails is a geometrical assembly of developable fabric sheets made of fibbers pasted on films. The reduction of sail weight particularly near head point increases the yacht performance. The gain is assumed to be relatively small in term of second/mile but sailing race can be win with just a small time difference (<1s), even after a 4 hours race. The stress map shows here after the principal stress contour of a Genoa. The figure shows one of our computed Main-sail. It is the second from the left on the figure.



Lessons learned and replicability

For academia, this join-venture in sport is successful by showing the powerful of applied mathematics endowing sailing race with research. Others ship designs, like sails cruising-boat, multihull yachts, mast manufacturers, has used this kind of computation. The methodology is useful to compute new designs and give performance predictions.

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Mathematical modelling of complex materials in underwater sonar systems

Executive summary

A long term collaboration between the University of Manchester (UoM) and Thales UK is helping to understand, model and improve the properties of complex materials used in advanced sonar systems.

Challenge overview

Thales UK's underwater systems business specializes in acoustic, sonar and anti-submarine systems serving a broad range of platforms. The Royal Navy's latest generation submarine, the Astute-class, can detect the quietest submarines thanks to the planar flank arrays, and active low frequency sonar, which form parts of the integrated sonar system, S2076, provided by Thales.

Many sonar systems rely on knowledge of the constitutive behaviour of inhomogeneous visco-elastomeric (VE) materials. The VE acoustic baffles are often subjected to massive compressional forces, leading to a large deformation and nonlinear pre-stress of the material. The study of the subsequent incremental response of the materials can assess their stability, incremental constitutive behaviour and fitness-for-purpose. Their inherent inhomogeneity and complex microstructure leads to large gaps in the understanding of the constitutive behaviour of such materials in a number of regimes, including that of pre-stress. The aim of the current project is to build mathematical models in order to improve this understanding.

Implementation of the initiative

Thus far, two EPSRC CASE PhD studentships and the award of a Royal Society Industry Fellowship have supported these aims. Two new CASE PhD studentships have just started, together with an EPSRC postdoctoral grant and a Leverhulme Trust award. Various Masters and Undergraduate projects have also been carried out. All these diverse mechanisms of funding have supported and will continue to support progress in this area. In particular they have enabled the growth of a large group with expertise in wave propagation in complex materials in the School of Mathematics at the UoM.

The problem

The broad problem investigated by the group at the University of Manchester and Thales UK is to characterise the wave propagation properties of the acoustic baffles used in underwater applications when subjected to large hydrostatic loading. David Abrahams and William Parnell of UoM comment "in order to model such complex heterogeneous materials it is necessary to employ fundamental mathematical tools such as the techniques of asymptotic homogenization, multiple scattering theory, finite elasticity and viscoelastic theory." Phil Cotterill from Thales UK, and a current Royal Society Industry Research Fellow at UoM, adds "only by developing a detailed mathematical understanding can one obtain a phenomenological picture of the wave processes at work."

The physical and mathematical models developed by the team at the UoM, which presently consists of over ten active researchers, are helping Thales predict the behaviour of current acoustic materials and assist in the design of future sonar systems.

Results and achievements

The varied projects have provided training for many researchers, a number of whom have gone on to work in related industries. The team has derived the first theory pertaining to wave scattering and homogenization in pre-stressed media in the presence of inhomogeneous deformation. Results from the studies have been fed into software at Thales thereby providing an improved modelling suite. Future (larger) projects will permit even better predictive capability within such modelling tools. The theory developed has potential applicability for materials used in many other areas including environmental, industrial and biological applications.

Contacts

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THALES

EPSRC
Engineering and Physical Sciences Research Council

THE ROYAL SOCIETY

Optimization Algorithms in Electronics Design Automation

Executive summary

The aim of the research was to find an efficient algorithm to solve a problem of nonlinear global optimization connected to the design the doping profile of semiconductor devices as well as to circuit design problems.

Challenge overview

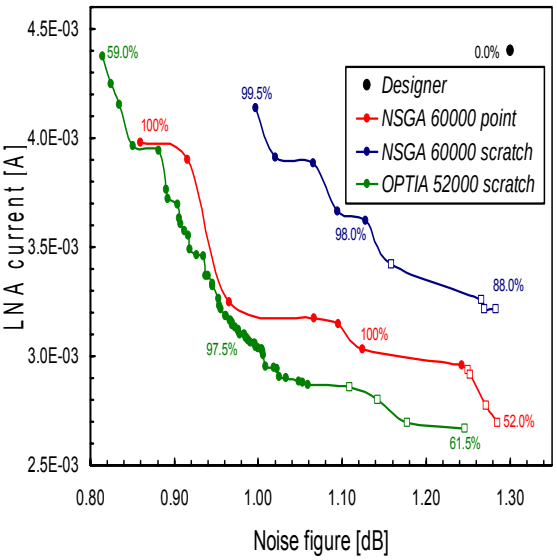
The ever increasing computing power and the development of fast and effective simulation tools, has contributed, in the last years, to an increasing interest in the optimal design of semiconductor devices, analog circuits and systems, which can nowadays be based on robust and effective optimization algorithms. For the semiconductor devices, the most prominent design variable (and correspondingly the unknown in the associated optimization problem) is the device doping profile, which describes the (charge) density of ion impurities in the device and a typical objective of the optimization is to improve the current flow over some contacts by a slight modification of the device doping profile. The mathematical version of this optimal design problems it is important to find suitable functionals to be minimized; on the other hand one has to choose an appropriate mathematical model to describe the physical device behaviour. Nowadays, there is a whole hierarchy of semiconductor device models available, ranging from the microscopic Schrödinger–Poisson model to the classical energy transport or the classical drift diffusion model. Obviously, one has finally to choose an appropriate class of optimization algorithms for the solution of the respective design problem.

Implementation of the initiative

In the engineering community, global optimization algorithms are most frequently used, since they only require a simulation tool for the forward problem. Our research adopted multi-objective optimization algorithms in Electronics Design Automation (EDA). In fact, this class of global optimization algorithms has been the “choice” for such a large class of systems in EDA, and, in particular, such usage of black-box optimization is the best way of tackling many of these problems

The problem

The effective optimization algorithms have to balance accuracy, robustness and computational effort. Typical analog integrated circuit optimization problems are computationally hard and require the handling of multiple, competing, conflicting, and non-commensurate objectives having strong nonlinear interdependence. Our methodology tackles the problem by non-linear global optimization algorithms to produce trade-off solutions on the Pareto Frontiers. In this research, device and circuit design problems have been modelled as a constrained multi-objective optimization problem defined in a mixed integer/discrete/continuous domain.



Results and achievements

The following real-life case studies, Low Noise Amplifiers, Leapfrog Filter, Ultra Wideband LNA, silicon diodes, and different MOSFETs were selected as “test bed”. The proposed class of derivative-free optimization algorithms was shown to produce acceptable and robust solutions in the tested applications, where state-of-the-art algorithms, commercial solutions and circuit designers failed. The results show significant improvement in all the chosen design problems

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Mathematical modelling of charge transport in semiconductors

Executive summary

We developed a macroscopic model and numerical code for the description of the heating of the semiconductor crystal due to the electron flow in nanoscale devices. In practical cases shrinking has an order of magnitude of some tens of nanometers and can influence considerably the operation of the devices.

Challenge overview

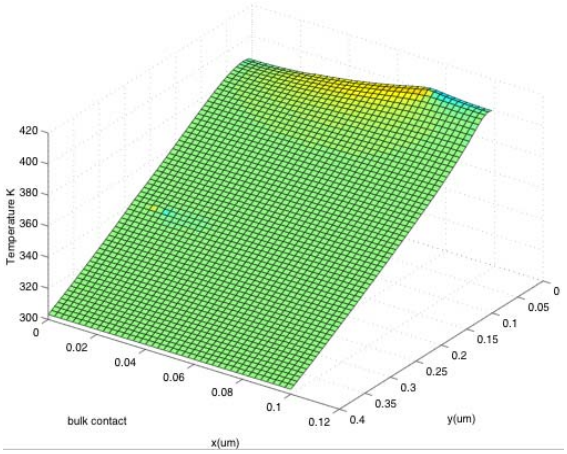
This research has involved the network COMSON (COupled Multiscale Simulation and Optimization in Nanoelectronics). It consists of five universities, Polytechnic of Bucarest, University of Calabria, University of Catania, Technical University of Eindhoven, University of Wuppertal, and three companies, the INFINEON (now QUIMONDA), site of Munich, the NXP in Eindhoven and the ST-Microelectronis, site of Catania.
The main objective of the Consortium was to realize an experimental Demonstrator Platform in software code, which comprises coupled simulation of devices, interconnects circuits, electromagnetic fields and thermal effects in one single framework. It connects each individual achievement, and offers an adequate simulation tool for optimisation in a compound design space. The platform is capable of analysing medium sized coupled problems of industrial relevance, thus offering a chance to develop advanced mathematics for realistic problems in nano-electronics

The problem

The task of the Catania group was the development of a macroscopic model and numerical code for the description of the heating of the semiconductor crystal due to the electron flow in nanoscale devices. Thermal lattice effects in electron micron devices are negligible, but shrinking the typical scale to few tens of nanometers they become relevant and influence considerably the operation of the electron devices. The model has been obtained by the moment method applied to the Boltzmann-Peierls kinetic equations for the electron-phonon system, closing the resulting evolution equations with an approach based on information theory. An appropriate numerical method has been formulated for the simulation

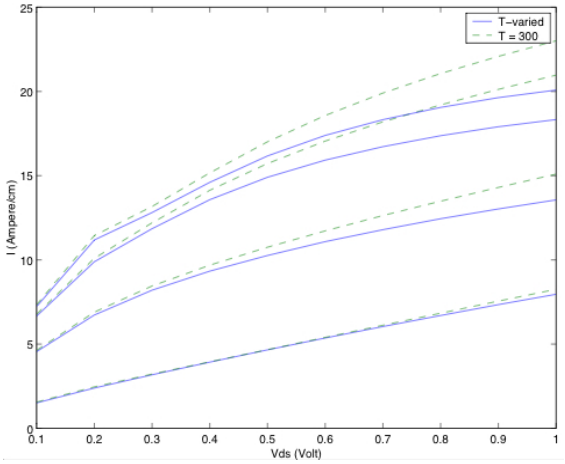
Results and achievements

As study case we have considered a particular semiconductor device, called MOSFET, which is one of the basic elements in integrated circuits. The importance of the thermal effects is shown by the following figure



It is possible to see in a MOSFET with a length of 50 nanometers, parts of the devices with hot spots, where the temperature is much higher (about one hundred degrees) than the room temperature. Similarly in the figure below, there is a clear influence of the temperature at high electric field on the characteristic current-voltage curves that synthesise the performance of the device and represent one of the main needs for the design of integrated electric circuits

Contact: Vittorio Romano, Department of Mathematics and Computer Science, University of



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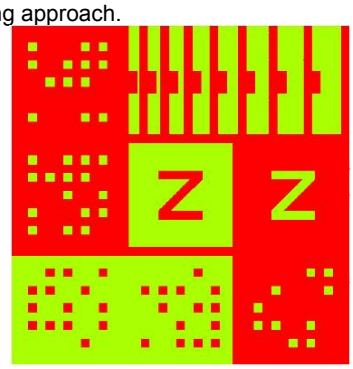
Online simulation of 3D nano-optical components

Executive summary

Modern information technologies are based on photonic and electronic components with feature sizes in the micro- and nanometer scale. Industrial production environments must be able to process and control the various parameters of production steps within an adequate accuracy. Regarding optical process steps, this requires the solution of the 3D Maxwell's equations. Moreover, the production flow demands that measurement and control processes must be carried out in real time, meaning that complex simulations must be done in seconds. We developed a reduced basis approach to the solution of 3D Maxwell's equations meeting these requirements. We have shown that typical tasks like pattern recognition, position sensing and shape optimization can be carried out both efficiently and reliably.

Challenge overview

The main challenge is to deliver simulation results supporting production processes in real time. Since conventional simulations involving 3D Maxwell's equations may take hours up to days this seems to be impossible at first glance. But as the structures under investigation usually depend only on a few parameters (geometry and material data) and the parameter range is known in advance, a reduced basis approach with a careful decomposition into online and offline parts accompanied with appropriate error estimation techniques offer a promising approach.



Test mask for optical lithography. The light passing the mask will be influenced by the geometry of the openings (green) and diffraction effects.

Implementation of the initiative

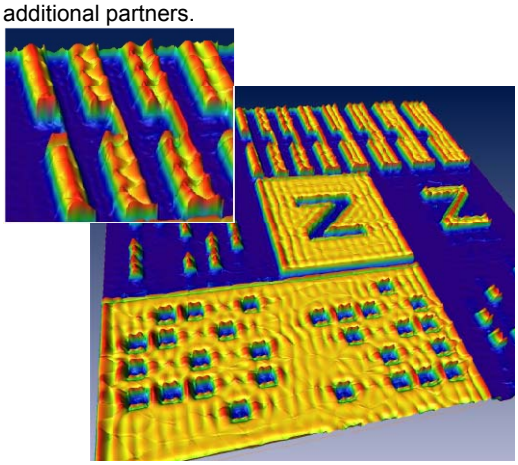
The first steps towards reduced basis techniques for 3D Maxwell's equations were motivated by companies in the business environment of optical micro-lithography. Recognizing the technology as a door-opener for many different nano-optical applications from lithography over metrology to component optimization we decided to develop the approach in three phases: a) theoretical investigation of the method and its potential, carried out by the Zuse Institute Berlin (ZIB) and JCMwave GmbH, partly together with Cadence Design Systems, Inc., b) the phase of industrial research, currently carried out by JCMwave and supported by research results from ZIB, c) subsequent product development led by JCMwave.

The problem

The theoretical part of the project encompassed three major problems. First, we derived a general framework for object parameterizations yielding an affine structure with respect to the parameters. Second, we developed an efficient offline/online decomposition of the solution process. Third, we developed a new error estimation technique essential for both the online and the offline part based on the residual error estimation approach.

Results and achievements

We have shown that our reduced basis approach developed in the project enables real time solution to parameterized 3D Maxwell's equations. First applications were realized in optical lithography and metrology. Based on the success, different major companies and institutions, including Nicon Corporation, Cal., and Physikalisch-Technische Bundesanstalt, Germany, initiated joint research and development projects. For JCMwave the results stimulated a new product development plan with additional partners.



Optical near field after passing the mask and zoom into a detail.

Contact

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Energy

Bentonite Buffer in Nuclear Waste Management

Executive summary

Helsinki University of Technology[1], University of Jyväskylä and Numerola Oy have co-operated in a research project which investigates the numerical modeling of bentonite buffer in nuclear waste management.

Challenge overview

Professor Rolf Stenberg from Helsinki University of Technology suggested Numerola Oy to take part in the Finnish research programme on nuclear waste management to develop the numerical modeling of bentonite buffer. Motivation for the initiative was to improve the software development in the project, especially to make it more continuous and consistent. During the past ten years, Numerola has developed its own software platform called Numerrin for numerical modeling and optimization. This was seen as a suitable tool to continue the development of numerical models and methods to study the behaviour of bentonite buffer.

Implementation of the initiative

The project was initiated by preparing a research plan for a funding application to the national research programme. The Department of Physics at the University of Jyväskylä participated in the application as a third partner. Their role was to coordinate experimental studies and to develop physical modeling of the bentonite buffer. The group at the Helsinki University of Technology concentrated on the development of numerical methods while Numerola was responsible for the software development.

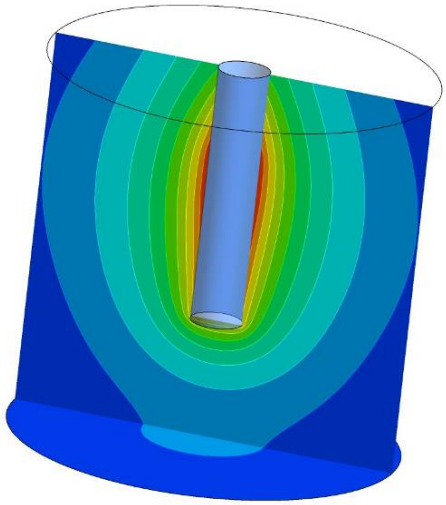
The problem

Previous research work had already resulted in a thermo-hydro-mechanical multiphase model, which gave a starting point for this project. However, more efficient and robust methods and implementations were needed for the numerical solution of the equations. Also the models needed to be improved and extended to more complicated situations. Currently chemical reactions are being coupled to the physical equations.

[1] Starting from 2010 Helsinki University of Technology is a part of the new Aalto University.

Results and achievements

The project has proceeded as expected in the research plan, and is still active. Both the mathematical models and numerical methods have been improved as a result of the co-operation. Recently the Technical Research Centre and Geological Survey of Finland have joined the project as two new partners.



Lessons learned and replicability

The co-operation has been fruitful and it has provided a concrete sample problem to test and develop the capabilities of the Numerrin platform. It has turned out to be a flexible and efficient tool for various modeling purposes and it is currently used in many research projects around Finland as a computational tool. It thereby supports both academic work and practical utilization of the research results.

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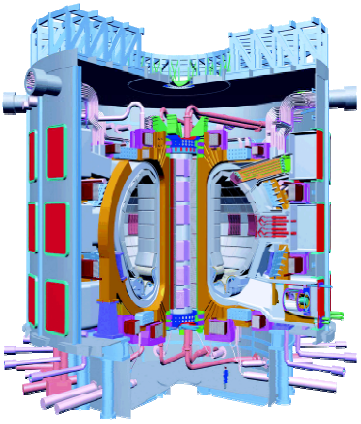
Intelligent Video Understanding Applied to Plasma Facing Component Monitoring

Executive summary

Infrared thermography has become a routine diagnostic in many magnetic fusion devices to monitor the heat loads on plasma facing components (PFCs) for both physics studies and machine protection. In ITER[2] perspective, the development of a versatile, reliable and fully automatic system for the real-time monitoring of PFCs becomes essential.

Challenge overview

The understanding of the observed phenomena is not a trivial task and requires a high degree of expertise in both image/video processing and plasma physics. This research project aims at applying the scene understanding framework developed at INRIA for activity recognition to PFC monitoring during plasma operation.



ITER

Implementation of the initiative

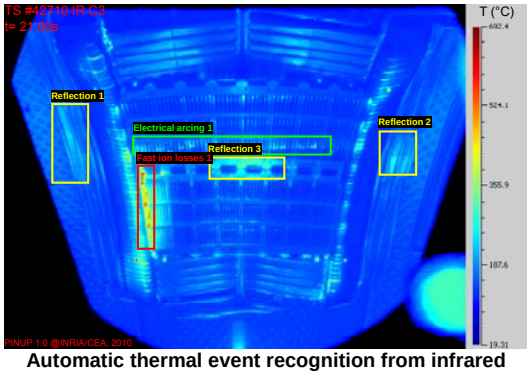
The cooperation between INRIA and CEA is born in September 2005 from the common goal to put together efforts for the success of ITER. In 2008, a research collaboration project named *moniTORE*[3] between INRIA team-project PULSAR and the PFC group of CEA/IRFM at Cadarache and financially supported by INRIA has permitted to recruit a post-doctoral researcher and several master trainees. This project is now supported at national level by the French Federation for Magnetic Fusion Research and at European level by EFDA (European Fusion Development Agreement) through a research fellowship.

The problem

Many operational tasks as machine protection functions can be assured on the basis of qualitative imaging. The main problem is thus to be able to automatically perform a semantic interpretation of a dynamic scene from multi-sensor numerical data. In a mathematical point of view, semantics can be extracted using statistical models or fuzzy logic. The second problem relies on real-time constraints imposed by the control system during plasma operation. Vision algorithms must then be designed with the help of high computational performance hardware as FPGAs to perform in real-time.

Results and achievements

A major achievement resulting from this partnership is the implementation at Tore Supra (a French Tokamak producing long plasma discharges) of an unique prototype of infrared imaging diagnostic relying on intelligent reasoning for real-time detection and recognition of abnormal thermal events during plasma operation. This constitutes a good starting point toward a real-time automatic feedback control system based on intelligent signal and image processing. We hope that this control system will be part of the foreseen infrared viewing system of ITER, which aims at protecting its PFC components.



Automatic thermal event recognition from infrared images of Tore Supra PFCs during plasma operation

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INRIA
centre de recherche SOPHIA ANTIPOLIS – MÉDITERRANÉE

[2] International Thermonuclear Experimental Reactor
[3] real-time *moni*toring of imaging diagnostic applied to *TORE* plasma operation

Modeling coal combustion

Executive summary

Mathematical models and numerical methods for the simulation of pulverized coal furnaces of power plants were developed under contract for the company ENDESA.

Challenge overview

The contact with ENDESA started in 1989 through Prof. Juan Casares, who was the director of the Department of Analysis of Results in the Power Plant of As Pontes (Spain). This plant had numerous problems with slagging, fouling and pollutant emissions (due to a more restrictive normative). The non-existence of well established commercial packages for numerical simulation of coal combustion prevented a good understanding of the phenomena taking place in the interior of a pulverized coal furnace. This lack of knowledge in turn prevented the company from adopting strategies to improve the installation through a modification in the operating conditions. The group then tried to establish and numerically solve a 3D mathematical model for the behaviour of a pulverized coal furnace. The results provided by the program were used by the engineers to improve the efficiency of the generation groups of the As Pontes power plant, as well as to state guidelines for their adaptation to the combustion of coal blends (lignite of the local mine and imported sub-bituminous coals).

Implementation of the initiative

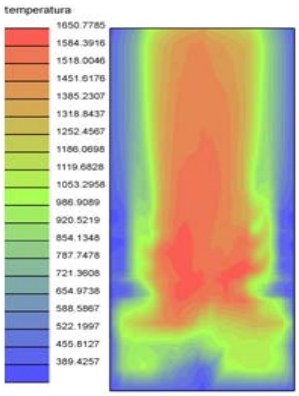
Using funds of the PIE program, an investigation project was agreed for a period of three years (1991-93) with a equivalent budget of 127,000€ between ENDESA and the Department of Applied Mathematics of the USC. This project gave rise to the group in mathematical modeling of combustion, directed by Prof Alfredo Bermúdez, and complemented with two pre-doctoral students. The international expert Prof. Amable Liñán provided an introduction into the theory of combustion. The project was subsequently extended for a period of one year and a budget of 87,500€, with the objective of including a graphical user interface and the corresponding user guides in the computer code, as well as a training program for the technicians of the company in the As Pontes power plant.

The problem

The mathematical model must contain the fluid dynamics equations for a turbulent, multiphase and reactive flow, where the energy transport by radiation is important. The disperse character of the coal particles led to an Eulerian description for the gas phase and a Lagrangian description for the solid phase being considered. The main outcome was the development of a completely new model for the combustion of coal particles by using the high activation energy asymptotics methodology. With respect to numerical solution, we developed high-order semi-Lagrangian finite element methods for the discretization of the partial differential equations of the gas phase model. This choice was encouraged from the experience of the group in the analysis of this kind of methods. Finally, in order to determine and adjust the boundary conditions and some of the parameters involved in the models, the staff of the Plant carried out different measurement campaigns.

Results and achievements

From the obtained results, some of the problems observed in furnaces were justified and thereby some modifications in operating conditions or in the geometrical design could be proposed in order to improve the efficiency. New projects have since been agreed between ENDESA and the research group for simulating new installations and operation conditions.



Lessons learned and replicability

This initiative has been the seed of the research group in combustion which is now composed by 3 permanent positions and 3 doctoral students. Other students subsequently secured positions in private companies. The computational tool SC3D, which can be seen as a precursor of the present combustion commercial packages, is now being updated to include new models and improved numerical methods.

endesa generación

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Optimal Flames

Executive summary

Temperature distribution in industrial furnaces strongly affects the quality of ceramic products: optimal control techniques may help to improve the production.

Challenge overview

Edilcuoghi, a leading Italian producer of ceramic tiles, estimated that 12% of the production did not satisfy the high standards of the company. This was mainly due to excessive temperature oscillations inside the furnaces in which the tiles were processed. Moreover, it was observed that changing the furnace burners, flames with different shapes are obtained, causing very different temperature distributions. Hence, the R&D department came up with the idea of finding an "optimal flame shape" that makes the temperature of processed tiles as close as possible to a desired value. Indeed, based on this information, the corresponding optimal nozzles can be designed. However, the available commercial softwares were inadequate for such analysis. *Edilcuoghi* contacted the Modeling and Scientific Computing Laboratory (MOX, Politecnico di Milano) to develop in-house optimization algorithms and softwares that could serve their purposes.

Implementation

A two-year research contract was signed between MOX and *Edilcuoghi*. The research was initially set up based on internal resources, including a Master degree student, and later by hiring an engineer working on the established guidelines. First, a mathematical model of heat exchange was developed. Radiative heat transfer was taken into account by representing flames as radiating surfaces at high temperatures, and by non-local boundary conditions for the heat equation inside the furnace walls. Then, Optimal Control techniques were used to derive the equations expressing the sensitivity of the temperature with respect to surface variations. The numerical approximation of the model was performed by the Boundary Element Method. A Constrained Gradient Method was developed for the minimization of a "cost functional" measuring the deviation of the temperature from the target profile. Different optimization algorithms (genetic algorithms) and more complex heat transfer modes (convection) were considered as well.

Results and achievements

The critical dependence of the temperature profile on the radiative shapes was confirmed by computer simulations. Moreover, the optimal shapes were found to be non-symmetric, with a reduced width and an increased height. The quantitative results on the optimal shapes and on the temperature profiles were useful for *Edilcuoghi* to design specific nozzles for their furnaces.

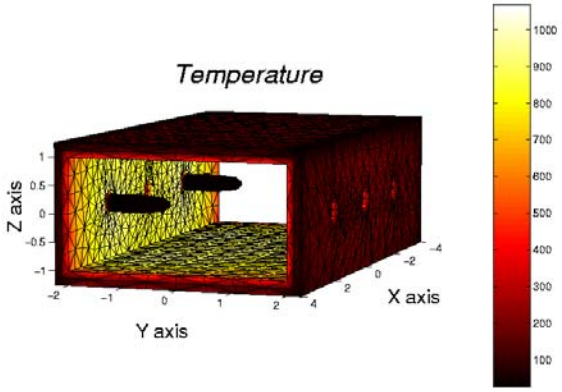

Figure A: Temperature (Kelvin) inside a section of the furnace. The internal, lower horizontal surface is where tiles are processed and temperature is controlled.

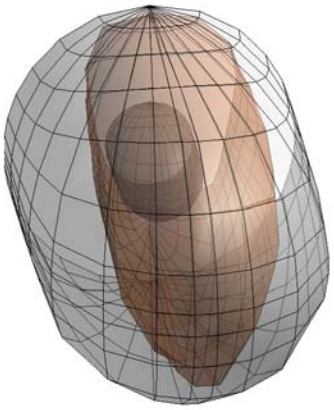

Figure B: Optimal radiative shape (enclosed between the maximal and minimal admissible shapes).

Replicability

The scientific consultancy conducted for *Edilcuoghi* proved that optimal control techniques and shape optimization can be effective tools to improve industrial production involving thermal processes, also when complex radiative heat exchange conditions have to be accounted for. The developed software can be used or expanded to treat similar problems, supporting the engineers in designing radiative surfaces and heat exchangers.

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Optimizing a complex hydroelectric cascade in an electricity market

Executive summary

In hydroelectric power stations it is possible to manage the storage of water in reservoirs and to release water downstream, thus producing energy. The profit resulting from this process depends on the price of energy at times of energy consumption and energy production. Having the possibility of pumping water upstream at times when the energy price is low, the energy stored may then be made available at a later time when prices are higher. This study considered a branched model for a hydroelectric power station interacting in a cascade arrangement, in order to provide guidance in decision-making aimed at maximizing the profit.

Challenge overview

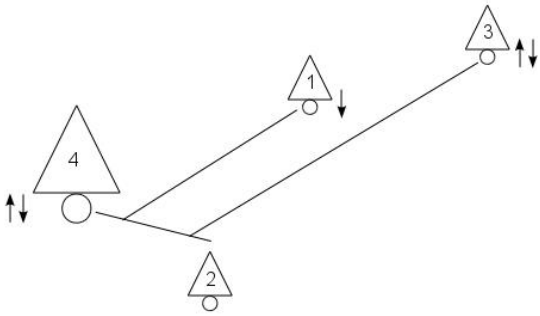
The problem involving a specific hydroelectric cascade power station was posed as a case study by the Portuguese electricity and gas transmission supply operator, “Redes Energéticas Nacionais, S.A.” (REN), to the 69th European Study Group (ESGI69) which took place at the University of Coimbra in 2009. Some turbines in that power station are able to pump water up from a downstream reservoir to an upstream one. Pumping water upstream can be advantageous, for instance if done at times of low demand for electricity, to build up reserves in order to be able to produce energy during peak hours, thus balancing the load. The problem proposed was focused on profit maximization when operating such a system, and on how to decide which upstream reservoir to pump to, when there is a choice.

Implementation of the initiative

A team of mathematicians from European universities participating in the ESGI69 gathered for one week to learn about and discuss the problem and to mathematically model it. A representation of the hydroelectric cascade as an optimal control set of equations was formulated and some conclusions were drawn for particular cases and simplified versions of the whole model. Finally a non-linear optimization program resulting from the discretization of a one day period into one hour time steps was developed. After the meeting was over the team associated with this problem presented a report of the study.

The problem

In the case of reversible hydroelectric power stations it is possible to bring water from a downstream reservoir to an upstream one. This is usually desirable at times of low demand, in order to be able to produce energy during peak hours. While this might not be worthwhile from an energy point of view, the fact that the price of electricity varies along the day makes it possible to use cheaper energy to produce energy at future times when it will be more expensive. While in the case of one single power station the solution of the problem is more or less straightforward, it becomes more complex in the case of a system of power stations in a cascade configuration with the possibility of pumping water from one reservoir to two reservoirs. Moreover, the different characteristics (dimension and location) of reservoirs give rise to different consumptions and productions of energy. This type of problems can be treated by various fields of mathematics, from optimal control to network flow optimization, among others. In practice major model simplifications often lead to inaccurate solutions, which can have a high impact on companies' revenues.



Results and achievements

The report produced presents the models and the conclusions drawn during and after the ESGI69, as well as recommendations to REN. It includes also a detailed analysis of a simple reservoir configuration, some simple relationships between price and timing of decisions, and a numerical algorithm based on the non-linear program. A paper based on this final report has been submitted for publication in a scientific journal.

Lessons learned and replicability

The complexity of the hydroelectric power station and the multiple variables involved made it difficult to come up with an accurate system's representation in terms of the problem formulation, capable of answering the issues raised by REN. Nevertheless the process benefited from an intensive contact with the industry representative, and in the end it was possible to point out models and ways to find an (eventually approximate) optimal solution.

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Mathematical Problems in Oil Pipelining

Executive summary

We have developed some mathematical models for wax precipitation in waxy crude oils (oils with high content of heavy hydrocarbons), studying the dynamics of wax deposition in pipelines crossing cold regions (subsea pipelines).

Challenge overview

The research is the result of a contract with Eni (Milan). The main objective was modelling the mechanism of the segregation of wax, of its migration induced by temperature gradients, and its the deposition on the pipeline walls. This was the first research contract of the company with mathematicians. We were asked to develop mathematical models and numerical codes apt to predict the possibility of occurrence of precipitation and deposition of wax on the walls of pipelines, depending on the temperature of the environment.

Section of a pipeline with deposited wax

Implementation of the initiative

The research was carried in continuous contact with the company. Every step was checked by means of experiments carried out by the company itself or by other departments of our university. Concerning the confidentiality issues, they just caused delays in the publication of the results.

The problem

We have modelled various aspects of wax precipitation and deposition, both in the cases when thermodynamical equilibrium (between solid and liquid phases) can be assumed and when a kinetics of precipitation has to be taken into account. We have considered static and dynamical situations in laboratory devices (cold finger, loop) and in real field pipelines. We have developed models for predicting wax precipitation, wax deposition and wax gelification.

We adopted a multi-scale approach, taking into account microscopic phenomena (such as crystal nucleation and growth) and studying the time scale at which different phenomena occur. A main encountered in the research consisted in the lack of the experimental data which are useful for the development and validation of the model. In recent years this problem has been overcome thanks to the collaboration with the Department of Chemistry of the University of Florence where some experiments were performed and the input data for the model were found.

Results and achievements

The models we have proposed are capable to predict the amount of precipitated wax in specific thermal conditions. Moreover they can predict the amount of deposited wax (by molecular diffusion) on the pipeline walls.

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Let the oil flow!

Executive summary

Bringing together the IFP and the Laboratoire Jacques-Louis Lions, a technological research team was set up to develop new computing methods to improve the simulation of multiphase flows in pipelines.

Challenge overview

A mixture of hydrocarbons flowing in a pipeline usually gives rise to very complex phenomena because liquid and gas coexist over very long range and under highly varying temperature and pressure conditions. The challenging case of the « severe slugging » is the paramount of a violent chaotic problem. Oil companies request numerical simulations that are robust, accurate and fast in order to pilot the installations. Stemming up from a long-run collaboration between the two institutions, through thesis and internships, the idea of tackling this difficult problem originated during Cemracs 2003 with a project involving Quang-Huy Tran (IFP), Frédéric Coquel (LJLL) and Marie Postel (LJLL) .

Implementation of the initiative

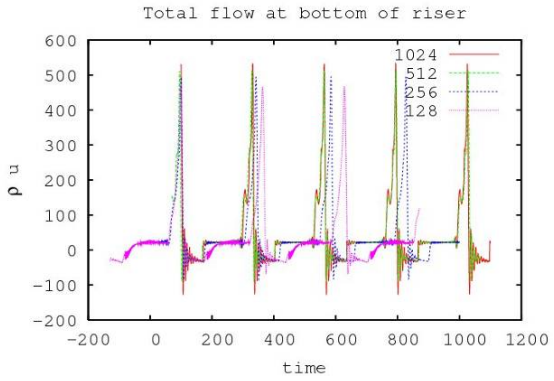
An “internal technological research team” was formed and financed by both the IFP and the French Ministry of Research. Experts in complex fluids and in adaptive methods for hyperbolic systems were already in the LJLL, and just had to be motivated on this specific problem. IFP was willing to involve one permanent researcher and to welcome temporary staff. It turned out that for almost four years a base kernel of two academics and one industrial researcher met weekly at the LJLL. They carried out in their stream two master internships, one post-doc (N. Andrianov) and one PhD thesis (Q.-L. Nguyen) and occasional collaborations. Most of the numerical algorithms were designed during the weekly sessions at the LJLL, and then checked, implemented and tested by both partners. A C++ program was developed jointly at IFP and at LJLL with a huge effort made on collaborative development. Four papers and numerous proceedings were published to formalize and illustrate the results.

The problem

The transport of hydrocarbons from the well site to the separation facility can be modeled by a system of hyperbolic PDEs whose unknowns are the density, speed of the different components of the fluid mixture, as a function of time and position in the pipeline. The main difficulties encountered in the design of numerical schemes to solve these equations are three-fold: physical laws linking the gas and liquid phases of the mixture are highly non-linear and very costly to evaluate. In operating mode, the transport is monitored at both ends of the pipeline by pumps, which amount to very stiff time varying boundary conditions. Last but not least, the changes in the pipeline geometry induce source terms and non-conservative terms in the PDEs. We have attacked these challenging issues from two fronts, both ensuring the robustness of the resulting schemes: large time-steps relaxation methods to handle the non-linearities and multiresolution analysis to monitor a space and time varying grid.

Results and achievements

The difficult part for the academics was to confront our algorithms and programs to realistic test cases. If no real comparison with experimental results was possible at this stage, at least a good knowledge of the expected qualitative behaviour of the solution was available. The software developed during the project was able to reproduce difficult test cases already handled by the company home software TACITE. The adaptivity in time and space allowed drastic computing time reductions.



Lessons learned and replicability

This type of collaboration has proved itself fruitful for both parties. At the end of the four-year contract a new « technological research team » has been set up on another challenging problem, namely, in oil reservoir modeling.

Partners in the project

http://www.ann.jussieu/ERTint

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Ministère de l’enseignement supérieur et de la recherche

Near Real-Time FCC riser simulation and visualization

Executive summary

A lightweight physical model and a fast numerical solver have been designed for the near Real-Time rendering of fluid catalytic cracking (FCC) in the riser cylinder reactor part. For Real Time requirements, a trade-off between the model fidelity and the numerical complexity was needed. The choice of the physical model and numerical schemes are here completely driven by the requirement of Real Time rendering virtual reality on a standard (powerful) PC. It has been possible to design a real time numerical rendering model able to show the three-phase flow dynamics depending on design parameters (number of oil injection inlets, injection angles, flow rates, temperature of catalyst powder). Open source technologies were used for the software design: gcc, python, SWIG C++ Python wrapper, wxPython, pyVTK.

Challenge overview

The problem was expressed by the French Petroleum TOTAL company, Head of scientific Division. The challenge was to produce a software able to "render" in quasi Real Time on a standard PC a three-phase three-dimensional flow into a Fluid Catalytic Cracking riser reactor with runtime visualization and human interaction capability. The model is expected to return most of the expected flow feature like gas expansion near liquid oil inlets, turbulent fluidized bed, emergence of privileged gas paths, recirculation patterns, etc. The goal was also to be able to directly act on some design parameters like the number of oil inlets, the inlet attack angles, the oil flow rates, the temperature of regenerated catalyst powder. The industrial interest for such a tool is the use of a lightweight simulator for training and understanding of the process but also for numerical Engineering design. Because of internal review deadlines, it was asked to produce such a tool in record deadline: 3 months!

Implementation of the initiative

So the duration of the contract was three months. A multidisciplinary academic team of 5 persons was set up: three specialists of fluid mechanics and particle methods, a software engineer and an expert of scientific visualization and VTK toolkit. A transversal manager was also chosen for project coherence: interfaces between the model components, interface between the models and the visualization component, interface between the models and the interactive graphic user interface. During the first month, weekly meetings between academics and the company were necessary for a precise definition of the requirements. Then each 15 days, a project review in the company was scheduled to check the agreement between the industrial expectations and the work in progress. The software was delivered on a laptop PC with dedicated integrated development environments and high-performance graphic hardware accelerator.

The problem

From the mathematical and computational point of view, multiphase flows are known to be very difficult to model and simulate. A model designed a full system of volume-averaged multiphase flow equations would require several weeks of CPU time for only a few seconds of physical time! Therefore a strong effort of model reduction was necessary in this work. Moreover, very fast solvers were designed in order to reduce the CPU time of about one or two orders of magnitude. It appeared that a coupled system of Lagrange particle solvers for both liquid and solid phase and an Eulerian finite volume solver for the gas were good candidates to get a good trade-off between performance and accuracy of the whole numerical model.

Results and achievements

The work and the resulting software were much appreciated by the company. Almost Real-Time was reached on the PC laptop with the expected flow description. The software was built using pure open source tools under GPL-like public licences. A company's internal project review highly rated the project. Now the labs involved in this success story are still working with TOTAL on related projects. We thank Bruno Frogé for his advices concerning VTK.

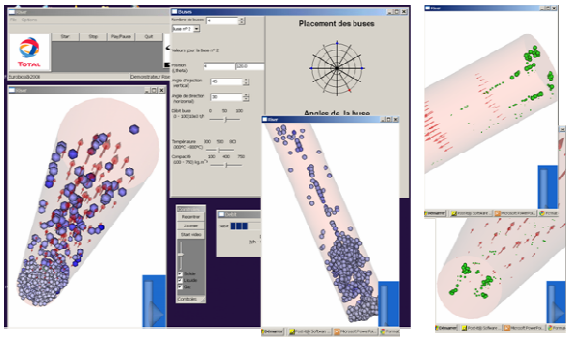

Figure – FCC riser software: near real-time simulation with interactive graphic user interface and three-dimensional three-phase visualization during runtime.

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SmartGrid.gc: Intelligent agent based modeling and simulation of electrical grids

Executive summary

This project deals with the development of a framework that allows simulation of island power systems at market and operational levels. Complex situations that occur in the management of electricity networks are modelled based on the interaction of multiple decision making units, with bounded rationality and self-interest. For system behaviour studies is used the paradigm of Agent Based Modeling and Simulation (ABMS). It is conceived as a tool for modeling and simulating scenarios, that is configurations and situations in electrical grids. Special emphasis is focused on the study and simulation of the effects of technological trends regarding generation, storage and processing in order to evolve towards future smart grids. This project has received financial support from by the Canary Islands Agency for Research, Innovation and Information Society (ACIISI) of the Canary Islands Government and with the participation of the important utilities sector, UNELCO-ENDESA (Canary Islands electrical generation company) and *Red Eléctrica de España* (Spanish electrical transportation company).

Challenge overview

The results of this project are:

- The study of solutions to future scenarios for restructuring and management of island power systems (like Gran Canaria island electrical grid) can simulate situations in order to maximize renewable energy sources (RES) integration into the grid, ensuring the service quality and reducing dependence on fossil fuels and environmental contamination.
- Studies towards the definition of smart power grid management solutions, like the ones related to the maximization, the RES integration and use of electrified vehicle fleet as storage element.

Implementation of the initiative

The initiative has been developed by the Artificial Intelligence and System Division with Prof. Mario Hernández (fhernandez@siani.es) as scientific director. The research group is composed by a multi-disciplinary team of engineers, computer science graduates and scientists working together in research and innovation for industry and government departments.

The problem

Electrical systems are facing major challenges due to:

- The new environmental needs related to climate change control.
- The introduction of market structure at different levels of electrical business.
- The economic and geostrategic problems related to the electrical energy production from fossil fuels.
- The massive introduction of unmanaged RES in the electrical grid.
- The revolutionary changes that are occurring in the automotive industry due to the planned production of plug in electrical vehicles (PHEV).
- The technological changes that are necessary to grid management with the introduction of the Smart Grid concept.

Lessons learned and replicability

Over 97% of domestic energy demand of Gran Canaria is covered with refined oil (more than 10 million barrels per year), with an annual consumption of oil of 1.4 million Tm of which 0.8 million Tm are dedicated to produce electricity and 0.6 million Tm. to transport and others. This situation occurs in the island of Gran Canaria with the best wind resources in Europe. The integration of a substantial amount of RES in an isolated electrical system of medium size like the island of Gran Canaria grid (3800 GWh of annual production), demand intelligent management systems to guarantee their effectiveness and stability. Both of them can be increased if it is done with storage systems, acting in a buffering mode, as can be PHEV. The case of Gran Canaria electrical grid is similar to many other medium size grids around the world and is a good laboratory exemplar to evaluate different technological approaches and market solutions for future grid studies.

Contact

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A Kinetic Model of Blast Furnace Automation

Executive summary

Blast furnaces have been used for iron production for centuries. In today's competitive engineering markets, math-based furnace simulation can cover operating conditions which are not accessible by experiment.

Challenge overview

Siemens VAI is one of the world´s leading engineering and plant-building companies for the iron & steel industries, based in Linz, Austria, which has been cooperating with mathematical research institutions since the 1980s. They became a partner in the Industrial Mathematics Competence Center (IMCC), which was established in 2002 and is co-financed between industry and the public sector. The support of the Austrian Ministry for Economy and Labor and the Upper Austrian Government is gratefully acknowledged.

The modernisation of steel-mills around the world requires a thorough understanding of the processes going on in a blast furnace and quantitative simulation tools for analysing the influence of different raw materials and of different operatiing conditions.

Implementation of the initiative

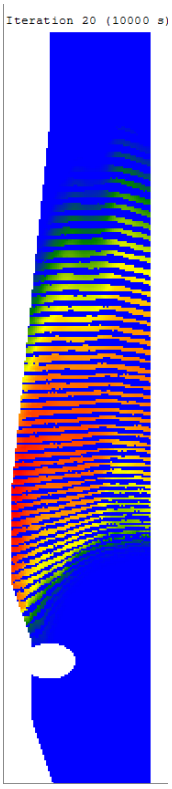
The joint research team consisted of experts in metallurgical and chemical engineering, in numerical mathematics and in computer science. Regular meetings between the team members, especially in the modeling stage, were essential for success.

The problem

The mathematical model of a blast furnace should cover at least: (a) the transient movement of layers of coke and of iron ore and the shrinking of the coke layers, (b) the movement of gas through the furnace, (c) the chemical reactions taking place (up to 50 of them taken into account), (d) balances of energy. This leads to a system of (around 50) highly nonlinear partial differential equations with the unknowns depending on position and time. Assuming a rotational symmetry seems reasonable, leading to a (2D + time) problem. The discretised version (finite elements combined with method of lines for some reactions) led to systems with up to 800,000 unknowns.

Results and achievements

The simulation tool which was developed is able to simulate e.g. various mixings of raw materials. The computation of one real-world blast furnace day takes typically 3 hours on a standard PC and therefore allows the user to simulate different operating conditions and thus to optimise, e.g., energy consumption. The kinetic blast furnace model is part of Siemens VAI's automation offerings. From the academic point of view, such cooperations allow for industry-driven PhD theses, as the complexity of the coupling between the differential equations is extremely high, and to prepare young scientist for industrial problem solving. Other projects for the iron and steel industry carried out at math institutions in Linz were in the fields of sintering, continuous casting of steel or hot rolling.



Concentration of FeO (red = high) in the layers of a blast furnace. Note that there is no FeO in the (blue) coke layers.

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Numerical Modeling of Heterogeous Porous Media

Executive summary

Numerical modeling of the flow and transport of radionuclides in heterogeneous porous media

Challenge overview

I was contacted by the responsible of the division modeling and scientific computing IRSN/ Radioactive Waste Safety Department for collaboration in the upgrade of the 3D MELODIE code to perform radionuclide transport calculations within the field of technical expertise of the French radioactive waste underground repository project.

Implementation of the initiative

The collaboration began in 2000, it has mobilized research engineers from IRSN, Professors from the University and Master, Ph. D and Post-doctoral students.

The problem

Perform efficient and robust numerical methods for the numerical simulation of coupled systems arising in multiphase flow in porous media: finite volume methods & upscaling.

Results and achievements

During this collaboration, several codes have been performed, a Ph. D. thesis, several publications and reports. The contract is ongoing until at least 2012.

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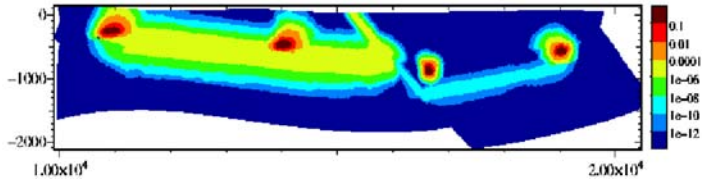
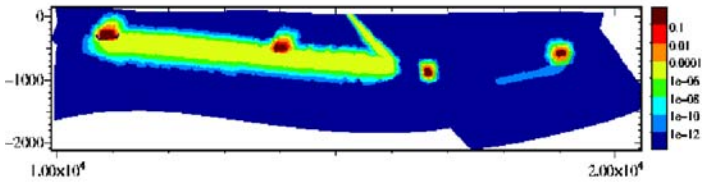


Radionuclide transport calculations by finite volume method for a scenario of radioactive waste underground repository.



IRSN
INSTITUT
DE RADIOPROTECTION
ET DE SÛRETÉ NUCLÉAIRE

Aero-acoustic virtual design of exhaust systems

Executive summary

Swenox is a leading manufacturer of exhaust systems for the European car industry, with an established cooperation with the Marcus Wallenberg Laboratory for Sound and Vibration Research (MWL) at the Royal Institute of Technology (KTH) in Stockholm. Applied mathematicians of the Computational Technology Laboratory (CTL) at KTH now participates in a project together with Swenox and MWL to develop new tools for modelling and simulation of turbulent flow fluid-structure-acoustic interaction in exhaust systems.

Challenge overview

After a discussion at a chance meeting in 2007, the project was initiated when it was realized that the work at CTL on simulation of blood flow in flexible arteries relied on similar mathematical technology as would be needed to address the outstanding problem of simulating aero-acoustics of the flow of air in exhaust systems. The use of existing simulation tools for such problems is limited since the problem is too challenging to address without extensive simplifications, so that many aspects of key importance for design are not part of the model.

Implementation of the initiative

The collaboration was in 2007 funded by Swenox and the Swedish Governmental Agency for Innovation Systems (Vinnova), and was later continued in 2009 as a new 3-year project funded by Swenox and the Swedish Energy Agency. Swenox acted as project coordinator through regular meetings and workshops with a core group of 3 senior researchers and 3 PhD students, of which one of the students was recruited specifically for this project. The meetings were the key to find a common language between the engineers, experimentalists and mathematicians involved, and to indentify suitable project goals to both break new ground in mathematics research and to advance the frontier of aero-acoustics simulation in industry.

The problem

An exhaust system consists of flexible parts interacting with the airflow from the engine, and the problem is to predict aero-acoustic properties of such a system. The basic model is the Navier-Stokes equations describing velocity, pressure and density of the exhaust air, together with corresponding equations for the solid structures of the system. The main challenges are: (i) to model turbulent fluid flow, with several open problems with respect to the mathematics of the model and the computational cost of resolving the turbulent scales, (ii) coupling of the fluid and the structure models, which is typically very unstable, and (iii) extracting acoustic information from the model, in the form of very small pressure fluctuations.

Results and achievements

The mathematical technology used in the project to simulate both the turbulent airflow and the solid structure is adaptive finite element methods. The algorithms are implemented in the open source software project fenics.org, in the form of the simulation software Unicorn, developed by CTL. To address the industrial problem of complex geometry and realistic physics, the computer code had to be redesign to run efficiently on the most advanced supercomputers available in Sweden. The coupling of the fluid and the structure was handled by a monolithic approach where the fluid and solid were formulated as one unified continuum, to achieve robustness. The project is still running, and today fluid-structure interaction simulations are routinely carried out at CTL, which are validated against experimental tests at Swenox and MWL. The aero-acoustic sources can now be extracted from the simulations, and the next step of the project is to allow for a fully coupled fluid-structure-acoustic coupling of the problem. Dissemination of the new technology developed at CTL is also in process, in the form of software tools adapted to the needs of Swenox.

Figure 1: Simulation of the turbulent flow of air past a mixer plate in an exhaust system (simulations by Rodrigo Vilela De Abreu and Johan Jansson at CTL).

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Environment

Numerical simulation for environmental prediction

Executive summary

This project deals with the numerical simulation of four important environmental problems: the realistic prediction of wind fields, solar radiation, air pollution and forest fires.

Challenge overview

Three groups (Laboratori de Càlcul Numèric, LaCàN, from Universitat Politècnica de Catalunya, Instituto de Física Fundamental y Matemáticas from Universidad de Salamanca and Instituto Universitario de Sistemas Inteligentes y Aplicaciones Numéricas en Ingeniería, SIANI, from Universidad de Las Palmas de Gran Canaria) have been working from ten years ago on these environmental problems and they have finished together three previous coordinated projects sponsored by Spanish Goverment and FEDER. At present (2009-2011) these groups are develoving the project entitled Predictive Numerical Models for Environmental Management where the Agencia Estatal de Meteorología (AEMET), Desarrollos Eólicos, S.A. (DESA) and Instituto Tecnológico de Canarias, S.A. (ITC) are the three main companies involved.

Implementation of the initiative

The present environmental problems (wind fields, air pollution, fire propagation and solar radiation) have a great social, economic and scientific impact. Nowadays, climate change is being considered as one of the most important problems of our planet. Because of that efficient use of renewable energies (as wind and solar) is increasing exponentially. Moreover, decreasing of air pollution and forest fires is needed for maintaining quality of ecosystems and human environment. Many companies and institutions are interested on the results of this project.

The problem

The main objective of the project is the combination of our local approaches with predictive mesoscale models such as MM5, WRF, HIRLAM or HARMONIE for weather, and CMAQ or MOCAGE for air quality. These models usually solve the problems by using finite difference methods on an structured grid (defined on several nested domains) and can predict atmospheric magnitudes with a maximum resolution of about 1km. The combination of these predictive models with our adaptive finite element models (see figure), which work with triangular or tetrahedral unstructured meshes, allows us to carry out predictive simulations in a local scale accurately (about a few meters). In this way, the terrain characteristics and solution will be efficiently approximated according to a desired precision.

Results and achievements

The scientific aims proposed in this project are clear, reachable and suitable. We do not try to reproduce tools that already exist. We try to solve problems that cannot be solved by known standard codes. Our wind model will be able to construct a wind field starting from few experimental measures. This is important for the diagnosis or evaluation of the wind power in a zone. However, companies are also interested on the prediction of such power. For this purpose, our adaptive local models (with a resolution of a few meters) must be connected with predictive mesoscale models (with a resolution about kilometres). We have initially focused in the MM5 and WRF codes since they are widely used by the community of meteorological phenomena prediction, although other predictive mesoscale models are also considered. In the framework of air pollution, the aims are similar. The adaptive local code that we are developing will extract the meteorological and air quality information from the MM5-CMAQ codes. The forest fire model will also be connected with MM5. The solar radiation model will be designed for both diagnosis and prediction. The integration of GIS tools will provide all these codes with the necessary information for carrying out realistic simulations.

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Predicting climate change

Executive summary

Increasing global temperatures, rising sea levels and the disruption of fragile ecosystems: climate change is one of the greatest challenges humanity has ever faced, and could potentially affect billions of lives in the coming century. Scientists around the world are working to tackle the problem with detailed models of our changing climate, and mathematicians are at the heart of these models, solving the difficult equations that no one else can. Researchers in meteorology, physics, geography and a host of other fields all contribute their expertise, but mathematics is the unifying language that enables this diverse group of people to implement their ideas in climate models.

Challenge overview

At the centre of all climate models are the Navier-Stokes equations, which describe the movement of liquids and gases such as the atmosphere and ocean. Translating the Navier-Stokes equations into computational code is undertaken by Paul Williams, a Royal Society Research Fellow at the University of Reading, who aims to improve the time-stepping calculation, making it more accurate without losing computational efficiency.

The problem

As a linked set of four nonlinear partial differential equations the Navier-Stokes equations are impossible to solve analytically in all but a few trivial cases, hence the need for numerical approximation methods. These methods allow us to apply the Navier-Stokes equations to a range of practical situations.

There are a variety of time-stepping methods, each with their own strengths and weaknesses, but because climate modelling is so complex, the different methods don't always produce results that agree. Determining which method to use can be beneficial as it allows climate scientists to investigate uncertainties.

Other aspects of the climate aren't captured by the Navier-Stokes equations, and some atmospheric phenomena lack fundamental mathematical theory behind them. Clouds are the leading source of uncertainty in climate modeling because they occupy a scale much smaller than the 100 km grids currently in use in climate models, so the full details of their behaviour are lost.

These unanswered questions show that while current climate models have served us well, demonstrating that increased carbon dioxide levels lead to a rise in temperature, we must still gain a deeper understanding of all the mechanisms within our atmosphere and ocean if we are to effectively fight global warming.

Climate scientists use many different varieties of time-stepping methods to power their models, and the choice of method can influence the resulting predictions. The most widely used is the “leapfrog” method, so-called because the function and its derivative get from the previous time to the future time by “leaping” over the current time.

Results and achievements

The method's success is due to its ease of use and low computational complexity, but its jumping nature can lead to discrepancies between even and odd steps. This can be solved by using the Robert-Asselin filter to smooth the discontinuities, but at the cost of a loss in accuracy. Williams' research modifies the filter in a way that counteracts this loss, producing better models with no noticeable reduction in calculation speed.

University of Reading

THE ROYAL SOCIETY

Institute of mathematics & its applications

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Stepping in Sherlock Holmes's shoes: where is the underground water? Is it still drinkable?

Executive summary

This document describes the multidisciplinary collaboration between four universities, two in Europe (Oviedo and Bordeaux1 Universities) and two in Morocco (D'ElJadida and Meknès Universities). By putting together their knowledge in applied mathematics and optimization, geology, applied geophysics and geostatistics, a common language was created and we were able to solve important environmental problems using hydrogeophysical methods. These methodologies were then used to solve underground water problems in the Sahel des Doukkala and Saïss basins of Morocco. In particular, the contamination of underground water by salt water intrusion is a problem that interests most of the industries and local administrations in countries belonging to the Mediterranean basin. These methods are versatile and low cost in their implementation and can be easily applied to underground water exploration in countries where other geophysical methods cannot be used due to technological and economic constraints.

Challenge overview

First contact was made at the XI International Congress of Mathematical Geology held in Liège,Belgium in 2006. The Spanish and French teams quickly discovered our commonalities and that we had much to gain by sharing knowledge, experiences, software and data. An Atlantic Spanish-French team was immediately formed and was soon joined by our Moroccan colleagues who brought a wide variety of interesting environmental problems and a large volume of field data. Thus, our scientific and human collaboration was built across continents and now is based on strong cultural respect and friendship.

Implementation of the initiative

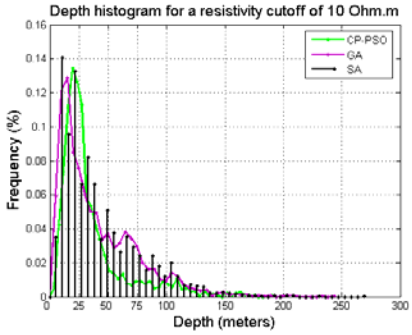
The first steps of our collaboration were facilitated by the exchange of professors and researchers of the different universities, first in France (Bordeaux) and later in Spain (Oviedo). Agreements were signed to share the available data and the mathematical models. Support was given by interchange programs: one Franco-Spanish (Hubert Curien PICASSO) and the other Franco-Moroccan (Hubert Curien VOLUBILIS).

The problem

Hydro-geophysics is made of a set of geophysical techniques that serve to study underground aquifers, and eventually all the problems (such as contamination) related to their exploitation and management. Currently it is a very active subject of research due to the increasing impact that drinkable water has in any country's economy. Some methods are more sophisticated, while others such as the Vertical Electrical Soundings or the Spontaneous Potential are more low-cost. Implicit to these methods are their respective inverse problems which are crucial for retrieving information from the underlying earth structure (including the aquifers). The low number of parameters facilitates the use of global methodologies to perform risk analysis on the final decisions that often have a very important environmental character.

Results and achievements

We were able to create simple methodologies to help assessment and risk analysis in applied hydrogeology. These methodologies have recently become very important for local industries and administrations that are highly dependent on the amount and quality of the underground water resources.



Depth of a salt water intrusion on a coastal aquifer in southern Spain.

Lessons learned

One of the most important lessons learned from this experience is that in science, problems have an international character and we should cooperate across borders in their solution. Usually teams compete to arrive first to the target, but when a common language is created that respects the uniqueness of cultures, the success is the normal outcome of these initiatives. These developments can have a great impact when knowledge is transferred to developing communities. Mathematics and science can be used to improve people's life.

Contact

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Modeling and simulation of environmental problems

Executive summary

Mathematical models and numerical methods for simulation of free surface flows including the treatment of the geometry, the turbulence, and the transport or dispersion of pollutants have been developed and applied to some aquatic environmental problems.

Challenge overview

The contact with the COTOP ("Consellería de Ordenación do Territorío e Obras Públicas") of the Government of Galicia started in 1986. They were interested in the construction and the location of submarine outfalls in the Galician coast. From the mathematical point of view, in order to solve the problem, it is necessary first to obtain the velocity fields and the water surface elevation in the coastal region, second to apply a mathematical model giving the evolution of the Dissolved Oxygen (DO) and the Biochemical Oxygen Demand (DBO) and third to formulate and solve some constrained optimal control problems. The non-existence of well-established commercial packages for this topic in 1986 was the motivation to develop our own codes. We considered two numerical strategies, finite elements and finite volumes methods in order to discretize the partial differential equations involved in the mathematical models. Non-standard finite elements were used for the shallow water equations. Concerning the finite volume approach, a new numerical treatment of the geometry terms (source terms) was proposed and analyzed.

Implementation of the initiative

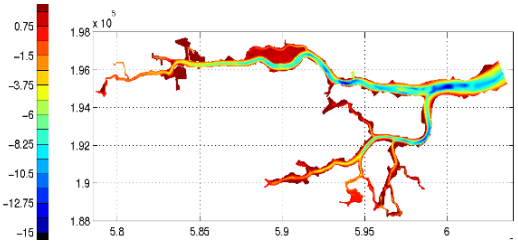
Using funds of the COTOP, three research contracts were agreed from 1986 to 1990 between this institution and the Department of Applied Mathematics of the USC. These contracts gave rise to a group in mathematical modeling directed by Prof Alfredo Bermúdez and complemented with four pre-doctoral students. For the finite volume topic Profs Alain Dervieux and Antoine Desideri, from the well-known French Institute, INRIA, were contacted due to a previous collaboration in the HERMES European project. At the end of this project the group developed a FORTRAN code to solve the problem and wrote a report with the proposed location for the submarine outfalls in the "rias" of Pontevedra and Vigo.

The problem

The mathematical model of the shallow water equations is a system of hyperbolic conservation laws with source term, the latter arising from the bottom geometry. The main outcome in the context of the finite volume methods was the development of a completely new methodology to upwind these source terms.

Results and achievements

This contract was the initial motivation of a now consolidated research line. Since the preliminary application to the Galician rias, other geographical areas have been considered. Moreover, many theoretical and numerical contributions have been published by the group.



From an academic point of view, the research led to four PhD theses.

Lessons learned and replicability

This initiative was the origin of the research group in hydrodynamics modeling which is now composed by 5 permanent positions and 2 doctoral students. The methodology developed, from this contract in finite volumes, was tested experimentally in the context of the CADAM (Concerted Action on Dam-Break modeling) project (1998-2000). The developed computational tools are now implemented in two codes: SOS with the finite element method, which also include optimization of systems of treatment plants, and TURBILLON with the finite volume method. The latter was registered in 2005 by the Universities of A Coruña and Santiago de Compostela and used to model shallow water flows in many coastal areas and rivers around the world (Arosa and Barqueiro rias in Galicia, Strait of Gibraltar, Ebro river in Spain, BioBio river in Chile, and the Crouch in estuary in the UK.

XUNTA DE GALICIA

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New Storm Surge Forecasting model in the Netherlands

Executive summary

The bottom topography of the North Sea used in a numerical tidal model was reconstructed more accurately by using a new parameter estimation method.

Challenge overview

Operational storm surge forecasting is very important for the Netherlands. The forecasts are computed by using a detailed numerical tidal model of the North Sea and adjacent areas developed by the research institute Deltares. A weak point in the model is that the bottom topography is not known very accurately.

At Delft Institute of Applied Mathematics (DIAM) of the Delft University of Technology research has been carried out on efficient methods for parameter estimation in large scale numerical models. Deltares and DIAM corporate all ready for many years with each other on different research topics, so it was quiet natural to formulate a joint project where the new parameter estimation algorithm would be applied to reconstruct the bottom topography of the storm surge forecasting model.

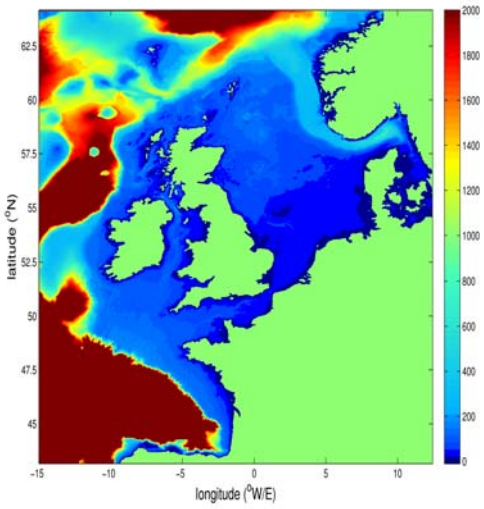
Implementation of the initiative

The initiative was carried out in the framework of a PhD project, partly financed by Deltares. Here first the general methodology was developed and tested for relatively simple problems. In the last year of the project the methodology was applied to the new tidal model of Deltares.

The problem

The so called adjoint method has often been used for the calibration of large scale numerical flow models. Here a number of unknown parameters is introduced into the numerical model. Using the given data these parameters are identified by minimizing a cost function that measure the difference between model results and data (observations). The drawback of the adjoint method is the programming effort required for the implementation of the adjoint model code. In this research, a method of parameter estimation has been developed based on model reduction using Proper Orthogonal Decomposition (POD) for a large scale shallow sea model of the entire European continental shelf. The POD based method shifts the minimization problem into lower dimensional space and avoids the implementation of the adjoint of the tangent linear approximation of the original nonlinear model.

Results and achievements



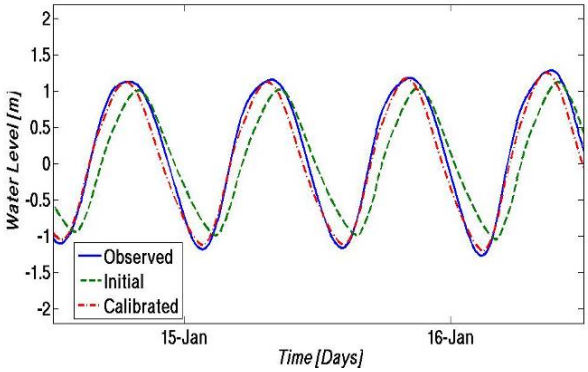


Figure above: The bathymetry in meters. Bathymetry greater than 2000 m is shown as 2000 m. The North Sea is much shallower, with maximum depth around 200 m.

Figure below : Water level time series at tide gauge station Delfzijl for a two days period from observations and the numerical model before and after calibration.

Validating the new model using long series of data showed that the Root Mean Square error reduced from approximately 20 cm to 10 cm.

TU Delft

GOFIM – simulation and optimization of waste water filtration

Executive summary

Mathematical models have been the basis for a new management protocol to improve the filtration process for drinking water treatment.

Challenge overview

The initiative started by the collaboration between our Department and the one of Environmental Engineering of our University. The latter has many collaborative projects with *Publiacqua*, the company in charge for the management of municipal waters in Firenze (Italy) and a wide region around the city. The continuous discussions taking place within this network led to the idea of applying mathematical models in order to improve the efficiency of the filtration plants, focusing on water treatment based on membrane filters.

Implementation of the initiative

The start of this collaboration was the contribution made by the Fondazione per la Ricerca e l'Innovazione – Firenze. Publiacqua decided to join the project GOFIM, coordinated by our Department, in which the company contributed by making available one of the filtration plants managed by the company. Such a plant was the reference point for the initiative, started in January 2009 for the duration of one year.

The problem

We studied the filtration process based on hollow-fibers made of polymeric membranes. These fibers are arranged in cassettes like the one shown in the figure. The problem consists of describing the evolution of the transmembrane pressure, which is the quantity driving the filtration. To address this problem, a set of ODEs was defined and the system was solved numerically. The major challenge of the research was the experimental determination of parameters involved in the model, since it is difficult to link the qualitative description of the process taking place closer the membranes with the experimental results referred to the global plant.

Results and achievements

The numerical code was implemented in the language Python, developing also a prototype for a graphical user interface to simulate the filtration process, and so a useful tool for managing the plant has been obtained. The methods experienced in this initiative were used by our Department in participating in a larger project with a similar subject. The project (named PURIFAST) has been funded by the European Community, within the programme LIFE+.

Company: ***Publiacqua S.p.A.***

Publiacqua

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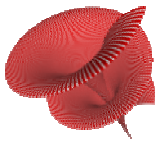


Solar Reflector Design

Executive summary

Methods were investigated to optimise the collection of solar energy on a roof.

Challenge overview

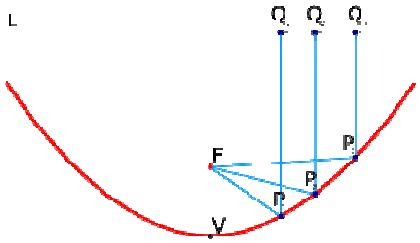
Erin Energy initiated contact with MACSI and sought help to optimise the design and cost of solar reflectors.
The company were aware that their panels were too thick. They needed guidance on how to approach this problem and required theoretical knowledge on how to solve it. The depth of the panels was also problematic for the construction industry. The company needed to find an economical way of reducing the depth of panels without compromising energy efficiency.

Implementation of the initiative

After initial analysis of the problem MACSI decided that the problem would benefit from an intensive brainstorming session involving using experts from a wide range of mathematical disciplines. Therefore the problem was included in the 70th European Study Group with Industry: the second industrial study group held in Ireland, organised by MACSI at the University of Limerick. The study group format also simplified the consideration of intellectual property and confidentiality issues since results obtained by study groups are released into the public domain.

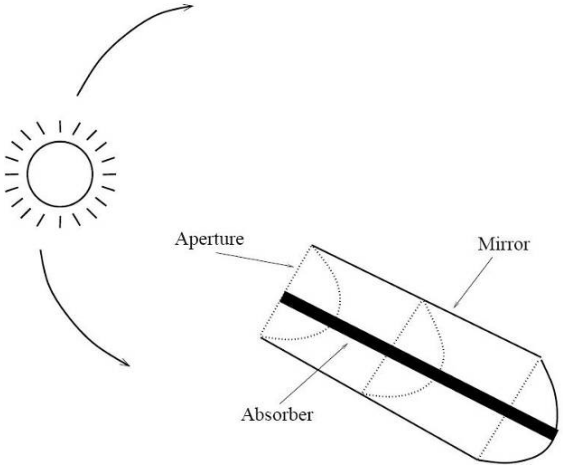
The problem

The device considered in this study collects solar energy on the roof of a house using an energy absorber. The solar energy is first collected, then transported and stored in a chemically based energy tank. Ideally, the roof should be completely covered with energy collectors but they are quite expensive. To reduce the amount of collectors necessary, the roof is covered with mirrors. The challenge was to optimise their shape in order to maximise the solar energy collected and minimise the costs.



Results and achievements

The solar radiation was studied and a ray tracing algorithm was developed by the academics involved. These models were used in simulations during which several techniques were considered to calculate the shape of the mirrors. The optimisation process shows that wide mirrors are not as energy efficient as smaller ones when the depth of the mirror is forced to remain shallow as is preferred in the construction industry. This simple rule is now used in the design of the solar reflector.



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MACSI
Mathematics Applications Consortium for Science & Industry

sfi Science Foundation Ireland

The birth of CELMEC

Executive summary

The international meetings on Celestial Mechanics CELMEC, now worldwide recognized as focal points of the community, are born by a strong collaboration between the University of Roma Tor Vergata and Telespazio SpA, Roma.

Challenge overview

Modern Celestial Mechanics deals with the study of the motion of celestial bodies, natural or man-made. It can be approached from different points of view: a purely theoretical analysis of the models which may lead to results which are or little relevance for applications, a numerical investigation aimed to assess mission strategies but often without a solid theoretical foundation. We needed a bridge which would allow the merging of the mathematical analysis, the numerical experiments and the mission developments. A group of mathematicians together with some researchers working at Telespazio, Roma (Italy) decided in 1993 to try to find a common ground through the organization of a meeting encompassing both theory and applications.

Implementation of the initiative

The first meeting was organized on a national basis in 1993 at the University of L'Aquila in collaboration with Telespazio, Roma; it was followed in 1997 by a national second meeting. Due to the interest shown by the overseas community, the meeting was upgraded to an international congress in 2001. Since then, it is organized every 4 years by the Dept. of Mathematics, University of Roma Tor Vergata and Telespazio, Roma, which act as main sponsors of the meeting.

The problem

Modern Celestial Mechanics has a basic interdisciplinary nature. Its methods and applications are developed by mathematicians, physicists and engineers working in widely different contexts: universities, research institutions, astronomical observatories, space agencies and the aerospace industry. Within this framework the CELMEC meetings aim to establish a common ground among people working in this field, to provide a reference event open to discussions and collaborations, and to maintain a knowledge network at an international level.

Results and achievements

CELMEC is now recognized worldwide as the meeting point of the three "souls" of modern celestial mechanics: *Perturbation Theories* (stability and evolution of dynamical systems), *Solar System and Stellar Systems* (dynamics of solar system bodies) and *Spaceflight Dynamics* (near-Earth spacecraft orbits and interplanetary missions). The success obtained by the CELMEC meetings has brought to a steady increase in the number of participants, from 30 people in 1993 to 153 in 2009. The last meeting was attended by researchers coming from 25 countries. CELMEC contributed also to increase the development of common projects between mathematicians and space industries. The strong link between Universities and Telespazio established thanks to CELMEC have proven essential for building up the winning teams of contracts within the framework of the ESA NEO Space Mission Initiative, the ASI Vision for Moon Exploration and the ESA Space Situational Awareness Program. Moreover, CELMEC gave birth to the "Italian Society of Celestial Mechanics and Astrodynamics", which was founded in 2001 and it is presently composed by 130 members (http://www.mat.uniroma2.it/simca/). The association is very active in promoting collaborations between universities and industries.

Lessons learned and replicability

In the ever-increasing differentiation of the scientific disciplines CELMEC has demonstrated that there is a great demand for interaction among different topics, from purely mathematical subjects to space applications. CELMEC greatly contributed to the activities of the Space Academy Foundation, whose founder members are Telespazio, Thales-Alenia Space and the University of L'Aquila, and whose activities are devoted to high-level learning and training on space science. Science, technology and the socio-cultural aspects of merging together people working in different topics and institutions, all contributed to this end.

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TELESPAZIO
A Finmeccanica / Thales Company

Simulation of a moving bed reactor used in the pulp and paper industry

Executive summary

This project gathered a group of experts in mathematics and chemical engineering to model and simulate numerically the dynamical behavior of a moving bed reactor, the so-called digester, used in the pulp and paper industry. The main goal was to develop a software package, based on innovative numerical methods, to simulate experiments that could be expensive or risky in an industrial context.

Challenge overview

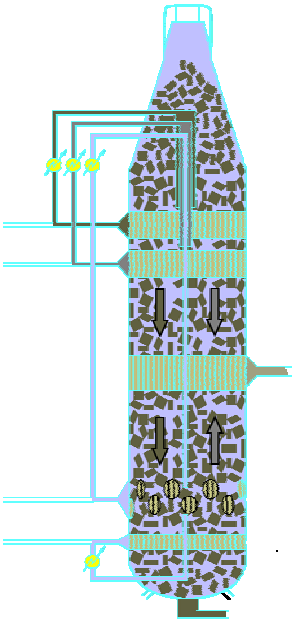
The pulp and paper business is one of Portuguese most important industries. Near Coimbra is located an important mill of the major Portuguese firm Portucel, which is one of the world's biggest producers of bleached eucalyptus Kraft pulp for the packaging industry and one of Europe's top five producers of uncoated wood-free paper. The most critical piece of equipment in a Kraft pulp and paper plant is the digester, known as the heart of the mill. It is a very special and complex heterogeneous reactor where a moving bed of wood chips contacts and reacts with sodium hydroxide and sodium sulphide in a liquid phase (Kraft process), in order to dissolve lignin and therefore to release the fibbers of cellulose. In order to optimize the quality of the pulp, this industry has a real need for tools that enable the simulation of experiments that cannot be afforded or that might be risky in a real industrial context.

Implementation of the initiative

The problem was tackled under the scope of a research project financed by the Portuguese Science Foundation. The project involved two chemical engineers, five mathematicians and three graduate students, and it was accomplished in three years. The incidence of the work was twofold: from an engineering point of view, the description of the transient behavior of the digester which allows the prediction of the quality of the pulp when some changes in the wood properties occur; from a mathematical point of view, the project gave the possibility to study new numerical methods, specially tailored to the phenomena that take place in each part of the digester.

The problem

The dynamical behavior of the reactor can be represented by a system of hyperbolic nonlinear partial differential equations. Among the equations of the system, we can identify three main types: the equations that describe the temperature and the concentration of the solid, the entrapped liquid, and the free liquid phase. Each one of these types of equations presents a certain complexity, making its numerical simulation a hard task. Several factors contribute to the complexity in the numerical simulation: (i) the high nonlinearity of the functions that represents the chemical reactions; (ii) the discontinuities induced by the extraction, enrichment and heat of the free liquor; (iii) the discontinuities in the convection velocity of the free liquor - positive where the liquid flown downwards and negative where the free liquid flows upwards.



Results and achievements

An open-source software package to simulate the dynamical behavior of the digester was developed and is available by request. This package was tested by the company to simulate the steady-state case with very promising results. The scientific activity is reflected in five papers in international journals and one PhD thesis.

Lessons learned and replicability

The translation of the mathematical technology into practical terms and its efficient implementation in applicable paradigm is not straightforward. To enhance the process of communication between academia and industry there is a need for academic careers in industrial mathematics to demonstrate the complexity and value of application-driven research.

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Dynamic image based lighting for highly realistic lighting in building design

Executive summary

Arup hosted an Industrial Mathematics Intern from the University of Warwick to assist in the production of algorithms for re-lighting virtual objects using videos.

Challenge overview

The natural world presents our visual system with an ever changing and wide range of light, colours and intensities. The difference in average luminance level between a starlit night and daylight scene spans eight orders of magnitude. A human eye can see detail in regions that vary by 1 in 10,000 at any given eye adaptation level.

Existing video cameras are only capable of capturing a limited part of this wide range of light, colour and detail with sufficient resolution. High Dynamic Range (HDR) imagery can represent most real world luminances, but until now the capture of HDR images with a linear response function has been limited to static scenes rather than 'moving images'. In July 2009, the University of Warwick took delivery of the world's first true HDR video system.

Image Based Lighting (IBL) is a technique for artificially re-lighting real world or synthetic objects. The project sought to develop a new mathematical approach to IBL to cope with the dynamic nature of the lighting captured by the HDR video camera.

Additionally, the project sought to integrate accurate dynamic real world lighting captured from this HDR video system into Arup's existing visualisation system in order to significantly improve the fidelity of images used for building design.

Implementation of the initiative

Arup and Warwick University successfully applied to the Industrial Mathematics Knowledge Transfer Network for an Industrial Mathematics Internship, a mechanism which is co-funded from the UK's Engineering and Physical Sciences Research Council and is designed to expose current PhD students to real industrial problems in a business environment for 3-6 months to stimulate new relationships between industry and academia.

The problem

Dynamic IBL will play a key role in improving the visual fidelity of computer generated imagery for building design. High-fidelity rendering techniques, such as image based lighting are physically based and thus require a robust mathematical foundation in order to deliver the desired perceptual equivalence between the real scene and its virtual counterpart. A novel mathematical method for dynamic image based lighting is required to cope with the nature of the video streams now possible with the HDR video camera.

The new mathematical method can then be used to define algorithms for IBL using images or videos. Of particular interest are temporal IBL algorithms applicable to the newly acquired HDR video.

Results and achievements

An important achievement of the project was the production of a series of algorithms for re-lighting virtual objects using videos. Of particular interest was the re-lighting of high contrast videos, i.e. videos with a high dynamic range.

ARUP
www.arup.com

WARWICK
www.warwick.ac.uk

Knowledge Transfer Network
Industrial Mathematics

Technology Strategy Board
Driving Innovation

EPSRC
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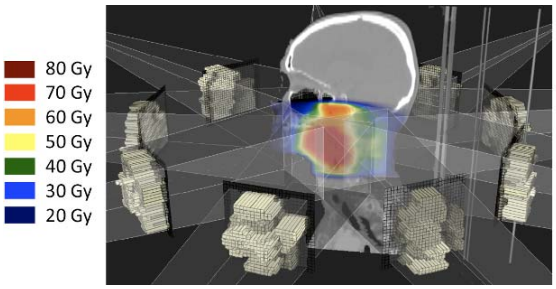
Health

Optimization of Radiation Therapy

Executive summary

The project concerns new optimization methods for intensity-modulated radiation therapy.



Challenge overview

RaySearch Laboratories, which was founded in 2000 as a spin-off from Karolinska Institutet, is a medical high-tech company with a strong research profile. The CEO and founder has an undergraduate degree from KTH, and he had good connections with the Division of Optimization and Systems Theory at KTH. The initiative to launch an industrial graduate student project jointly with KTH was made to take a deep look at the mathematical aspects of the optimization models and optimization problems that the company faces. The project was financially supported by the Swedish Research Council (VR) and RaySearch.

Implementation of the initiative

The first part of the project was carried out as an industrial graduate student project during 2003-2008. The setup was such that the student was employed by RaySearch and a graduate student at KTH. Besides his research project and PhD student courses, he also had part-time company duty at RaySearch, making him well acquainted with the academic environment at KTH as well as the industrial environment at RaySearch. A reference group with members from KTH and RaySearch was formed to support the project. The group usually met twice a year. Informal meetings were held more frequently between advisors from KTH and RaySearch, so as to make the project run smoothly. The Swedish Research Council provided a contract regulating confidentiality issues, which was helpful.

The problem

The optimization problem arising in intensity-modulated radiation therapy is an inverse problem in that certain requirements on the desired dose distribution in the patient are typically known. These requirements are in general conflicting since high dose is required in tumor cells whereas sensitive organs must be spared. A major challenge is how to formulate the optimization problem so that the solution obtained is clinically acceptable while it at the same time best fulfills the given requirements. The PhD student project was aimed at utilizing problem structure to analyze and design methods for solving the optimization problem in order to achieve these goals.

Results and achievements

The PhD student project led to significantly deepened understanding of the optimization problems that arise. The interaction between problem structure and behavior of methods led to important insights into how the problems can be solved efficiently.

Lessons learned and replicability

An important lesson in this project is the interplay between practice and theory. The understanding of the behavior of methods required a deep understanding of properties of the optimization problems. Conversely, practical aspects of the optimization problems led to new interesting fundamental research questions on optimization methods. Another important lesson is the close interplay between industry and academia which is necessary for such a project to be successful. Trust and openness from both parties is essential for success. The PhD student project discussed above was successfully completed in 2008. It has been succeeded by two new PhD student projects, using the same framework for cooperation between RaySearch and KTH.

Partners in the project

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Simulating Atrial Fibrillation

Executive summary

In a series of collaboration projects with AstraZeneca, the Fraunhofer-Chalmers Research Centre for Industrial Mathematics (FCC) has implemented mathematical models of canine heart muscle cells and performed simulations of the electrical activity in realistic atrial geometries. These projects have increased the understanding of atrial arrhythmias and have enabled quantitative evaluation of treatment strategies *in silico*.

Challenge overview

Mathematical modeling of biological systems that are of interest in the pharmaceutical industry is a rapidly growing area. AstraZeneca, a world leader in cardiovascular medicines, became involved with FCC in 2005 through a joint project focusing on mathematical modeling and computational analysis of canine atrial action potentials. Having previous experience of mathematical modeling, AstraZeneca believed that this approach would give insight in the interplay by which different ionic currents shape the action potential, knowledge that could assist in the screening of novel anti-arrhythmic drugs.

Implementation of the initiative

Upon completing the initial project, the ambition of a long-term collaboration was realized through a number of consecutive projects where the scope was extended to investigate the electrical activity at the tissue and organ level. During each project, there was a continuous dialogue. In addition to informal research discussions a status report were given at each meeting and all projects were thoroughly documented in written reports. The gradually established confidence in FCC during the course of these projects contributed strongly in the engagement of a new coworker at the centre.

The problem

Atrial fibrillation is the most common form of heart arrhythmia and is associated with a 5-6 fold increase in the incidence of stroke. Computer models make it possible to relate the dynamics of the action potential propagation in realistic atrial geometries to drug effects at the single cell level. This in turn permits *in silico* reconstruction and investigation of phenomena like atrial flutter and fibrillation.

FCC has developed a framework for modeling and simulation of electro-chemical activity in large scale cell networks. A geometric model of the canine atria has been constructed utilizing ultra sound imaging data and a realistic fiber structure and cell type distribution has also been incorporated. The complete atrial tissue model consists of about 2,000,000 coupled nonlinear ordinary differential equations. To meet the computational demands of this model the framework has been translated and deployed onto Chalmers high performance computational centre (C3SE).

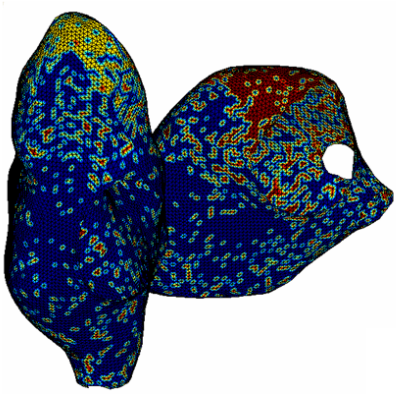

Figure 1. Color coded cell type distribution.

Results and achievements

The simulation framework has been used to induce fibrillation and flutter like electro-dynamic activity in cell networks from simple sheets up to realistic atrial geometries. In addition, the effect of ion-channel modulation on this behavior has been investigated. The simulations are in good accordance with *in vivo* observations, have great potential to provide insights into the underlying mechanisms of atrial fibrillation and flutter, and can serve as a tool for prediction of drug effects. Valuable results for academia have been made available through international conference contributions and journal manuscripts are in preparation.

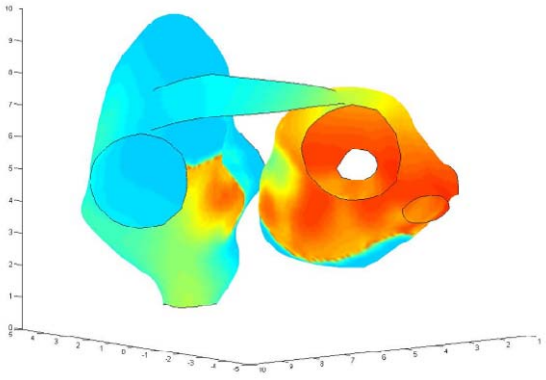

Figure 2. Action potential propagation in left and right atria.

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Realistic Modeling of Human Head Tissues Exposure to Electromagnetic Waves

This research project is concerned with the numerical modeling of the propagation of an electromagnetic wave emitted by a mobile phone throughout the head tissues. This has been achieved through the development of state of the art finite element solvers able to deal with realistic geometric models built from medical images.

Challenge overview

This research was initiated in the context of the HEADEXP multidisciplinary project which took place from January 2003 to December 2004 and which was funded by the scientific direction of INRIA. This project aimed at filling the gap between human head magnetic resonance images and the efficient and accurate numerical modeling of the interaction of electromagnetic waves with biological tissues. This required the development of specific image analysis tools and automated unstructured mesh generation tools for the construction of realistic discretized, human head models on one hand, and of unstructured mesh based numerical methods able to take into account the heterogeneity of the electromagnetic characteristics of the propagation media on the other hand.

Implementation of the initiative

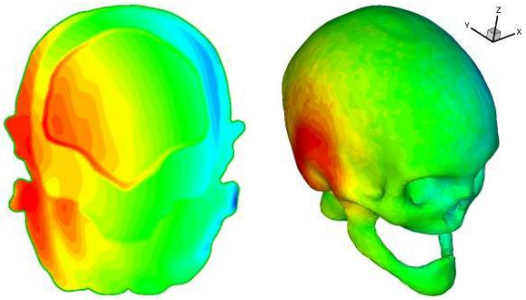
The HEADEXP project involved specialists from medical image processing (the EPIDAURE and ODYSSEE project-teams from INRIA Sophia Antipolis – Méditerranée and the medical image processing group from ENST in Paris), geometrical modeling (the GEOMETRICA project-team from INRIA Sophia Antipolis – Méditerranée) and applied mathematicians and specialists of scientific computing (the CAIMAN project-team from INRIA Sophia Antipolis – Méditerranée and the POEMS project-team from INRIA Paris – Rocquencourt), In addition, two non-academic partners have also participated to this project: INERIS (a French public research body of an industrial and commercial character which is a national expert at the service of environmental safety) and the WAVE group from France Telecom R&D which is specialized in the study of human exposure to electromagnetic waves. Since 2005, this research is going on in the context of an industrial partnership between the Orange Labs (formerly France Telecom R&D) and the NACHOS project-team (formerly the CAIMAN project-team). Two research grants between 2005 and 2009 have allowed the hire of a PhD student for working on the subject in close collaboration with researchers from the NACHOS project-team and research engineers form the group of Joe Wiart at Orange Labs (head of the WAVE group)

The problem

The propagation of electromagnetic waves in biological tissues is modeled by the system of 3D Maxwell equations. The great majority of numerical dosimetry studies make use of finite difference type methods working on Cartesian grids. With such methods however, the discretization of interfaces between tissues suffer from the so-called stair-casing effect, which affects the accuracy of the calculations. This problem is only partially solved thanks to the use of highly refined discretized models and more elaborated numerical methods are required if a realistic modeling is the objective.

Results and achievements

The research partnership has led to the development of a new modeling approach based on a highly accurate discontinuous finite element method (so-called discontinuous Galerkin method) particularly well suited to the discretization of heterogeneous propagation media and that can easily handle locally refined unstructured meshes.



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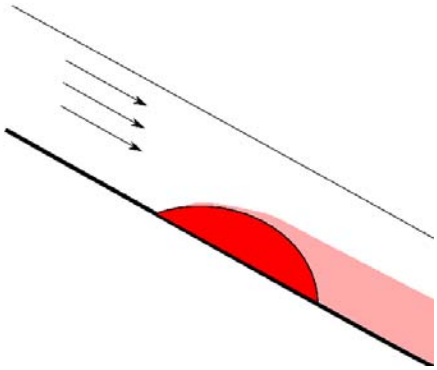
INRIA

Mathematical modelling of a decontamination process

Executive summary

An industrial mathematics internship has improved theoretical understanding of a decontamination process in which a contaminating agent is removed through delivery of a decontaminant solution.



Challenge overview

Dstl is the main research organisation of the Ministry of Defence. The problem investigated falls under the auspices of the Hazard Management team, whose brief is to develop methods to minimise the hazard resulting from the use of chemical, biological or radiological weapons. The team's activities increasingly supprot civil as well as military hazard management.

Implementation of the initiative

Dstl expressed interest in the Industrial Mathematics Internships programme co-funded by EPSRC for this problem and the Technology Translators at the Knowledge Transfer Network helped them to identify a student and supporting University department (DAMTP, University of Cambridge) to participate.

The problem

The aim of the Internship was to analyse fundamental problems associated with the removal of a contaminating agent from a surface. A drop of agent may be made safe through delivery of a decontaminating reagent in solution. The agent dissolves into this solution, and is then neutralised through chemical reaction. As this process occurs, the agent diffuses into the decontaminant solution and is then swept downstream of the drop. This method of decontamination has several civilian applications, such as the cleaning of railway stock, removal of traffic film from road vehicles, and graffiti removal.

There are several possible ways in which the decontamination process may be improved. For example, the efficiency of the decontaminant solution may be enhanced by increasing the reactivity between the decontaminant and the agent, or by increasing the solubility of the agent in the decontaminant solution. Another important aspect is the method by which the decontaminant is delivered. A large delivery rate of decontaminant may quickly `wash off' the drop from the surface, but may also result in wastage of decontaminant. A smaller delivery rate would minimise wastage, but at the expense of the speed of decontamination.

The focus of the internship was to develop mathematical models in order to determine which aspects of the process were most important to the efficiency of decontamination, and thereby guide future research and development.

Results and achievements

The transport of the agent into the decontaminant layer outside the drop was predicted using a theoretical model that included the key effects of advection, chemical reaction and diffusion. This model provided insight into the gains in efficiency that would result from optimising parameters such as the reactivity with, or solubility in, the decontaminant solution.

The spread of the agent droplet across the substrate is one of the aspects of the process of interest to Dstl. One of the main outcomes of the internship was the delivery of a computational simulation of the motion of the droplet throughout the process.

The decontamination process analysed during this internship is the subject of ongoing research at Dstl, The mathematical approach taken throughout the internship has provided important guidance for future work, and the theoretical and computational techniques used will be developed further by Dstl, towards the most effective and efficient decontamination strategies.

www.dstl.gov.uk

www.cam.ac.uk

Knowledge Transfer Network
Industrial Mathematics

Technology Strategy Board
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Engineering and Physical Sciences Research Council

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Mathematical modeling of an ultrasound sensor for bioprocesses

Executive summary

The focus of this project was to further develop the acoustic component of the mathematical modeling associated with ultrasound sensors for bio-processing.

Challenge overview

Bioprocesses such as microbial fermentation and cell culture are fundamental for the production of a whole host of products ranging from pharmaceuticals, specialty chemicals, food ingredients and bio-fuels. At present, these processes operate in a sub-optimal fashion because of the lack of available monitoring, and optimisation technologies which could "control" the biological system, and lead to maximised yields and product quality.

Bioinnovel is a new biotechnology venture developing novel in-line process sensors and associated bio/chemo-informatics and control software for bio-processing, agro-food processing and specialty chemicals processing. Its vision is to revolutionise the way that these industries develop, monitor and control their production processes.

This project contributed to the ongoing development of Bioinnovel's ultrasound probe technology which aims to significantly increase the capacity and productivity of these industrial sectors by introducing effective real-time process performance monitoring and optimised control. This technology is being developed using a multi-disciplinary approach that combines mathematical modelling with ultrasound engineering, chemistry, biology and software engineering.

Implementation of the initiative

Bioinnovel and Strathclyde University successfully applied to the Industrial Mathematics Knowledge Transfer Network for an Industrial Mathematics Internship, co-funded by EPSRC. Two interns gained experience in working in a multi-disciplinary environment involving engineering, bio-processing, mathematical modeling and business planning. By the end of the internship they had not only gained experience in applying mathematics to a real world problem they have also become very familiar with how a small company operates, how it finances and markets itself, and manages projects.

The problem

The literature survey identified the Epstein, Cahart, Allegra Hawley (ECAH) model as most appropriate for the task. The model provides estimates for the attenuation and phase velocity of ultrasound waves in suspension as a function of the system parameters and frequency. This is precisely the form of the data that is captured by the experimental apparatus and so a direct validation can be performed.

The model relies on a number of assumptions such as the particles are spherical and small compared to the wavelength, any changes in temperature or pressure due to the absorption of waves can be neglected, the velocity and pressure of sound waves are small, and the particles are well dispersed so can be considered as isolated scatterers. With these assumptions equations for the propagation of a compression, transverse and thermal wave in particle-laden fluid can be derived by considering conservation laws, a stress-strain relationship and thermodynamic equations of state.

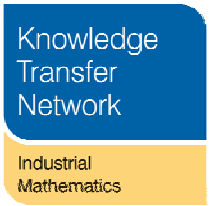
Both the full model which includes some time consuming matrix inversions and an approximate model were then implemented. The model output was then compared to a range of experimental data such as suspensions of silica particles and titanium dioxide particles in water. In each case the theoretical attenuation and velocity spectra had reasonable agreement with the experimental data.

The sensitivity of the model to each of the system parameters was then explored to assess the viability of an inverse problem methodology in recovering each of these parameters. A methodology for the inverse problem was then designed involved the minimisation of the least squares calculation between the theoretical and experimental data. This was subsequently implemented and a range of system parameters recovered. The methodology is fairly robust and the company will be testing and assessing its ability against a range of bioprocess data.

Results and achievements

All of the project's objectives were met and in some instances surpassed. The company intend to employ Anna to continue this modelling work and this further underlines the success of the internship.

www.strathclyde.ac.uk



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Minimal Paths and Virtual Endoscopy

Executive summary

We proposed a minimal path approach for extracting a path along a tubular shape in a 3D image and used this path as a trajectory for a virtual camera inside the body.

Challenge overview

Following a workshop presentation of our primary work on using minimal paths for 2D vessel tracking, we got in contact with people from Philips Medical systems, who build Medical imaging devices like scanners. They were interested to an extension of our methods to 3D medical images. After a few months of collaboration, an application to virtual endoscopy appeared as an important target.

Implementation of the initiative

Once we decided to work together, the natural way was to supervise a PhD student together through a CIFRE grant available for three years for collaboration between Industry and University.

The problem

Our method for finding a minimal path for extracting a tubular shape in a 2D image was extended to 3D images. This was a natural extension of the Fast Marching method to solve the Eikonal equation in the 3D domain of the image. We then obtain a path that is globally minimizing a functional based on the grey level of the image. This can also be seen as a minimal geodesic path according to a metric defined from the image. We thus had an easy interactive tool where the user provides a starting point and the output is a path of a given length going through the structure of interest, like colon, trachea, aorta, or any vessels. In order to use the path as a trajectory for a virtual camera, another challenge is that the path had to be centered inside the tubular shape. We proposed a variation on the initial approach that allowed finding a centerline of the structure. Once a path is centered in the vessel, it is used as a trajectory for a virtual camera inside the body. Rendering a sequence of images along the trajectory leads to virtual endoscopy. This means the physician can have a look at the 3D shapes along a part of the body without any device other than a scanner image.

Results and achievements

The proposed method was the subject of many publications in international conferences and journals, as well as a patent. Other authors made a comparison of different approaches that ranked ours as the best one to find a centerline. The interactive tool was made available by the company for the Medical Imaging workstations they provide to physicians.

Figure 1: extraction of the aorta vascular tree using the Fast Marching algorithm in a 3D MR image. The user just provides an initial point.

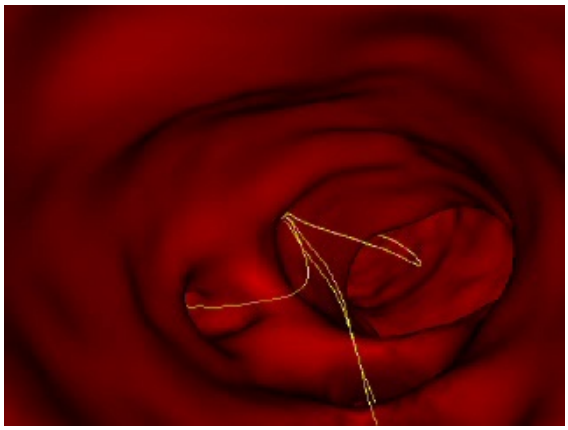

Figure 2: an image extracted from the virtual endoscopy along a path inside the aorta. A set of centerlines from the initial point to the ends of all branches is obtained. Some of these paths are shown in yellow in the figure.

PHILIPS

CEREMADE

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Simulation of a Bone-Prosthesis System

Executive summary

Prototype software, KneeMech, has been developed to assist surgeons by simulating the structural strain and stress distribution in a bone-prosthesis system of a knee, under various load conditions.

Challenge overview

The project saw a collaboration between the LIMA group S.R.L. and the University of Catania, after a contact started by Prof. Angelo Marcello Anile, from the Department of Mathematics and Computer Science (DMI) of the University of Catania. The objective was to provide a tool that is able to simulate the stress distribution in the prosthesis and in the bones as a result of the implantation of a knee prosthesis. The results depend on a large set of parameters, such as the mechanical properties of the bone and the geometry of the cut.

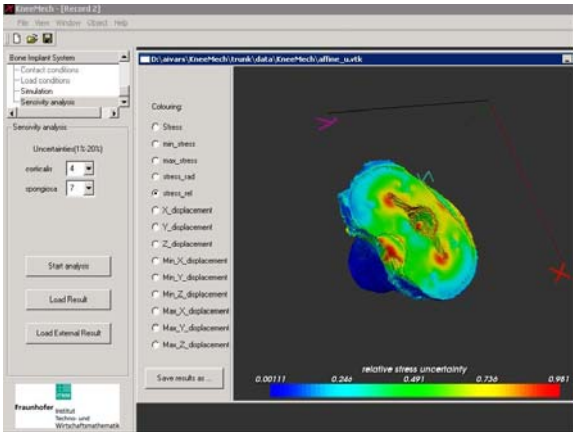
Implementation of the initiative

The initiative was so complex that several groups were involved in the project: the LIMA S.R.L. the DMI (applied mathematics group, conducted by Prof Anile, and image processing laboratory, conducted by Prof Gallo) and the DIIM (Prof Risitano). The research was carried on with the help of a foreign partner, the Fraunhofer Institute ITWM from Kaiserslautern, with the group conducted by Dr Heiko Andrä. The Vittorio Emanuele hospital in Catania, Sicily, was involved in the project, providing CAT scan of the bones, and consulting about the surgical process. The total duration of the project was two years. Some permanent staff were directly involved in the project, mainly for coordinating and supervising the activity of several post-doctoral fellows, who were specifically hired to perform the various tasks required by the project. The industrial partner provided all the necessary data about the prosthesis and much information about the process of prosthesis implantation. For more details about the actual surgical operation, a surgeon from the Catania hospital has been consulted.

The problem

The bone is modeled as a five-parameter viscoelastic material; the parameters were determined by fitting the measured response using the analytical solution of the relaxation predicted by the model.
A three dimensional geometric model of the bone was constructed by the image processing group from several 2D section images obtained from CAT scan. The geometrical data were integrated with the mechanical properties of the bone, obtaining a complete 3D description of the object. Great care has been used in the modeling of the bone-prosthesis contact: highly accurate multi-scale modeling provides the determination of effective parameters to be used in the numerical simulation.

The final problem is discretized using finite element on a tetrahedral mesh, obtained from the voxel representation of the bone. For the prototype, only an elastic model has actually been implemented. The final large sparse linear system is then solved by preconditioned conjugate gradient method. Once the displacement vector and stress tensor have been computed, the results can be displayed on arbitrary cross section of the bone (see figure).



Typical screen shot of the KneeMech software, with the visualization of the Von Mises stress in a bone cross section

An important aspect of the package is the possibility of performing uncertainty analysis, to establish the range of variation of the results upon uncertainty in the knowledge of some parameters, such as, for example, Young modulus of the bone. A suitably adapted affine arithmetic technique has been used for such purpose. The result of the collaboration was the realization of the software prototype KneeMech, and a scientific publication, and represented an excellent example of successful team work.

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Unravelling the genetic code

Executive summary

Knots crop up in all sorts of places: shoe laces, computer cables, and in our DNA. The difference is that while untangling the mess of wires behind your desktop is merely frustrating, knots in DNA molecules are life-threatening. Learning to control these knots could lead to new treatments for genetic disorders and diseases such as cancer or MRSA, so biologists and mathematicians are collaborating to help unravel the problem. Dorothy Buck at Imperial College London is using knot theory to understand why DNA becomes knotted, and how our bodies react to the tangles. It is all down to the unique packaging of our genetic code.

Challenge overview

The DNA molecule is a double helix, with two long strands joined together by a series of paired molecules, the particular order of these forms the genetic code for creating life. DNA replicates by splitting down the middle, so that each strand contains one half of the genetic code. The molecules in the rungs will only join with their opposites, the two strands each act as a template for reconstructing the entire genetic code, resulting in two identical copies of DNA.

The human genome stretches for nearly two metres, so it is wrapped to fit inside our cells. It is compact, but not always convenient, as our cells sometimes need to make minor rearrangements to their DNA. To achieve this, specialised enzymes called recombinases cut out small parts of the genetic code and replace them with DNA from elsewhere. We also use these enzymes as molecular scissors for inserting genes in genetic engineering. This procedure, known as recombination, involves repeatedly winding and unwinding the DNA parcel, inevitably creating knots and tangles. They make it impossible for the DNA to replicate, so other enzymes called topoisomerases act to keep the ball organised by tidying up after the recombinases.

Although biologists have known about these enzymes for some time, we don't fully understand what combination of tugs and cuts unpicks a particular DNA knot. The same problem is at the heart of knot theory: for a given knot, what set of moves will unknot it? Buck and her colleagues have recently helped narrow down the scope of the problem by showing that DNA can only form a certain family of knots. Buck hopes that this research will help characterise newly discovered recombinases, expanding the biologists' genetic engineering tool kit and allowing them to treat genetic disorders. Buck's work could also help improve existing treatments for a variety of diseases.

The situation is described mathematically by an equation relating the tightness of the double helix coil to the extent of supercoiling. These two quantities, called twist and writhe, add together to make the linking number, a value that describes the number of times two strands cross. Decreasing writhe automatically increases twist, leading to increased tension. Topoisomerases act to reduce the linking number, relieving the extra tension.

Cancer is essentially uncontrolled cellular growth caused by genetic errors, so the DNA within cancer cells is constantly replicating. Some chemotherapy treatments work by disabling the straightening topoisomerases, halting tumour growth. Unfortunately, this also affects DNA replication in healthy cells, leading to side effects such as hair loss. A better understanding of how the topoisomerases work within cancer cells could allow specific targeting, sparing enzymes in healthy cells and reducing the harmful side effects.

Another variety of topoisomerase can also act upon circular DNA, which is formed by the double helix looping back on to itself and joining together. This kind of DNA is found in bacteria and also in mitochondria, the small parts of a cell that convert glucose into energy. Unlike in normal DNA, the two strands of circular DNA remain intertwined during replication, resulting in two linked molecules. These circles must be separated before they can be placed into separate cells, so this second variety of topoisomerase cuts through one loop and pulls the other free before repairing the cut. This action also serves to reduce the linking number, simplifying the knot.

Results and achievements

Fluoroquinolones, an effective type of antibiotic, work by inhibiting these unlinking enzymes within bacterial cells, preventing them from replicating and killing the bacterial infection. As with all antibiotics, there is a danger that overuse will lead to bacteria developing resistance, rendering the drugs useless against diseases like MRSA. By revealing how the bacterial topoisomerases work, knot theory offers the possibility of developing new variations of fluoroquinolones to attack the enzymes in a variety of ways, reducing the chance of resistance.

Imperial College London

EPSRC Pioneering research and skills

Institute of mathematics & its applications

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Forecasting for urgent medical care call centres

Executive summary

Durham University developed statistical assessment and forecasting processes to underpin quality of service measures, to manage uncertainties in day-to-day operations, and to provide forecasts for resource needs for future operations for urgent medical care call centres.

Challenge overview

Northern Doctors Urgent Care (NDUC) is a not-for-profit organization which delivers out-of-hours urgent medical services to around 1 million patients in North East England.

Patients who call their own doctor out of hours are referred to NDUC. Calls are received by trained call handlers who record details from the patient and determine priority. The calls are then triaged by trained medical staff and patients are offered the most appropriate care for their condition including telephone advice, a visit to an Urgent Care Centre, a home visit, or direct admission to hospital. NDUC must deliver a high quality of service and value for money. 64% of service costs are to pay for clinician time.

NDUC needs to forecast call volumes and daily patterns of call arrivals to allocate appropriate staffing, both to provide a good level of service at times of peak demand and to avoid paying for under-utilised clinical staff time. A secondary problem is management of performance of clinicians and identifying good and bad practice.

Implementation of the initiative

NDUC approached Durham University in 2007 with the gist of the problem. David Wooff, an academic statistician and director of the university's Statistics & Mathematics Consultancy Unit, met with NDUC's executive manager John Harrison and suggested a number of alternatives. The result was that a two-year Knowledge Transfer Partnership (KTP) was established between NDUC and Durham University in August 2008, funded by One North East and the Economic and Social Research Council.

The problem

There is little extant methodology available to provide forecasts for call-centre volumes and daily patterns of arrival for this kind of problem. Forecasting is difficult because (1) there are structural daily effects - the call centre is closed during normal working hours, but open Saturday and Sunday; (2) there are thought to be different typical caseloads for different days of the week, e.g. Friday night heavy loads; (3) there are calendar effects, e.g. national holidays, Easter, Christmas, New Year; (4) general seasonal effects; (5) occasional epidemic effects, such as swine flu; (6) drift in demand because of population change or policy changes affecting service provision or organisation. We chose to model the daily volume of calls using regression models to identify and adjust for the crucial factors. We modelled daily arrival rates using a mix of generalized smoothing and a Poisson approximation to arrival times.

Results and achievements

The statistical methods provide NDUC with a forecast of numbers of calls arriving during every 30 minute. The model is periodically updated as fresh data arrives. The forecasts are made up to a year in advance if desired, and turn out to be highly accurate. For a recent three-day bank holiday we forecast 2116 calls and NDUC received 2113. The forecasts are used for staffing and resource allocation. The methods have been implemented using the statistical language R sitting behind Excel, and operated by NDUC staff with a small amount of training. NDUC also now has routine access to diagnostics such as queue build-ups and monitoring of clinicians triage-time performance in addition to a wealth of management information. This has allowed the saving of considerable money, whilst in parallel delivering an enhanced service to patients. There has been much interest in the methods for roll-out to similar organizations in the UK, and more widely to industries with queueing and service as an important component of their activity.

NDUC
Durham University
one NORTH EAST
E·S·R·C ECONOMIC & SOCIAL RESEARCH COUNCIL

http://maths.dur.ac.uk/stats/people/daw/daw.html

Three-dimensional X-ray imaging for dentists

Executive summary

Dentists often need three-dimensional information about teeth, for instance when planning how to attach an implant. Standard X-ray devices at dental clinics produce only two-dimensional images that are not sufficient for this. In the project, a panoramic X-ray imaging device was reprogrammed to take a few X-ray images from different directions, enabling three-dimensional reconstruction of tissue. The data set is sparse and collected from limited angle of view, so the inverse problem of reconstruction is sensitive to measurement noise and mathematically challenging. A clinically useful reconstruction algorithm was developed as a joint project between the Finnish Centre of Excellence in Inverse Problems Research and the company Palodex Group, with partial funding from the Finnish Technology Agency. The resulting product has been in the market for several years now, see http://www.vt-cube.com/.

Challenge overview

The contact between industry and academia was made in 1999 when a mathematics PhD from our team was hired to the research and development group of a company called Instrumentarium Imaging (later part of GE Healthcare and now Palodex Group). At that time, the need of affordable three-dimensional dental X-ray imaging was already acknowledged and research work started. The mathematical complexity of the problem encouraged the company to seek help from academia.

Implementation of the initiative

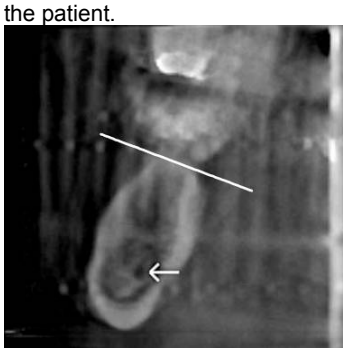
Three interdisciplinary projects were conducted in 2000-2008 with partial funding from Finnish Technology Agency. Involved were about a dozen mathematicians and physicists from various Finnish universities, and several company engineers with backgrounds in mechanical, electrical and software engineering and signal processing. The academic partners developed a variety of approaches to the ill-posed inverse problem of reconstructing tissue from sparse and limited-angle tomographic data. The company people in turn developed the hardware, converted the research codes into more effective production software and provided information about the needs of end-users. The scientists needed to learn how to communicate mathematical ideas to people with backgrounds in medicine, engineering, or marketing.

The problem

X-ray images can be interpreted as collections of line integrals of a nonnegative attenuation coefficient. As different tissues attenuate X-radiation differently, the coefficient can be seen as a three-dimensional image of tissue. In computational inversion, the unknown attenuation function is represented by dividing the region of interest into small cubic voxels. There are two basic problems in reconstructing the voxel values from the measurement data. First, the solution is not unique as several different tissues may produce the same sparse X-ray data. Second, the reconstruction process is very sensitive to noise in the data so specially regularized methods are needed. Bayesian inversion does the job by complementing the insufficient measurement data by incorporating *a priori* information about the unknown. The main challenges in the project were related to representing expert knowledge about dental tissue in the form of a computationally effective probability distribution. Out of the many approaches developed in the project, the wavelet-based Besov space priors were most successful.

Results and achievements

The project has so far produced 13 scientific publications and 4 patents. Also, the company now has a unique and cost-effective three-dimensional imaging product to offer for dentists. The figure shows a two-dimensional slice through a three-dimensional reconstruction of a mandible (jawbone). The nerve channel is marked with an arrow. A tooth implant is mounted by drilling a hole to the jawbone and then screwing a titanium screw into the hole. The implant is then attached to the screw. Before drilling the hole, oral surgeons need to measure the length from the level of teeth (marked with a line) to the nerve channel. Namely, drilling too deep would damage the nerve and lead to irreparable injury to the patient.



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Finnish Centre of Excellence in Inverse Problems (http://wiki.helsinki.fi/display/inverse/Home),
Professor S. Siltanen, University of Helsinki, Finland. Email samuli.siltanen@helsinki.fi

HELSINGIN YLIOPISTO
HELSINGFORS UNIVERSITET
UNIVERSITY OF HELSINKI

Computer simulations in electrocardiology

Executive summary

A mathematical model has been devised to describe the three dimensional electrical activity of the heart. Coupled to the torso, it allows in particular to compute numerical electrocardiograms (ECG). The simulation tool can be used by a pacemaker manufacturer to assess algorithms embedded in the device.

Challenge overview

Modern pacemakers, including or not a defibrillator, can provide measurements of the electrical potential at several locations in the heart. Rather than these raw data, a clinician would prefer something more familiar to him, that is, closer to a standard ECG, which corresponds to measurement on the skin.
The idea is to get a rough instantaneous ECG, just by remotely questioning the pacemaker, without setting up all the skin electrodes needed to get a 12-lead standard ECG. Of course, this cannot replace a genuine ECG but since the data are available for free, it could be used as a simple routine clinical examination. This project was supported by ELA Medical, a Sorin group company.

Implementation of the initiative

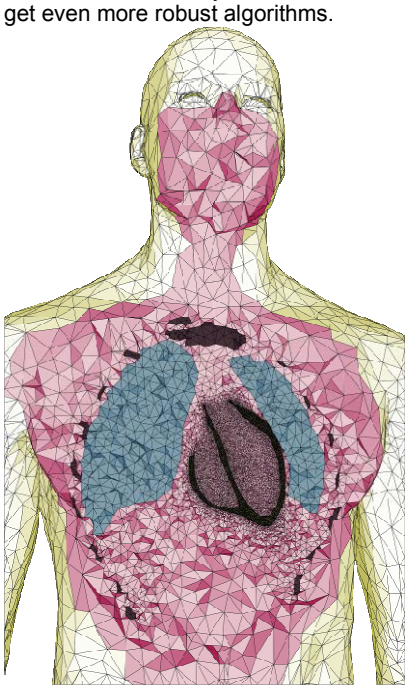
There are two difficulties related to the problem: first, devise an algorithm to build the “pseudo-ECG” from the measurements on the pacemaker; second, assess the quality of the algorithm. The second point being complicated to carry out on real patients, our industrial partner was interested in our capability to generate “computational ECG”. The simulation tool was therefore used as a virtual patient to test the reconstruction algorithm. A post-doc was hired in our research team and supported by the company for a year.

The problem

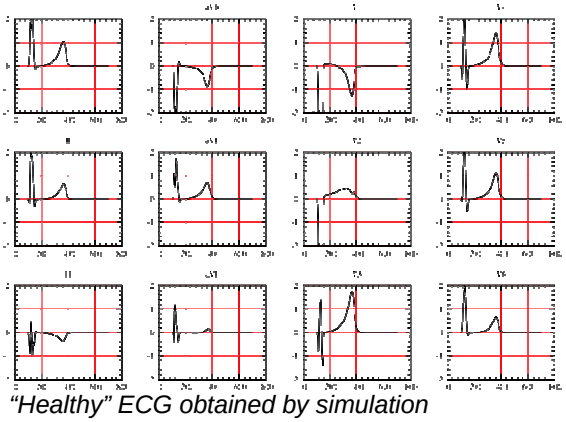
On the one hand, the electrical activity of the heart was modeled through nonlinear diffusion reaction partial differential equations, coupled to a system of ordinary differential equations describing the cardiac cells membrane activity. A specific software, based on finite element and domain decomposition methods, was developed to solve the problem in the heart and the torso. On the other hand, a machine learning algorithm, based on Reproducing Kernel Hilbert Space, was proposed to quickly deduce the ECG from the measurements on the heart. The numerical tool was used to assess the quality of the machine learning algorithm.

Results and achievements

The simulation tool was able to generate synthetic ECGs corresponding to different pathological situations (fibrillation, bundle branch blocks,…). The machine learning algorithm could therefore be tested in various configurations much more easily than with real patients. In the future, with the increasing power of pacemaker chips, real data could be enriched by simulation results in order to get even more robust algorithms.



The computational domain



“Healthy” ECG obtained by simulation

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SORIN GROUP
AT THE HEART OF MEDICAL TECHNOLOGY

Non Fickian diffusion in polymers and medical applications

Executive summary

The aim of the project was the design and the production of ophthalmic therapeutic lenses characterized by a controlled drug delivery .The lenses are polymeric platforms with silicone micro particles dispersed, the whole being loaded with drug which are used in the treatment of pathologies of the anterior segment of the eye. The need for an interdisciplinary approach put together a team composed by mathematicians, ophthalmologists and material scientists.

Challenge overview

Topical administration of eye drops is very inefficient because a substantial volume of drug is lost and there is a short residence time in the tear film. One of the most active areas of research and development in drug delivery involves "controlled-release" systems, which deliver a drug at a slower rate and for a longer period. The dosage form contains more drug than a conventional system but delivers the medication far more slowly: over a period of hours or days, rather than seconds or minutes. Three main disciplinary areas have been involved in the production of such devices: Mathematics (robust and accurate mathematical models which simulate drug delivery in polymers and allow an a priori control of delivery rate and total mass released); Ophthalmology (specification of the therapeutic properties of the devices); Material Science (synthesis of polymers in laboratory).

Implementation of the initiative

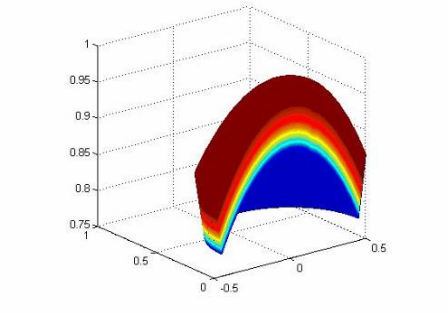
The project has been supported during three years and a half by the Portuguese Science Foundation. It has involved two chemical engineers specialized in polymers, three mathematicians, one of them being a PhD student, and an ophthalmologist. The work evolved in three steps. Firstly several mathematical models, describing the diffusion, transference and possible reversible and irreversible reactions occurring in the polymer platform, have been studied. Qualitative properties and numerical simulations were compared with experimental results obtained in laboratory. Secondly, the ophthalmologist in the team selected a set of drugs and established the optimal properties of the delivery - for the treatment of pathologies as for example glaucoma- concerning therapeutic flux rate, total mass and period of delivery. In a third step mathematicians selected the parameters of the model that produce solutions with the desired properties. Polymers characterized by such parameters were then synthesized.

The problem

From a mathematical point of view the problem is represented by a system of partial and ordinary differential equations with initial conditions - the concentrations in the polymeric matrix and in the micro particles - and natural boundary conditions. The study began by the qualitative behaviour of a one-dimensional system with the Theory of Laplace transforms. Expressions for transient flux and mass were established. An expression for a time constant-effective time- was also computed analytically. The dependence, on the parameters of the model, of these quantities was then studied. The models have been extended in three dimensions to shells and microspheres and solved numerically. Numerical codes for shells and micro spheres have been developed.

Results and achievements

Therapeutic lenses prototypes have been produced in laboratory. These therapeutic lenses have delivery characteristics a priori known (flux and effective time) resulting from the analytical approach and numerical experiments. An open-source software package to simulate the delivery behaviour has been developed. This package contains several routines to compute time dependent concentration, flux and mass; effective time and a tracking strategy that consists of a set of a priori estimations fluxes and the times it takes to reach these values. The external robustness of the models, in the sense of the agreement with laboratorial results, was very effective. A coupled model that simulates the behaviour of concentration, mass and flux in the anterior camera of the eye is also included in the package.



Lessons learned and replicability

As traditional in interdisciplinary work we mention a certain difficulty in the dialogue between the different fields involved. However a continuous work of three years and a half has given mathematicians a certain expertise in diffusion through polymeric platforms.

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Prof. José Augusto Ferreira (ferreira@mat.uc.pt)

Statistical testing of molecular motion inside living cells

Executive summary

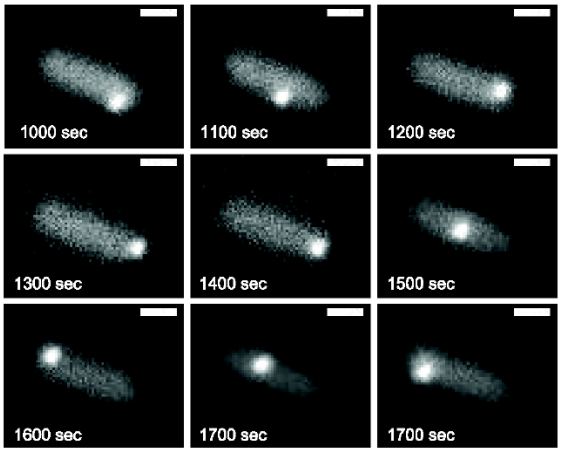
A new statistical test, basing on the so-called p-variation technique, is introduced to analyse and detect anomalous behavior of individual molecules inside living cells [1].

Challenge overview

A detailed understanding of the diffusion of single molecules in comlex biological systems is a challenging and timely problem. Such an understanding is necessary to model intracellular transport, regulation of cell polarization, gene transcription, kinetics of reaction, to name only few. It is also useful in other scientific disciplines, including physical chemistry and polymer physics, where the clarification of the mechanisms that govern the dynamics of single chains in polymer solutions is one of the most fundamental problems. Also, in pharmaceutical research, it could possibly improve the speed of release of drugs from polymer matrices.

Implementation of the initiative

Statisticians from Hugo Steinhaus Center, led by Professor Aleksander Weron, in close collaboration with Professor Joseph Klafter from Tel Aviv University, analyzed experimental data describing random motion of an individual molecule inside the *E.coli* cell (see Fig. below). The experiment was performed I. Golding and E.C. Cox at the Department of Molecular Biology, Princeton University, in 2005. The main goal of the analysis was to explain origins of strong anomaly detected in the experimental data.



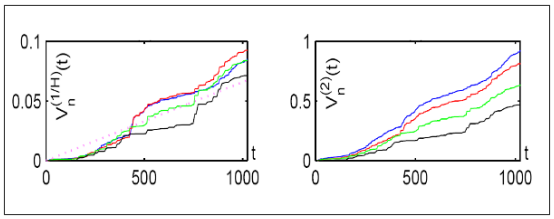
Source: I. Golding, E.C. Cox, Phys. Rev. Lett. 96, 098102 (2006)

The problem

Recent developments in single molecule spectroscopy enabled an accurate observation of random motion of an individual particle inside a living cell. The detailed analysis of experimental data revealed anomalous (subdiffusive) character of such motion. However, origins of subdiffusion in a given biological system are often unknown. It is not always clear which model applies to a particular system, an information which is essential when diffusion-controlled processes are considered. Therefore, determining the appropriate model of subdiffusive dynamics is an important and timely problem. Its solution could have strong impact on both theoretical and application-oriented disciplines.

Results and achievements

The introduced statistical test is capable of verifying origins of subdiffusive dynamics in complex systems. The test is based on the analysis of p-variation $V^{(p)}(t)$. It exploits different critical values of $V^{(p)}(t)$ corresponding to different theoretical models. The proposed method is very easy to implement, universal (it works for finite and infinite systems, with or without external potential), it requires only one appropriately long trajectory of the experimental data. The test was applied to the experimental data (random motion of an individual mRNA molecule inside the *E. Coli* cells.) The results (see Fig. below) resolved a recent controversy on the origin of the anomaly in Golding-Cox data. It was demonstrated that the observed subdiffusion cannot stem from a broad distribution of waiting times. It is more likely that fractional Brownian (or stable) motion is the underlying process.



References

[1] M. Magdziarz, A. Weron, K. Burnecki, J. Klafter, Phys. Rev. Lett., 103, 180602 (2009).

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Non-invasive test for monitoring diabetes

Executive summary

An industrial mathematics internship has helped to bring closer a non-invasive eye test for glucose monitoring, which will save 2.6 million people with diabetes in the UK from taking blood samples.

Challenge overview

More than 280 million people around the world have diabetes. The usual method of monitoring blood glucose involves pricking the fingertip to get a blood sample. This is a simple, but not a pain-free or risk-free procedure. People with diabetes tend to have impaired healing, and fingertip pricking can lead to complications such as nerve damage, elevated infection risk and skin toughness. A reliable, non-invasive measurement method would greatly help people with diabetes.

Implementation of the initiative

Lein Applied Diagnostics, a healthcare technology SME, is developing a non-invasive technology to measure blood glucose levels through eye measurements using a confocal system.

Lein first came into contact with the Industrial Mathematics KTN through a Study Group in 2004, and then attended presentations and networking events for the next few years.

In May 2009 a six-month KTN internship began, co-funded by EPSRC, which focused on signal processing to improve the quality of clinical trial data and improving the correlation model between the eye and blood glucose.

In October 2009, the results of this internship helped to secure £1.3 million of venture capital funding to develop the product. This enabled Lein to hire another full-time engineer, and begin investing in industrial mathematics for itself. The KTN intern has returned to his PhD, but is also working part time at Lein tackling a variety of mathematics problems.

“The Industrial Mathematics KTN’s Internships are great for SMEs as they address an industry problem within a short time-frame,” says Graeme Clark. “Unlike large businesses, our main focus is the next six months, and *then* the next five years. PhD projects are great for big industry but take a long time, and the main priority is broader research rather than our specific technical needs.”

"Working in Lein Applied Diagnostics enabled me to certainly gain a better understanding of how research in industry differs from that in academia. I learnt many valuable lessons during my time at Lein which not only will help me with my PhD project at Southampton, but help me with my life and future career. Being able to work with experienced consultants also formed a great part of my learning curve at Lein as I became more familiar with the physics of optics (by working with Professor Tony Wilson), and experiment design and experimental result interpretation. I also learnt to work as a part of a group and that will indeed help me with my future experiences. In short, my time was well spent at Lein," said the intern Shayan Motamedi Fakhr, University of Southampton.

The academic supervisor Mohamed Torbati, University of Southampton, said, "There are certain competencies that are essential for a PhD candidate, such as time management, communication, team working, etc, which this internship has helped Shayan in obtaining them. This internship has been a perfect demonstration of how research can be applied to improve people’s quality of life. Furthermore, some of the techniques and skills learnt during the internship can be directly applied to his PhD project."

Results and achievements

Key impacts include:

- £1.3m of venture capital secured
- Product closer to market
- Two extra staff – including a direct investment in industrial mathematics
- Successful demonstration of Industrial Mathematics KTN’s industrial Internships.

www.lein-ad.com

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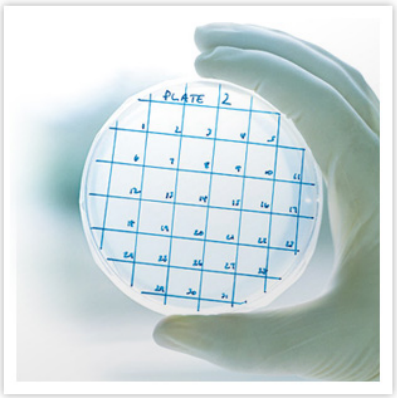
Qlucore-Bioinformatics

Executive summary

The first steps towards the birth, in 2007, of the bioinformatics software company Qlucore were taken in Lund, Sweden, in 2001. Researchers from the Departments of Mathematics and Clinical Genetics at Lund University then teamed up to attack the explorative challenges posed by the huge amounts of high-dimensional microarray data that was starting to emerge from high-throughput gene expression experiments. It early became clear that a fast and interactive software tool for visualization and statistical analysis was needed to conceptualize and explore the data. The project started as an academic research project, but after some years resulted in the creation of the company Qlucore. Today, in 2010, Qlucore is a world leader in bioinformatics, providing software to highly prestigious research institutes, as well as to several of the largest international pharmaceutical companies.



Challenge overview

Thanks to technological advances during the last decades, there has been an explosive increase in the amount of collected "high-through-put" measurements of so called Omics-data. Companies such as Illumina, Affymetrix and Roche provide platforms for collecting millions of measurements from hundreds or thousands of patients/samples in one single experiment. The big challenge for the entire research community is to draw biologically useful conclusions from this rapidely growing collection of data.

Implementation of the initiative

The project started as an academic research project. The goal of the project was to develop new models and algorithms to explore the gigantic Omics-datasets that were being generated in life science. It gradually became clear that an interactive software tool was needed.

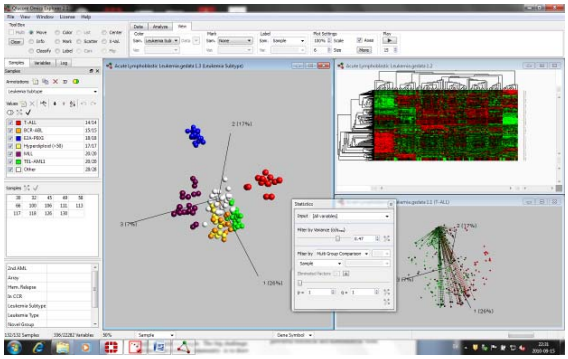
A first prototype of the software was developed within the academic project. But in order for the project outcome to be widely useful in the long run to the medical and biological research communities commercial software had to be developed. A company had to be formed in order to secure continuous development and general support.

The problem

The underlying idea in the initial project and behind the commercially developed Qlucore software is to provide a tool that can take full advantage of the most powerful pattern recognizer that exists - the human brain. This is made possible through a very fast interactive visualization tool. In order to secure full interactivity on a normal laptop for exploring datasets containing more than 100 million data points a new software architecture had to be developed and new algorithms had to be implemented.

Results and achievements

The result is a core software engine that supports e.g. PCA to interactively visualize the data in 3D and which helps the user to identify hidden structures and patterns. The visualization is combined with powerful statistical and mathematical algorithms.



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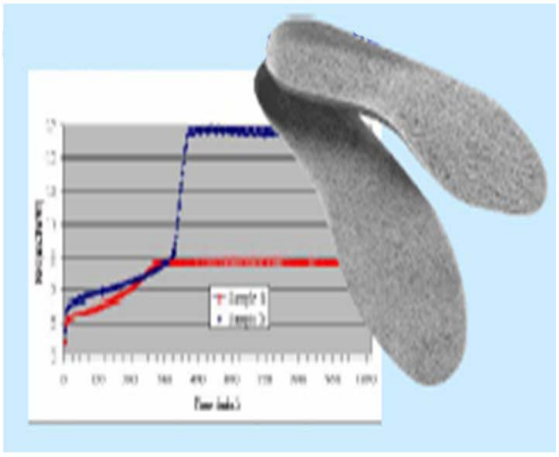
QLUCORE

Qlucore : www.qlucore.com

DINIS--Design of Innovative Nonwovens to be used as Insole in functional Shoes



Executive summary

The project DINIS was implemented by a research consortium involving 3 shoe factories and three research centres. Its goal was to optimize the structure of the insole by nonwoven material with respect to the customer's comfort.

Challenge overview

The initiative was proposed by Next Technology Tecnotessile - Prato (Italy) and involved several partners in four European countries (Italy, Germany, Spain and Denmark).
The final goal of the project was to identify, by means of numerical simulations, the best structure of a shoe insole made by nonwovens, so that it could achieve the target quality requested by the market.
The research was funded by public sources as well as by investments made by the partners.

Implementation of the initiative

The project had duration of two years and required continuous interactions of the partners. Moreover also the providers of the shoe factories were involved for a better understanding of the constraints of the problem.

The problem

The task of our research group was to develop mathematical models in order to estimate the comfort of an insole and in particular:
1. The mechanical response of the insole to different loads.
2. The evolution of temperature and retention of water and vapour within the insole, so that an estimate of the thermal comfort could be provided.
The problem was modeled in terms of a system of partial differential equations; the qualitative properties of the solutions were analyzed and numerical simulations were performed under different input parameters. The results were compared with the experiments performed on samples and on full-scale insoles. The comparison was successful, so that a series of virtual experiments were possible in order to perform a trial-and-error optimization.

Results and achievements

The experimental procedures and the mathematical simulations led to identify the best setting for producing optimal insoles for different type of shoes. One of these insoles was really produced by the companies and it resulted in a success story of innovation. Moreover, it was a very good example of technological transfer from research institutes to industry.
Our association (a not-for-profit organization linked with the Mathematical Department of the University of Firenze) keeps excellent contacts with some of the companies and possible future developments are currently under consideration.

Innovazione Industriale Tramite Trasferimento Tecnologico

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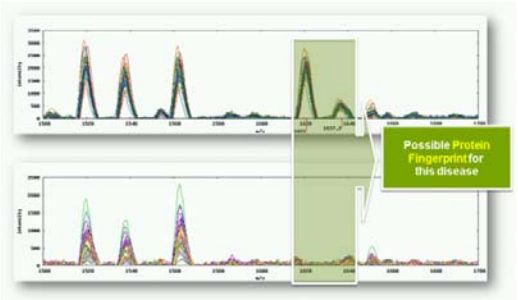
Early cancer detection by proteomics fingerprinting

Executive summary

Almost every disease changes the molecular constitution of an individual's blood (the proteome), following a pattern that seems to be unique for each disease. Mass spectrometry (MS) based screening methods have recently been introduced into clinical proteomics. This technology allows to display the current molecular contents of a biological sample, i.e., gives the approximate copy number of all types of molecules contained.. This is presently boosting the development of a new approach for early disease detection: proteomic pattern analysis.
In our project, new statistical-based algorithms for finding these disease specific patterns (fingerprints) in MS data were developed that run very efficiently on IBM's Cell/BE processor. This allows the application in time-critical environments like in clinical diagnostics in hospitals.



A possible (particularly simple) disease fingerprint. The shaded area highlights the difference between diseased (top) and healthy patients (bottom).

Challenge overview

Acquiring MS data from a complex mixture, such as blood, typically results in a dataset several gigabytes in size and containing tens of millions of signals. The challenge is to extract reliable signal patterns in short time from hundreds of these datasets that are unique to a given disease, such as cancer. If such a pattern exists in a patient's dataset it could help medical doctors to target subsequent clinical tests towards this disease.

Implementation of the initiative

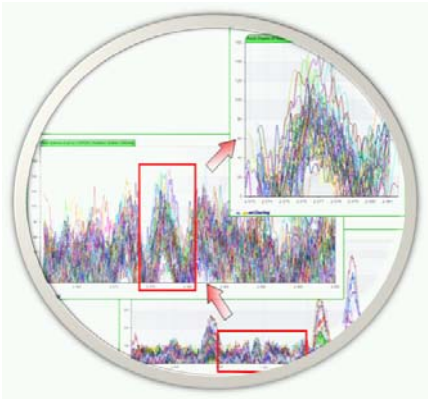
The project started with initial contacts between the Biocomputing Group at FU Berlin and Microsoft Research (MSR) regarding numerical problems in statistical feature extraction. Joint research quickly turned towards fingerprinting in proteomics and attracted Bruker Daltronics and the University Hospital Leipzig to join the team, finally the cooperation with IBM has boosted the reduction of computing time and a new level of statistical reliability.

The problem

This project required to solve three main problems. First, data from high-throughput platforms is often noisy and blurry and the signals sought for are frequently even smaller than the noise level in the acquired data. Second, small changes in the way the samples are treated before data acquisition can have a dramatic impact on the results. Third, the algorithms processing these huge amounts of data need to be efficient and very robust since a patient's further treatment might depend on it.

Results and achievements

The project partners could show that it is possible to solve the aforementioned issues and detect fingerprints for several cancer types. A standard operating protocol (SOP) has been developed that describes how to handle blood samples such that reproducible results can be generated.
On the data analysis side new algorithms have been developed that can detect disease-specific fingerprints with intensities as small as or even smaller than the noise level inherent in the data..
To reduce computation time algorithms were optimized for parallel computation to take advantage of state-of-the-art multi-core processors. IBM's Cell/BE chip was chosen as hardware platform. This technology satisfied all requirements such as speed, low energy consumption, reliability and is even suited to be used as coprocessor in future integrated systems.



An example for a signal (framed by the red box) as small as the noise level.

Contact

Prof. Dr. Christof Schütte, Dr. Tim Conrad, Biocomputing Group, Institute of Mathematics, Freie Universität Berlin

Partners in the project

Bruker Daltronic GmbH, Bremen
IBM GmbH, Böblingen
Microsoft Research, Cambridge
University Hospital Leipzig
University Hospital Charité Berlin

Services

MONOLIX

Executive summary

Monolix: a powerful tool for population pharmacology

Challenge overview

The pharmaceutical field is an area where conventional software tools have often been found to lack the power necessary to deal with complex models: pharmacokinetics-pharmacodynamics, viral dynamics, glucose-insulin, epilepsy…. A working group of academic statisticians and biostatisticians from INSERM began in 2003 *i)* to address the development of new statistical methodologies for the analysis of population pharmacology models, *ii)* to implement these methodologies in a software, *iii*) to apply these methodologies on real challenging applications.

Implementation of the initiative

For several years now, the pharmaceutical industry has shown considerable interest in Monolix. Between 2005 and 2008, Johnson & Johnson has lent its support to the development of the software by funding a post-doc.
In 2009, INRIA has launched a software development project that today brings together four engineers co-funded by the industry. The MONOLIX Scientific Guidance Committee involves representatives of the sponsors in order to define the specifications of the software. Members of the project are: Novartis, Roche, Sanofi-Aventis, Johnson & Johnson, Exprimo. Furthermore, several collaborations around the use of MONOLIX were established with other companies.

The problem

In order to evaluate a drug's impact, trial researchers must confront the need to model biological phenomena that evolve over time and present a high level of inter-individual variability. These highly variable systems are depicted by so called non-linear mixed effect models, often defined by systems of differential equations and for which it is particularly hard to estimate their numerous parameters. For 30 years now, pharmacologists wanting to interpret their clinical trials in preparation for market release applications have been using software programs that employ model linearization. This solution, however, raises major practical problems. MONOLIX implements several stochastic algorithms for parameter estimation that are known to have good theoretical and practical properties. The proposed methodology was recently extended to complex models (hidden Markov models, stochastic differential equations, mixture models…).

Results and achievements

Having started out initially just as a modest piece of code, Monolix has developed significantly over the years and is now widely used both by people in academic research as well as those in the industry itself. In particular, it allows the industry to solve some of the most complicated problems and models they face, such as complex viral dynamic modeling, issues that they can't solve with the usual tolls that they use. Development of these new methodologies and software has led to several successful collaborations with the pharmaceutical industry: HIV dynamic modeling (Pfizer, Tibotec), HCV dynamic modeling (Roche), epilepsy activity modeling (Pfizer). This project is also successful from the academic point of view (international collaborations, publications, conferences, PhDs in mathematics…).

Lessons learned and replicability

The Monolix software provides a clear example of the way close inter-disciplinary scientific collaboration can bring tangible benefits on a practical level. Balance between methodological development, industrial applications and software implementation is one of the reasons of the success of this project.

Contacts

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http://www.monolix.org

Shopper behavior modeling

Executive summary

This internship project contributed to Unilever's aim of developing a holistic model of shoppers' behaviour, taking into account heterogeneity in their demographic profile, as well as past responses to pricing, promotion and marketing strategies. Using large disaggregated panel data sets of supermarket transactions, this work developed, implemented and validated an agent-based model (ABM) of consumer choice.

Challenge overview

150 million times a day, someone somewhere chooses a Unilever product. A key challenge for Unilever's researchers has been to come up with a validation methodology using real-life data for the choice models that they have been developing. Stephen's contribution as an Intern goes a long way in taking those very important first steps in the validation exercise. These are important steps, not only for this project, but also as a contribution to the growing literature on the use of ABMs to study consumer markets. Unilever are not only more confident now of the use of the ABM methodology for business purposes, but will also benefit from the increased visibility of their research group within the ABM community.

Implementation of the initiative

Unilever expressed interest in the Industrial Mathematics Internships programme co-funded by EPSRC for this problem and the Technology Translators at the Knowledge Transfer Network helped them to identify a student and supporting University department (Mathematics at UCL) to participate.

The problem

The Internship project involved modeling and analysing large disaggregated panel data sets of supermarket transactions. The overall aim was to develop a holistic model of shopper behaviour, taking into account heterogeneity in the demographic profile, and past responses to pricing, promotion and marketing strategies. Using real-life data, the project sought to validate an agent based model of consumer choice within a particular product category (fruit juice) in an internet supermarket.

The project took an agent-based consumer choice model developed at Unilever and followed an iterative process of developing a simplified version of the model and implementing it as a computer simulation with the intention of applying validation techniques in order to assist the validation of the full model.

The final simplified model incorporated a weighted consumer choice function of net product price and product characteristics. Product characteristics refer to quantities or qualities of the product, such as brand or pack size, which are mapped to the interval [0,1] based on the volume of sales of categories within each characteristic. Each product was mapped to a point of the unit cube in a three-dimensional characteristics space.

Results and achievements

Following the development of the computer simulation model, panel data of the sales of fruit juice in 2007 from an internet shop were used in the initialisation of agents' characteristic preferences, calibration of parameters and subsequent testing of predictions out of sample. Out of sample tests gave the team greater confidence on the ability of the model to predict real life sales.

The validation exercise involved statistical techniques comparing the outputs of the simulation for a three month period to the real data covering the same period. Related ideas on probability evolution are currently being explored.

Industrial partner Dr. Abhijit Sengupta said, "The project has been a great success. It has played a key role in taking a step towards one of the challenges we were facing – i.e. validation of agent based consumer choice models. As industrial supervisor, I found the experience extremely rewarding and I look forward to future collaborations and publications."

Unilever

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UCL

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Generation of assignments of products to consumers

Executive summary

In market studies based in sensory analysis it is usually necessary to determine the products that each consumer of the sample will test, and the specific order in which he/she must do it. This assignment should follow some balance criteria, so that the conclusions are as unbiased as possible. A complete software solution was developed for the company Product Sensory Consulting Group (PSCG) to address this problem.

Challenge overview

A former student of the Degree in Statistics in our university, working in the company, contacted us for a consultation on how to do the assignments in the most balanced way. He usually did the job by hand, it took him several days of concentrated work, and the results were sometimes far from optimal. The company asked for a complete solution, from a friendly input of data to an output on an Excel file suitable for direct use in the field work. The final aim of the company was to offer their clients (major companies in the food sector) the guarantee of an accurate statistical analysis, based in the quality of the gathered data.

Implementation of the initiative

The 5-month project was led by a senior researcher, with experience in programming GUI in C++, and a young Ph.D. student, proficient in algorithmic low-level programming. No more than personal computers were really needed to develop de project, although a cluster of unix machines was used to test the memory load in problems of high dimensions. An evolving document with the specifications of the final product was continuously maintained between us and the person at charge in PSCG.

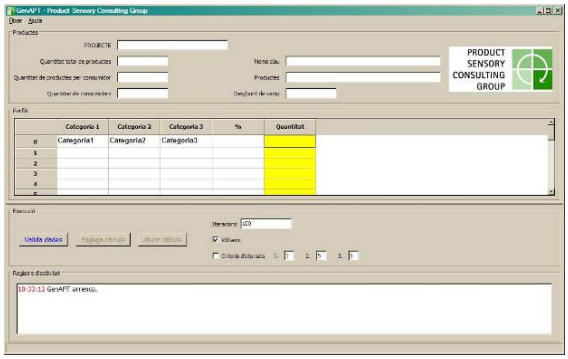
The problem

The difficulty lies in the fact that all products have to be tested a similar number of times in each position, and a similar number of times after each of the other products. This balance must hold at a global level, and also at a local level, for each of the profiles (gender, age, city, etc) in which the consumers are divided, and their combinations.

Results and achievements

The solution is based in latin squares, but they do not guarantee the required balance by themselves. A large number of columns of latin squares are generated at random, and the best solution is kept. It turns out that this simple strategy gives acceptably good solutions in a short time, and very good solutions when the software runs for several hours.

Some colleagues from the universities of Santiago de Compostela and Zaragoza helped with the initial idea.



The product is now being used in the company. The contact with PSCG has continued with a different project, which is presently in a preliminary stage.

Lessons learned and replicability

The idea can be used in other contexts. However, PSCG requested us not to offer the product to other companies of the same sector. Of course, the computer code can always be reused. The biggest technical challenge was to produce the output in an Excel sheet. The documentation on MS Object Linking and Embedding technology (OLE) for accessing their application programming interface from a C++ program is almost inexistent.

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PLATEA 4D: A decision support platform

Executive summary

The Geotemporal Exploitation and Analysis Platform (PLATEA 4D) is a platform to help the decision making process necessary for optimal response planning in emergency situations such as contaminant events in the environment, accidents where hazardous substances are involved, adverse meteorological phenomena, forest fires, etc.

Challenge overview

The platform has emerged from the evolution of several Interreg III B projects like ALERMAC (an Integrated Network for monitoring, alert and management of risks from spilled pollutants and catastrophic incidents in the Maritime Zone of Macaronesia), or like SAMM 2.0 (Alert and Environmental Surveillance System), contracted by the entity in charge of the environmental care in the Canaries (Dirección General del Medio Natural, Viceconsejería de Medio Ambiente, Consejería de Medioambiente y Ordenación Territorial del Gobierno de Canarias). Currently, PLATEA 4D is being equipped with new supporting modules to face contingencies such as adverse meteorological phenomena and forest fires. This has been possible by means of an agreement with the entity in charge of the management of emergencies in the Canaries (Gestión de Servicios para la Salud y Seguridad en Canarias S.A.).

Implementation of the initiative

The initiative has been developed by the Evolutionary Computation Division (CEANI, http://ceani.ulpgc.es) with the Prof. Gabriel Winter (gabw@step.es) as scientific director and the Assist. Prof. Blas Galván (bjgalvan@siani.es) as coordinator. The CEANI team include a multi-disciplinary group of engineers, computer science graduates and scientists working together in research and innovation for industry and government departments.

The problem

Several mathematical models were developed or enhanced along the research tasks included in the initiative, among them Sea Currents Fields, Wind Fields, Transport/Chemical simulation of Oil Spills at sea and Complex Rule based Systems. The major challenges of the research were the need of models' self-adaptation to real time situations with different available data set and/or geographical zones, sometimes large sometimes short, as well as to provide solutions with the precision required by the different users which are involved at the same time in emergency scenarios.

Results and achievements

PLATEA 4D has achieved optimized results in relation to its functionality, user driven characteristics and configuration capacities. The platform has an interactive user-friendly interface. It is possible to manage a large amount of heterogeneous data that can be simultaneously analysed and processed. These characteristics allow varying the configurations of the platform, providing different functionalities and applications as the mentioned above. All of them provide an important real time support decision system in emergency situations.

Lessons learned and replicability

The main impact of PLATEA 4D lies in its capacity of integrating new modules and processing data in real time. This feature allows adapting this platform to a wide range of new different applications for public services and industry, like maintenance strategies using monitoring, logistic management, etc. PLATEA 4D can be used also as tool for collaborative research activities among partners allocated in different places (cities or countries), being ideal for large R&D projects.

Contact

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INSTITUTO UNIVERSITARIO SIANI INGENIERIA COMPUTACIONAL

"HSC Populus" system helps control the job market in Lower Silesia (Poland)

Executive summary

The 'HSC Populus' system is used to analyze and forecast the evolution of human potential and the job market in Lower Silesia (Poland).

Challenge overview

What is the structure of the Wroclaw and Lower Silesia job market? How many people are seeking employments and in what fields? How many graduates will be entering the job market soon? These and other questions were of interest to the local government in Wroclaw in 2006. Wroclaw and Lower Silesia needed a system to analyze the changes in population, education and the job market in the coming years. The software was created at the request of the president of Wroclaw.

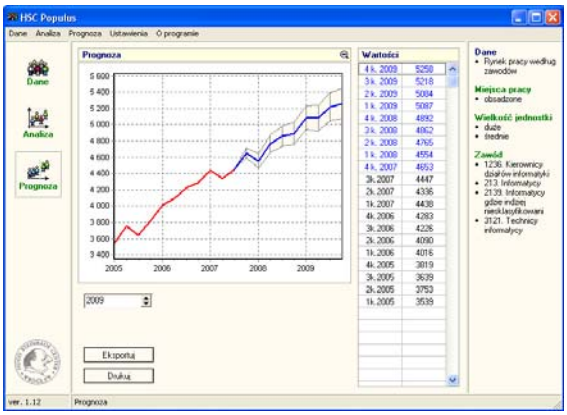
Implementation of the initiative

Ten specialists from the Hugo Steinhaus Center, headed by Professor Aleksander Weron, worked on the system from April to November 2006. HSC Populus costed approx. €40,000. It is jointly owned by the Wroclaw University of Technology and the Wroclaw Agglomeration Development Agency (ARAW).

The problem

The system contains three categories of data. These include detailed information on the population of Wroclaw, the state and educational needs of the region and forecasts concerning the changing job market in Wroclaw and the surrounding nine counties for the next five years. HSC Populus contains a list of the unemployed and employed from the Statistics Office in Wroclaw and the District Employment Office in Wroclaw, as well as information about the number of workers and people who are unemployed in one of the 1707 job categories. It offers forecasts of the most needed specialisations in the coming years. HSC Populus 'knows' when and in which branch there will be a deficit and where there will be an oversupply of the workforce**.** HSC Populus can provide the answer to the question: what specialisations will be the most wanted in 6 to 24 months?

The system is a type of a simulator, which analyses and models the trends on the job market. It constantly processes new data. It is an open architecture product and provides the opportunity to add new categories as new needs arise. Implemented forecasting procedures employ various time series models like, e.g., ARMA-GARCH processes.



Results and achievements

The HSC Populus system is the first of its kind in Poland. Thanks to the system, Wroclaw is at the forefront of the best prepared cities in Poland in terms of the job market, educational system, and business investments. Many investors have already submitted requests to obtain the analyses and forecasts from the system. Other Polish municipalities are also interested in having the HSC Populus tool.

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Using queuing theory to increase the effectiveness of physician staffing in the emergency department

Executive summary

Significant variation in emergency department (ED) patient arrival rates necessitates the adjustment of staffing patterns to optimize the timely care of patients. This study evaluated the effectiveness of a queuing model in identifying provider staffing patterns to reduce the fraction of patients who leave without being seen.

Challenge overview

Several US reports have documented a growing demand for care from emergency departments (EDs) and a simultaneous decrease in the number of operating EDs. The result has been increased crowding prolonged waiting times to be treated by an emergency provider, and high percentages of patients leaving EDs without being seen. A recent study found that 7.7% of the 36.6 million adults in the United States who sought care in a hospital ED reported trouble in receiving emergency care, and that more than half of these cited long waiting times as a cause. Timely access to an emergency provider is a critical dimension of quality for EDs, yet hospitals often struggle to provide adequate staffing to handle increasing demands for care. Constrained provider capacity relative to demand volume is exacerbated by the extreme variability in demand during each 24-hour period experienced by a typical ED week.

Implementation of the initiative

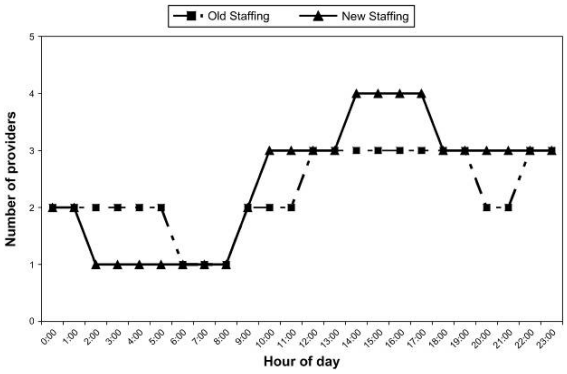
The project team collected detailed ED arrival data from an urban hospital in the US and used a Lag SIPP queuing analysis to gain insights on how to change provider staffing to decrease the proportion of patients who leave without being seen. The authors then compared this proportion for the same 39-week period before and after the resulting changes. More precisely, the study examined the response of one ED measure of performance, left without being seen (LWBS), to a provider staffing reallocation based on queuing theory. Two 39-week periods, one before the staffing changes (August 26, 2002, to May 25, 2003) and one after the staffing changes (September 1, 2003, to May 30, 2004), were studied. Matching weeks were chosen to better control for seasonal variation in both volume and disease states.

The problem

An M/M/s queuing model was used to estimate the number of providers needed during each staffing interval. This model assumes a single queue with an unlimited waiting room that feeds into s identical servers (e.g., providers). Arrivals occur according to a time-homogeneous Poisson process with a constant rate, and the service duration (e.g., provider time associated with a patient) has an exponential distribution. In this study, we used the Lag SIPP methodology, which was programmed using C as part of a prior research project, to identify provider staffing levels to achieve a given delay standard. The delay standard we chose was that no more than 20% of patients wait more than one hour before being seen by a provider.

Results and achievements

Despite an increase in arrival volume of 1,078 patients (6.3%), an average increase in provider hours of 12 hours per week (3.1%) resulted in 258 fewer patients who left without being seen. This represents a decrease in the proportion of patients who left without being seen by 22.9%. Restricting attention to a four-day subset of the week during which there was no increase in total provider hours, a reallocation of providers based on the queuing model resulted in 161 fewer patients who left without being seen (21.7%), despite an additional 548 patients (5.5%) arriving in the second half of the study.



Lessons learned and replicability

In an environment in which EDs are often understaffed, analyses of arrival patterns and the use of queuing models can be extremely useful in identifying the most effective allocation of staff.

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Air Elimination in Milk Pump Systems

Executive summary

This report summarises the work done by the Mathematics Applications Consortium for Science and Industry (MACSI) in Ireland on simulating a new design of milk metering equipment for Piper Systems Ltd.

Challenge overview

During collection, milk is pumped from a farm tank by a centrifugal pump into an air elimination vessel. After passing through the vessel, the volumetric flow rate is measured and the total amount of milk is calculated. Piper Systems manufacture the on board metering equipment carried by milk trucks. The managing director approached MACSI to ask for their help with

(i) modeling the existing setup (shown in figure 1) to understand and quantify any sources of error that might be introduced;

(ii) modeling a proposed new design of the milk metering equipment to see if it would improve the accuracy of measurements and to see if any optimization of the design could produce further reductions in errors.

Implementation of the initiative

After a half day MACSI workshop with postgraduates, postdocs and research fellows from MACSI as well as the MD of Piper Systems Ltd., a team with the most relevant experience was chosen to work on the problem over a 1 year period. A collaborative research agreement between the University of Limerick and Piper Systems Ltd. was drawn up.

The problem

The first stage of the problem was to simulate the entire system to demonstrate that the proposed design would successfully pump milk. This was modeled by a system of non linear ordinary differential equations which were derived and solved numerically. The next stage of the problem was to model the motion of the milk and the formation of bubbles within an air elimination vessel. Partial differential equations were derived for both cases, simplified and solved.

Results and achievements

Results were obtained by solving the equations described above and making recommendations regarding different parameters and physical dimensions of the system. These should help the company modify the design of the milk metering equipment for optimum performance which could potentially increase sales by up to €0.5 million.

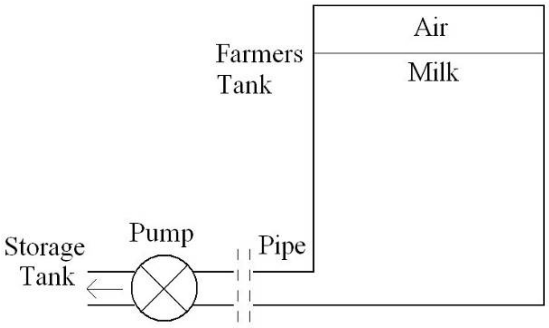

Figure 1: Generic farmer's tank and pump schematic.

PIPER SYSTEMS LTD.

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Optimal portfolio mix using insurance market data

Executive summary

The focus of this Internship project was to develop models that would help determine the mix of business in portfolios to provide the highest return or minimum risk. The tools developed during the project will be used to advise both individual Syndicates and Lloyd's of London themselves on how to manage the balance between risk and return.

Challenge overview

Lloyd's of London is one the world's best know insurance brands. It is however not an insurance company but a society of members, who underwrite in Syndicates on whose behalf professional underwriters accept risk. There are over 75 Syndicates who offer tailor solutions to respond to the specific risks of the client base. The syndicates operating within the market cover many classes of business including marine, aviation, catastrophe, professional indemnity, motor and many others.

Implementation of the initiative

Lloyd's of London expressed interest in the Industrial Mathematics Internships programme, co-funded by EPSRC, for this problem and the Technology Translators at the KTN helped them to identify a student and supporting University department (CARISMA at Brunel) to participate.

The problem

The main purpose of the this project was twofold:

- To determine the optimal mix of classes of business at Lloyd's level;
- To determine the optimal mix of classes of business at Syndicate level.

Mean – Risk models are tools for modeling choice under risk and widely used in the practice of portfolio construction. In these models, distributions are described and compared using 2 scalars: the mean and some suitable risk measure. In the mean – risk approach a random variable is preferred if it has greater expected value and less risk.

The project used variance as a risk measure and proposed two mean – variance models in order to determine the optimal mix of classes of business. An optimal mix portfolio is defined as a portfolio that achieves:

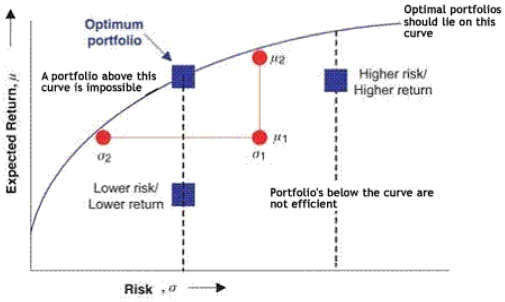
- minimum level of risk (variance of underwriting profit) at a given level of underwriting profit (mean);

or

- maximum level of underwriting profit (mean) at a given level of risk (variance of underwriting profit)

and by plotting the optimal portfolios, an Efficient Frontier is constructed.

Figure 1 is an example of an Efficient Frontier. All the portfolios on the frontier are optimal. The portfolio at (μ_1, σ_1) is not optimal; because at the same level of return (μ_1), a lower level of risk (σ_2) can be achieved and at the same level of risk (σ_1), a higher level of return (μ_2) can be achieved.



Results and achievements

The outcomes of the project will further go on to promote and help enhance the application of these mathematical techniques within the insurance industry, including all of the Lloyd's Syndicates.

Senior Analyst Michael Samuels said, "At Lloyd's, we had previously done some work on optimal portfolio mixes and we wished to take this further and refine it more extensively, using bespoke business constraints within the optimisation process. Having Nilgun as a 5-month intern from Brunel University via the Industrial Mathematics Internship Programme, really helped us to make significant progress in this regard, making full use of her supervisor at Brunel. Recently, she presented her main findings of her work to the Head of the Franchise Performance Directorate (FPD), who was very impressed. She has now subsequently been offered a role within our team to continue this good work going into the future and assist on other important modeling projects."

LLOYD'S
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EPSRC
Engineering and Physical Sciences Research Council

Faster calculations will boost business

Executive summary

A new approach to reinsurance risk calculation developed by UK mathematicians increases efficiency by 25-fold with no additional expenditure or carbon emissions.

Challenge overview

Catastrophe modelling and actuarial services are essential for reinsurance calculations to cover risk. These services rely on multifactor simulations and optimisation of complex contracts. Willis, a global insurance broker, wanted to increase processing capabilities without investing in expensive, energy hungry supercomputers.

Current simulations are so resource intensive that they take up to 24 hours, and are only run for 1 or 2 clients each year. Improving processing power will boost business by enabling Willis to run programmes for more clients. Such actuarial capability will be a unique offer to the reinsurance market.

Implementation of the initiative

The Environmental Risk Management Special Interest Group, set up in 2009 by the Industrial Mathematics KTN and the Natural Environment Research Council (NERC) to strategically address the challenges of the (re)insurance industry, determined that a small investment in this area would have major impact.

In October 2009 an intern successfully approached the problem with parallel processing, using computer idle time to perform calculations – 35 networked computers reduced calculation time by 25-fold, from 50min to 2mins. This time reduction scales linearly according to the number of computers.

A second KTN internship started in early 2010, using Graphical Processing Units, which also look very promising.

The first approach uses existing infrastructure, so no expenditure is necessary and there is no increase in carbon emissions. The second approach does require new hardware but it is considerably cheaper, smaller and produces less heat than current equipment. In contrast, a dedicated server network or supercomputer would have a significant cost and use large amounts of energy to run, meaning high levels of carbon emissions. Willis will implement the most efficient approach in September 2010.

“This increase in processing efficiency will enable us to run more simulations and optimise reinsurance programmes for prospective clients, and could tip the balance for winning contracts,” says Jurgen Gaiser-Porter, Willis. “Being strong in actuarial services and financial modelling is increasingly important as a market differentiator.”

The problem

Reinsurance provides protection for insurance companies against the risk of losses including catastrophic events such as earthquakes, floods and wind storms. Quantification of the associated risk relies on intensive simulations and the optimisation of complex contracts. The challenge of obtaining these calculations could benefit greatly from recent developments in parallel computing.

Willis is currently investing significant resources in the development of the next generation of catastrophe models for support of the transactional business. Willis has a new experimental prototype tool for optimising the placement strategy of client reinsurance programmes. This is particularly computationally demanding task demanding running tens of thousands of different strategies. However, timetables for their clients to make certain decisions about reinsurance placements can be measured in days so having fast tools is key.

Results and achievements

Key impacts include:

- 25-fold increase in speed of calculations
- No/minimal additional expenditure
- No increase in carbon emissions
- New actuarial service offering to the market
- Optimisation of complex contracts – many more can be evaluated and tailored to clients’ needs.

UNIVERSITY OF OXFORD

NATURAL ENVIRONMENT RESEARCH COUNCIL

www.ox.ac.uk
www.willis.com

Knowledge Transfer Network
Industrial Mathematics

Technology Strategy Board
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Networking for the future

Executive summary

Networks are all about making connections. The global internet and telephony networks form the largest and most complex machine the human race has ever constructed, allowing billions of people to exchange vital information in the blink of an eye. Equally important is the global transport network, which enables the mass movement of people and goods by land, air and sea. Understanding how these connections work is essential if we want to improve them, and only the mathematics of network theory can get the job done.

Challenge overview

A problem common to both communications and transport is the balancing of an individual's needs with the needs of the whole network. Individual car drivers pick the shortest routes to their destination based on personal knowledge of the network (road paths, average traffic levels, etc.), but these individual choices can actually cause the network to be less efficient overall. A similar problem arises in computer networking, with local routers having to decide which paths to direct individual data packets along.

One solution is to change the behaviour of individual drivers through incentives such as variable road pricing. The congestion charge zones in London and Stockholm encourage drivers to avoid paths through the city centres, even though this may be the shortest route for an individual. These kinds of changes are very different to traditional transport network modifications and they require a new kind of mathematical analysis.

Road pricing schemes need little in the way of civil engineering so can be rapidly implemented, while at the same time require the choice between a large range of options for zone boundaries and driver charges. In order to model the possibilities and find the best solution, mathematicians must develop faster and better network algorithms that can compare a larger number of options in a shorter amount of time.

Another solution is to provide people with new information that enables them to make more informed decisions.

Implementation & results

While working as Chief Scientific Adviser to the Department for Transport, Prof Frank Kelly assisted with the creation of a travel-time map of Cambridge in which journey times on public transport are represented by different colours. Someone moving to the city could use the map to quickly find a home that allows an easy commute to their workplace; information which is difficult to find by using a map alone. This work is now being developed into Mapumental, a user-friendly website created by mySociety.

Kelly believes the next mathematical challenge is to closely model the links between different types of networks. For example, modern smart-phones can connect to the internet through both the 3G mobile telephony network and local Wi-Fi hotspots, but this connection can often be unreliable, especially when browsing on the move, because only one connection is active at a time.

The next generation of smart-phones could allow simultaneous connections over both 3G and Wi-Fi, so that as one signal fades out another fades in to provide a continuous connection, but to do this mathematicians must design an algorithm that switches signals at the correct speed. Change too slowly and data packets will be lost, but change too quickly and packets will bounce between the two connections, creating problems when the data is reconstructed.

The travel-time maps created by mySociety software developer Chris Lightfoot offer a new way of looking at our transport networks. They allow users to make more informed decisions about their journeys by highlighting the relationship between travel distance and travel time to help identify the best routes.

The maps are produced by fixing a destination point and arrival time, then scraping the journey planner website TransportDirect for travel-time data between all of the transport interchanges in the region. The software then overlays the map with a grid of points and searches for all transport interchanges within a 15 minute walk from each point. Choosing the interchange that offers the shortest journey time to the chosen destination results in a grid of points at which we know either the journey time or that no journey is possible, and these points can be coloured according to the time.

Not every point on the map will have a defined travel-time however, so producing a smooth map requires a further step. The software extrapolates smooth contours using a solution to Laplace's equation, producing a map that is both useful and aesthetically pleasing.

Internet over cable networks

Executive summary

Cable networks were originally designed to broadcast analogue television signals from the service provider to its users. With the help of hybrid fiber coaxial technology, cable networks users could transmit signals to the service provider, which opened up a new world of interactive multimedia services with Internet browsing as most prominent application. This upgrade of cable networks asked for new ways to deal with the situation of bidirectional data transfer and presented challenging research issues. Mathematicians from Philips Research and the research institute EURANDOM explored new ways of dividing optimally the network capacity among its users, and of addressing the trade-off between capacity and delays.

Challenge overview

In 2000, Philips Research and EURANDOM joined forces to analyze reservation procedures for cable access networks with an approach based on mathematical modeling. The major challenge was to model the systems with its many users as stochastic networks. This gave rise to a whole collection of new multi-dimensional stochastic models. The analysis of these new models was used to assess the performance of the networks in terms of capacity and delay characteristics. Several new and patented protocols were developed and implemented on a large simulation platform.

A wide scope

The newly developed stochastic and queuing models are interesting in their own right. Queuing theory is concerned with the analysis of congestion phenomena and has developed hand in hand with communications for about a century. The research challenges in communications (first in telephone networks, then in wireless communications and the Internet) have spurred the development of the mathematical theory of stochastic processes; while conversely, a large number of applications in communications would not have been possible without the development of stochastic theory. This project moved at the interfaces of queuing theory, communications and analysis. The goal was to develop new mathematical theory for the performance analysis of large and complex stochastic systems and networks. The practical motivation stemmed from the explosive growth in the size and usage of the Internet and web-based applications, which asked for new paradigms as to how to design communication systems, schedule their capacity, and serve their users.

Mathematics was used not only for modeling purposes when dealing with immensely complex systems, but also for the management of a network, for understanding user behavior, for the development of algorithms and protocols, and for performance analysis, optimization and control. The dynamics and inherent randomness were described in terms of stochastic models.

Apart from their application in cable access networks, the models may find application in other fields. They incorporate characteristics of multi-access communication and resource sharing, issues that are the topic of ongoing research in fields like computer networks, radio frequency tagging, networks on chips, satellite systems, mobile telephony, wireless networks and many more.

Monograph published in 2008

Results and achievements

The research performed in the period 2000-2008 has resulted in a large number of conference and journal publications, a patent and two PhD theses, and a monograph published by Springer in 2008. The thesis was awarded the 2008 INFORMS Telecommunications Award for the best dissertation in operations research for telecommunications worldwide in 2005-2007.

EURANDOM

PHILIPS

sense and simplicity

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Smarter phones for all

Executive summary

There are more active mobile phones in the UK than people: over 70 million at the last count, thanks to multiple handset or SIM card ownership. The mathematical study of signal processing allows us to extract useful information from the noisy, invisible sea of radio signals above our heads. The rise of smartphones and mobile internet introduces new challenges to the mobile networks, but cutting-edge mathematics is set to provide cheaper, more energy efficient and better quality communications for all.

Challenge overview

Mobile phones transmit signals to a nearby base station via radio waves. Waves in the spectrum are described by their frequency, the number of oscillations per second, and two mobiles attempting to communicate with a base station using the same frequency will interfere with each other. This places a fundamental physical limit on how many mobile users can squeeze into the available frequency bands, making the spectrum a scarce natural resource that is be regulated by the Government to ensure it is used fairly. The spectrum is also an incredibly valuable resource, as demonstrated by the UK Government's £22.5 billion auction of the 3G frequency band in 2000.

Mobile networks, like all forms of communication, are underpinned by information theory, which was founded in the late 1940s by the American mathematician Claude Shannon, who realised there is an upper limit on the amount of information that you can send over a communications channel, such as a radio frequency band, before errors start to creep in. Reaching this “Shannon limit” requires a mathematical description of the message called an error-correcting code, but for decades the best codes could only achieve around half-capacity. It wasn't until the 1990s that researchers came close to unlocking the full potential of communications channels, with a new method called turbo codes.

Signals in a complex urban environment scatter when they bounce off buildings, causing echoes that take longer to reach their destination. These delayed echoes can interfere and cancel out when they meet again at the receiver, leading to dead zones and dropped phone calls. John McWhirter at Cardiff University has figured out ways to make these multiple-path effects actually improve signal transmission.

These improvements exploit an important new development in broadcasting technology called MIMO, or “multiple-input and multiple-output”. MIMO uses arrays of “smart” radio antennas in both the transmitter and receiver, combined with software that tunes in on the direction in which a signal is strongest. Currently used algorithms are inefficient because they can't solve the problem without an intermediate stage, but recently McWhirter and his colleagues have developed methods to tackle it directly.

The problem

Transmitting a signal with a MIMO system is a problem in linear algebra. The matrix in a MIMO system describes how a signal is transformed during transmission due to noise and other errors, and recovering the original transmitted signal by inverting the matrix.

Due to the time-delays introduced by multiple-path effects, MIMO matrices contain a polynomial in each cell. The current solution converts the polynomial matrices by first reducing them to a set of simple scalar matrices using a technique called orthogonal frequency-division multiplexing (OFDM), then inverting these scalar matrices with traditional algorithms. Each scalar matrix corresponds to a particular set of frequencies within the frequency range of the communication channel, but separating the frequencies in this way results in a loss of degrees of freedom and a less efficient use of the spectrum.

McWhirter hopes that removing this extra step will allow a more efficient use of the available spectrum. His new algorithms for inverting polynomial matrices directly could enable more mobile phone users to make better quality calls while also using less energy, an important goal when levels of mobile communication are constantly increasing.

CARDIFF UNIVERSITY
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http://www.engin.cf.ac.uk/whoswho/profile.asp?RecordNo=253

Transport and Logistics

Optimal trip planning in the presence of random delay

Executive summary

This project has provided train passengers a better way to plan their journey; it will provide the best route and the best starting time for their journey and the passengers will know that they will arrive to their destination on time even when the trains are delayed during part of the journey. The passengers will not need to worry about being late for the duration of the trip and they will not need to start their journey too early to compensate for the possible delay.

Challenge overview

Given the time a train passenger would like to reach his/her destination and some degree of certainty that he/she will arrive the destination on time, then using the probability distribution model for delays of each train, we will optimize the starting time of the journey, i.e. find the latest time the passenger should start the journey, such that the passenger will reach the destination on time within the given probability.

Implementation of the initiative

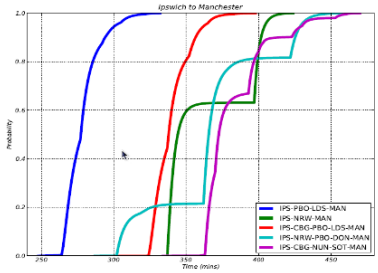
Birmingham University made the Industrial Mathematics Knowledge Transfer Network aware of its desire to work with industry on a discrete optimization project and they were subsequently introduced to BT who wished to develop a tool for planning train trips in the presence of random delays. The teams then applied for and were awarded an Industrial Mathematics Internship, co-funded by EPSRC.

The problem

The problem is bounded by the following assumptions: (1) the departure times of any two trains are statistically independent, (2) the order of the departure for any two trains may vary due to delay, and (3) passengers will always catch the first train that departs to their next station on their route after they arrive at the station. The project team also collected data for the delay of the trains which is found by comparing the actual departure times of the trains from different stations with the departure time scheduled on the timetable. Using the above assumptions and the data collected for the delay of the trains, the intern modelled the train delay for different stations as probability distribution function. From these distributions and with any given starting time, they developed a method of calculating the time a passenger will take to travel between two stations and subsequently the destination with the probability the passenger will arrive before this time.

Finally using the method they developed together with a bisection method, it is now possible to calculate the latest time the passenger can start the trip given the time the passenger want to arrive the destination and the probability the passenger wants to arrive on time.

CDF for journey times from Ipswich to Manchester



Results and achievements

The researchers were able to obtain some new results in generalized order statistics and have developed ways to decrease the number of calculations required in a problem with exponential computational complexity. The program can be used by public transport companies to improve their journey planning system on their website.

Industrial supervisor Dr Keith Briggs said, “This was an ideal internship project, combining rigorous mathematics and statistical modeling with a problem of genuine practical interest. Along the way we developed new results in the field of generalized order statistics (classical order statistics deals with e.g. the distribution of the minimum of a set of iid random variables; we are able to remove the iid condition and also compute conditional order statistics). And to write a program for the problem which is sufficiently fast was quite a challenge, since it must deal with a potentially large number of combinations of trains and routes. This was achieved by some clever programming.”

BT

UNIVERSITY OF BIRMINGHAM

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Knowledge Transfer Network

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EPSRC

Engineering and Physical Sciences Research Council

Aircraft icing

Executive summary

Ice accretion on aircraft poses a significant threat during flight. Consequently great efforts are made to prevent ice build-up. Since testing of new components is highly expensive and time-consuming improved mathematical models and numerical codes were required to cut down on development time and to reduce costs.

Challenge overview

Atmospheric clouds of liquid water droplets are frequently made up of supercooled droplets (without a nucleation site droplets may be supercooled down to -40C). If an aircraft encounters such a cloud droplets striking the surface are provided with a nucleation site and so begin to freeze. The resultant ice accretions may rapidly degrade the aerodynamic performance. Consequently nearly all commercial aircraft and some helicopters are provided with ice protection systems. However, these are expensive to run and it is not always clear where the ice will form.

The goal of this project was to develop a three-dimensional aircraft icing code which could be used in the future design of aircraft components. The project was carried out in collaboration with BAe Systems, Rolls-Royce, GKN Westland Helicopters, DERA and Cranfield University. Dunlop Aerospace and Airbus UK also became involved at a later stage.

The problem

The academic component was to develop a model for the ice growth coupled to the flow of a thin water layer and then develop and test subroutines to fit into the full icing code.

Mathematically this involved coupling a phase change model to one for thin film flow. The presence of two moving boundaries made both analysis and numerical solutions complicated. A further challenge was that the new component should not dramatically increase the run time for the existing code.

Results and achievements

The models developed were integrated into a number of subroutines which were then linked to the main code (from Rolls-Royce) for calculating air flow and water droplet trajectories. The full code was tested rigorously through comparison with existing two-dimensional codes and against experimental results from icing wind tunnel tests.

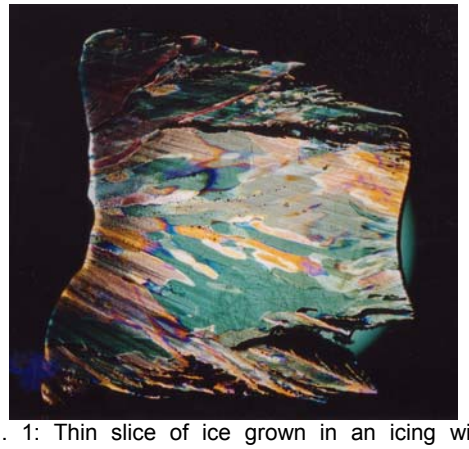

Fig. 1: Thin slice of ice grown in an icing wind tunnel. This shows the ice crystal structure and was used to verify the basic one-dimensional phase change model.

The success may be measured by the fact that all industrial partners now use the code as part of their development processes and that a follow-up project was funded. For a single case study it was stated that the ICECREMO code saved up to 1 million pounds :
http://www.aviationtoday.com/regions/usa/5135.html
ICECREMO has since been sold to overseas companies. There were also a number of spin-off projects, related to water flow through turbofan engines and accretion on rotating surfaces.

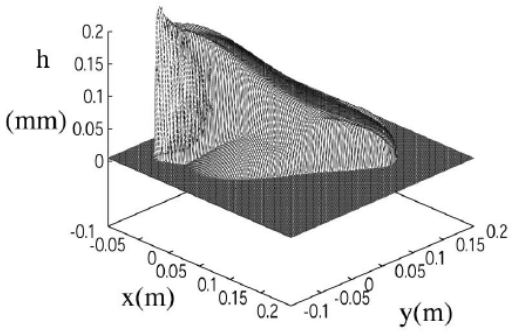

Fig. 2 : Shape of thin water layer on an accreting ice surface, subject to gravity (to the left) and air shear (to the right). (Reprinted from Phys. Fluids 14(1) 240-256 2002).

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Optimization of the “118” Emergency Management System in Milan

Executive summary

The project consisted in applying mathematical models and algorithms to develop a decision support system for the optimization at different levels of the operations performed by the Health Care Emergency Management System (EMS) in the province of Milan.

Challenge overview

The EMS serving the province of Milan is based at one of the major hospitals in the city and receives in average more than 1500 calls a day. About half of them generate missions for a fleet of 24 ambulances that are usually stationed at predefined parking places scattered in the metropolitan area and 28 ambulances located at some bases in the surrounding municipalities. The level of service to be provided is quite critical: urgent requests must be reached by an ambulance within 8 minutes. However this performance was achieved in less than 50% of the cases, resulting in complaints and even in negative articles on local newspapers. A constant increase in the demand over time and the need of keeping costs under control were additional reasons of concern. Though being well-equipped from an IT viewpoint, the operational centre responsible felt the need for an automated decision support system and more in general for a scientific, quantitative and effective approach to their everyday problems. The contact was established by a retired professional, member of the Italian O.R. Society (AIRO), who involved several research groups from different universities with complementary skills. The objectives were defined step by step in several meetings between the academicians and the prospective end-users. The project turned out to be made of many complementary sub-problems on optimal resource sizing, ambulance routing and allocation of patients to hospitals.

Implementation of the initiative

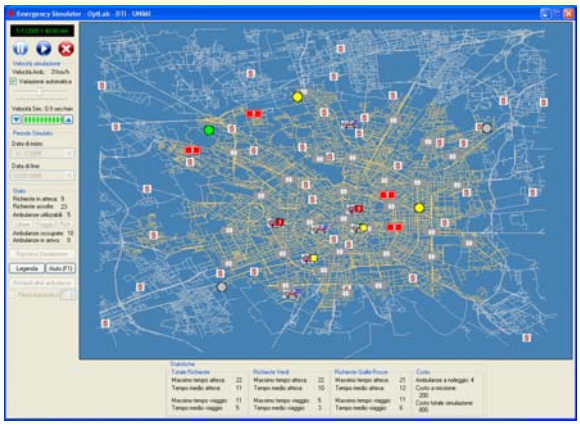
The research project, named « Decembria », lasted for two years and was funded by Regione Lombardia. It involved a dozen researchers from the academy and more than twenty young collaborators at different levels (graduate students to post-docs).
In spite of being developed by academic personnel, the outcome of the project has been actually implemented and is now integrated on top of the information system of the operational centre of the EMS. This integration was often the bottleneck, since the information system had not been designed to feed additional software modules with real-time data.

The problem

The project encompassed many different sub-problems related to the optimal execution of expensive and time-critical operations. Many different mathematical techniques were used, such as space-time statistical analysis of the demand patterns, forecasting techniques like time series decomposition, exponential smoothing models, kernel density estimate, discrete-event simulation, systems dynamics, game theory, queuing theory, mathematical programming, and online optimization.

Results and achievements

The models and the software developed within the project are now in use. In particular control charts are now used to forecast the demand for each week; systems dynamics models are used to predict the evolution of the seasonal flu every winter; a decision support tool is used to suggest mission assignments and ambulance relocations to the operators. A quantitative evaluation of the percentage of urgent calls reached within the eight minutes threshold is currently ongoing. Regione Lombardia is now planning to extend the project to the regional level.



Lessons learned and replicability

The project can be replicated in any other large city, where automated optimization tools are needed to support complex and life-critical decisions.

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Optimization of Public Transport Systems

Executive summary

The decision, planning, and optimization problems arising in public transport are highly complex and often of gigantic size. In the last twenty years, mathematical theory and algorithmic methods have been developed that make it possible to provide provably optimal solutions to many of the basic problems coming up here. These have made their way into the industry, and thus, mathematics helps to keep public transport systems affordable. Having the basic problems "under control" allows addressing more advanced questions like intermodal and integrated service design, disruption handling, and market aspects such as competition and user behavior.

Challenge overview

In the early 1990s the Zuse Institute Berlin (ZIB) was approached by public transportation companies in Germany − in some cases by the request of politicians who provide significant subsidies to keep the buses, etc. running − to help them plan the operation of their vehicle fleets and schedule their work forces. Among our main partners were the Hamburger Hochbahn and Berliner Verkehrsbetriebe (BVG), two of Europe's largest public transportation companies. At the time most of the planning steps were carried out manually. We initially addressed the bus circulation problem; many projects followed including driver scheduling, time tabling, network, line and fare planning. Some of the latter projects were carried out together with colleagues within the DFG Research Center MATHEON.

Implementation of the Initiative

The research took place in a series of projects funded by a variety of sources including the public transport industry, the Bundesministerium für Bildung und Forschung, and the Deutsche Forschungsgemeinschaft. All initial research activities were carried out at ZIB, mainly by PhD students and post docs, in close cooperation with the industry partners who also provided staff support and data. At the end of each individual project the industry partners and ZIB spin-off companies turned the prototype codes into commercial software products.

The problem

Optimization problems in public transport can, in general, be modeled in terms of network flow problems in suitable planning graphs (of very large scale). The whole range of methodology from integer programming (LP relaxation, cutting planes, branch & bound, primal heuristics, etc) was applied. Particularly important tools are column generation and multi-commodity flow techniques. Major challenges arise from the enormous sizes coming up. Bus circulation at BVG, for example, leads to integer programs with about 100 million variables, and driver scheduling problems may go even beyond this size.

Results and Achievements

The projects carried out have lead to a mathematical understanding of the basic problems of public transport. They have given rise to significant mathematical challenges in the fields of combinatorial optimization and mixed-integer linear programming. They have inspired new algorithmic developments coping with optimization problems with huge sizes. Public transport questions have also resulted in a fresh look at research fields such as robust and online optimization. We now have mathematical models for most of the basic problems arising; many of these problems can be solved to the satisfaction of the customers. The projects have resulted in spin-off companies (such as LBW GbR) providing today mathematical tools that are employed worldwide. Hundreds of million Euros are saved in this way annually. These tools have become best practice industry standards.

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DFG Research Center MATHEON
Mathematics for key technologies

Forecast Model Selection in FMCG Supply Chains

Executive summary

This project successfully developed statistical routines for selecting optimal forecasting models for fast moving consumer goods (FMCG) manufacturer Beiersdorf worldwide. Forecasting accuracy has been increased leading to substantial inventory savings.

Challenge overview

Beiersdorf (BDF) is a global fast moving consumer goods manufacturer of skin and beauty care brands, selling 100s of products across 150 affiliates worldwide. Planning and coordinating the supply chain is vital to ensure availability of the products to consumers. Here, forecasting plays a key role as its accuracy drives inventory, and hence supply chain efficiency and return on assets. Forecasting thousands of product/country combinations with different forms of seasonality and trends requires automation of model selection, which conventional approaches could not provide.

Implementation of the initiative

The Lancaster Centre for Forecasting, based at the Lancaster University Management School, has as its objective, developing new methods and approaches to forecasting focused on improved organisational practices. It has been particularly concerned with evaluating and improving company forecasting systems, funded by the EPSRC and a large number of companies. It has long standing relations to support Beiersdorf HQ in Germany and its UK division through a mentoring scheme. The project was conducted by a team of researchers, Lancaster PhD students and Masters students in operational research, who carried out a 14 week internship onsite.

The problem

The objective was to select the best forecasting algorithm for each product /country to forecast future demand as accurately and robust as possible. The project involved a large scale empirical evaluation of statistical forecasting algorithms and statistical model selection routines available in the in-house software SAP APO-DP, and recent state-of-the-art developments in maths & stats research. The team ran a large scale empirical evaluation on thousands of real-life time series of sales across product categories (lipcare, sun, deo, shower, etc.) and country clusters (Europe, LATAM, etc.) to identify optimal model parameters for unique, product- and country-specific consumption patterns. The analysis explored different algorithms of exponential smoothing, regression and artificial neural networks, and various routines for optimisation, e.g. with constrained parameter search spaces, all within a comprehensive rolling-origin design to mimic the performance of real planners over the last year. To limit complexity for the demand planners, similar products were assigned to 13 forecasting profiles, leading to a reduced model set within brand groups, within countries and globally, using sophisticated techniques of parameter clustering and time series clustering. The project estimated an optimal, reduced set of statistical forecasting profiles that (a) increases forecasting accuracy & reduces inventory costs, and (b) limits complexity to demand planners to enhance their understanding and acceptance.

Results and achievements

Results were presented to the HQ in Germany and are currently being implemented for world wide roll out. Key impacts include:

- Estimated improvements in forecasting accuracy of 2.4% - 5.1% (compared to using a single model)
- Estimated decrease in safety stocks of 5.8% - 12.5%, a significant reduction of excess stocks (at a constant service level)
- Time savings from enhanced automation of forecasting processes for 100s of demand planners globally

LANCASTER UNIVERSITY

BDF Beiersdorf

www.lums.lancs.ac.uk www.beiersdorf.com

www.lums.lancs.ac.uk/forecasting

Major Heathrow project takes off

Executive summary

A computerised scheduling system developed by UK researchers will help air traffic controllers improve efficiency at the world's busiest airport, which handles 67.5m passengers a year, by reducing delays and emissions.

Challenge overview

Aircraft scheduling is a high pressure world where lost seconds cost money, damage customer relations and have an environmental impact. Many factors affect aircraft take off – size, speed, direction, allocated time-slots – but safety is always paramount.

Reordering aircraft before they reach a runway is preferred, but Heathrow's layout means that it is more practical to do it once aircraft reach the runway queues, eliminating taxi-time unpredictability. The physical structure of the holding areas constrain what reordering is possible, sometimes making it difficult to achieve the most efficient take-off sequence.

Implementation of the initiative

The Industrial Mathematics KTN has been working with NERL, the R&D division of NATS which manages UK airspace, since 2001 when it brought a problem to the UK Study Group with Industry. This was followed by an EPSRC-funded CASE PhD through the KTN with NERL and the University of Nottingham's Automated Scheduling, Optimisation and Planning group (ASAP) that developed takeoff sequencing and scheduling algorithms for airport runways (2003-2006), and a follow-on research project on stand hold times (2008-2013).

These initial projects have contributed to a new, but separate, "intelligent decision support methodology – being implemented at Heathrow in late 2010 – that takes into account extra information (Fig. 1), enabling air traffic controllers to reduce delay and fuel burn.

The KTN projects have also helped build the UK's reputation and expertise in air traffic management. ASAP now has several related projects and other collaborations underway (all dated 2009-2013).

These include another KTN CASE PhD investigating sequencing of arrival aircraft, and several additional projects including a PhD project with NATS and a new research project with Zurich and Manchester Airports investigating ways to minimise environmental effects.

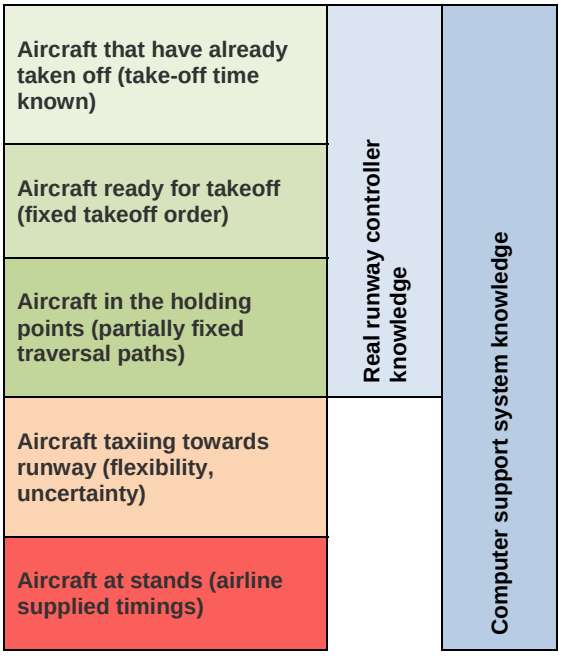

Fig 1. Knowledge base of controllers and computer support system.

Results and achievements

Key impacts include:

- Estimated idle time delay saving of 15-40%
- Estimated reduction in missed take-off time slots of 50%
- Significant reduction in fuel consumption and emissions
- Ongoing involvement with industrial mathematics – both with the KTN and external organisations
- Building of UK expertise and investment in air traffic management.

The University of Nottingham

EPSRC Engineering and Physical Sciences Research Council

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Oscillation-free Positioning of a Container Crane in a High Rack Warehouse

Executive summary

For the loading and unloading of high rack warehouses, floor driven shelf access equipments are the conventional solution. A new concept of ceiling driven storage systems consists of a trolley moving along rails at the top of the shelf. Via cable ropes it can lift and lower load-carrying equipment, which accesses the payload with a fork-like construction. For each positioning task, a reference trajectory has to be provided to ensure that the swinging of the crane system is under control during the movement and disappears at the final point. These trajectories can be obtained solving optimal control problems. In the industrial application, a model-based closed-loop control is used to follow the reference trajectories.

Challenge overview

Early tests of the company have shown that for a positioning task the usage of a feedback control law without reference trajectories only resulted in unsatisfying movements. Hence the company was searching for scientists, who could provide them with these reference data. We were able to produce a first set of data within 15 minutes using our software library NUDOCCCS to solve the optimal control problem. During the close collaboration within the next years, a stable tool was built for the generation and verification of reference data handling a large number of security requirements and additional requests. We convinced the company to skip their commercial feedback control and to give the mathematical closed-loop control a chance. Within two days it worked successfully on the industrial plant.

Implementation of the initiative

As our main goal was to see that our mathematics is actually working in industry, we agreed to a cost model where we participate in the sale of the final product. In addition, as several side projects emerged from this co-operation, a win-win situation for both partners was gained.

The problem

The container crane was modeled as a mathematical pendulum with a moving suspension and a varying rope length. Various tests have shown that this suffices in our case. This model is used to formulate an optimal control problem: The initial and final positions of the container crane are given by the positioning task. However, all velocities and accelerations have to vanish at these positions. During the movement constraints on the positions, velocities and accelerations as well as on the angle of the pendulum have to be fulfilled. The jerks of the horizontal movement of the trolley and the vertical movement of the load-carrying equipment are used as control variables and have to be chosen in order to minimize a combination of process time, energy consumption and average oscillation. For the Riccati model-based feedback controller the parameters of the weighting matrices had to be adjusted to follow the reference to the nearest millimeter.

Results and achievements

The criteria of the company grew as they understood the powerful capabilities of the solver for optimal control problems. The tool could be adapted easily to new requirements. The success of this mathematical adventure was crowned by the Bernd-Artin-Wessels-Award in 2009, which is conferred in recognition of outstandingly successful projects focusing on excellent co-operations between science and small and medium-sized companies. The success is measured against two further key criteria: the level of innovativeness and the benefit for the company.

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Modeling Vibrations and Noise in Complex Built-up Structures – a Wave Chaos Approach

Executive summary

We use tools from wave or quantum chaos, random matrix theory and the theory of dynamical systems to provide improved methods for modeling noise distribution patterns for large scale engineering structures.

Challenge overview

Finding the distribution of vibro-acoustic energy in complex built-up structures in the mid-to-high frequency regime is an extremely challenging task. Standard numerical methods such as boundary element methods (BEM) or finite element methods (FEM) scale with the wavelength which is often orders of magnitude smaller than typical dimension of components of the structure – examples are the vibrations of panels on trains, airplanes or ships. Modeling the vibrations and noise patterns of the structures based on finding numerically exact solutions of the underlying wave equations quickly becomes intractable even for modern computer architectures.

A range of high frequency techniques have been developed in the engineering community, such as *Statistical Energy Analysis* (SEA). However, this method is an expert tool and its range of applicability is still discussed controversially amongst engineers; in particular, the method is known to fail for non-diffusive wave energy transport.

Another challenge is the class of so-called mid-frequency problems; that is, structures with large variation of local wavelengths and/or characteristic scales. Dominant resonance behavior due to stiff or small scale parts of the structure cannot be resolved by SEA, however the models are still too large for a full FEM approach. Hybrid SEA-FEM methods have been developed to tackle these problems with the same shortcomings for the SEA component mentioned above. Still, software packages based on SEA and SEA-FEM methods have recently been introduced to the market by the company ESI (http://www.esi-group.com/ - VA-one) generating multi-million dollar revenues.

Implementation of the initiative

The initiative was seed-funded by an EPSRC spring board fellowship in 2006/7. The University of Nottingham together with the Institute of Sound and Vibration Research (ISVR) in Southampton and industrial partners such as the inuTech GmbH, Nuremberg, the Virtual Vehicle Centre, Graz and the Robert Bosch Gmbh, Stuttgart, have since successfully applied for an EPSRC grant (responsive mode) as well as an FP7 EU-grant (Industrial and Academic Partnerships and Pathways – IAPP) providing funding over 4 years for three research assistance positions (3+2+2 years) and covering salaries of senior members of staff for in total 4 years. The IAPP funding has a large secondment component exposing academics from Nottingham to working in a corporate environment and vice versa.

The problem

The goal of the initiative was threefold, namely
i) to analyse SEA in a wave asymptotics and wave chaos context and to give more transparent bounds for its applicability.
ii) to improve SEA including the description of non-diffusive wave transport and
iii) to develop hybrid methods based on these improved SEA methods.
This should make it possible to develop improved numerical algorithms and black box tools to aid the modeling work of structural engineers.

Results and achievements

As part of this ongoing project we have identified SEA as a course grained Markov process of the underlying (deterministic) ray dynamics. We have then proposed a new method – called *Dynamical Energy Analysis* (DEA) – which describes the flow of ray trajectories in terms of linear phase space operators (studied intensively in ergodic theory - Perron-Frobenius operators) in a complete basis set. The method interpolates between SEA and ray-tracing. We have developed a new SEA-FEM hybrid method based on a random wave field assumption for the SEA components and have extended the method to a DEA-FEM treatment.

The tools developed are met with great interest by the engineering community – discussions with customers of inuTech GmbH (Krones AG, Reckitt-Benckiser) for commercial applications are on-going.

The University of Nottingham | University of Southampton Institute of Sound and Vibration Research | inuTech

http://www.nottingham.ac.uk/mathematics

http://www.isvr.soton.ac.uk/

http://www.inutech.de/midea

MARIE CURIE ACTIONS

EPSRC Engineering and Physical Sciences Research Council

Guide to Load Analysis

Executive summary

The six European truck manufacturers DAF, Daimler, Iveco, MAN, Scania, and Volvo, in 2006 commissioned a research project to produce a guide to load analysis oriented towards fatigue design of trucks. The project was run by the Fraunhofer-Chalmers Research Centre for Industrial Mathematics FCC in collaboration with SP Technical Research Institute of Sweden, Chalmers Mathematical Sciences, Fraunhofer ITWM, and the industrial partners. The complete guide was available in 2009, as planned, after a joint effort of ten person-years.

Figure 1: Transport vehicles are exposed to dramatically different conditions in different parts of the world and different transport missions. The timber truck needs to sustain very high pay loads, as well as high dynamic loads.

Challenge overview

Transport vehicles meet very different conditions in their operations. The industrial parties had worked together on particular problems in this area. Some had run bilateral projects with the research institutes involved. They now decided to take a more fundamental approach combining front-line research in dynamics and statistics for durability. In 2006 an initial investigation was carried out of current practice and future needs within load analysis, together with a survey of the state-of-the-art in load analysis for automotive applications, Figure 2. After this pre-study the parties agreed on the main project.

Implementation of the initiative

During 2007-2009, the Guide was developed in close collaboration between all parties, including regular meetings and annual seminars at each company. The contract period on finances, results and confidentiality was done in parallel during the first half year. All parties made a point of carefully keeping deadlines.

The problem: load and strength balance

The ultimate goal for the manufacturer is to make a design that exactly meets the needs of the customers, neither too strong nor too weak. The requirements need to be converted into, e.g., a certain small risk of failure, a proper safety factor, or an economical expected life. In order to make a robust design it is as important to have good knowledge of the properties of the customer loads, as to have good knowledge of the mechanical behaviour of the material and structure in question.

Figure 2: The design specifications within the automotive industry are to a large extent based on testing and measuring loads on test tracks (courtesy of Volvo).

The Guide presents key analysis tools to meet the goal: *methods for load analysis* and *load analysis in view of the vehicle design process*. We give strategies for the evaluation of customer loads in statistical terms defining the load of interest and which population it represents, e.g. all potential customers, a specific application (e.g. timber trucks), or a specific market (e.g. the European market). We present derivation of design load time signals using simple synthetic loads, random load models, and modification of measured signals, standardized load sequences, test track measurements, or an optimized mixture of test track events. We present methods for verification of systems and components including generation and acceleration of loads, and planning and evaluation of verification tests.

Results and achievements

The quality manager of one of the industrial partners, Mr Eric Balligand, Vice president Quality at Volvo 3P, kindly stated that the 424 pages long Guide “should be the "bible" for all our new design and test engineers for the 15 coming years”.

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Calibration procedure for a height measurement system for excavators

Executive summary

For a new portable depth and grade control system for excavators a calibration procedure was developed which allows for an easy and quick setup of the system while achieving a high accuracy for its operation at the same time.

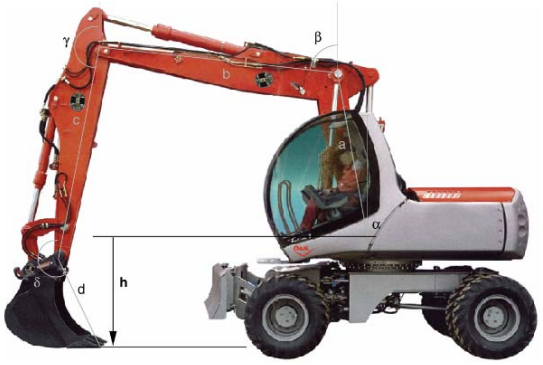
Challenge overview

AGATEC, a company located in Le Mesnil le Roi, France, develops and distributes laser tools and laser based control systems for construction machines. One of their latest developments is a portable measurement system for excavators, which provides the operator with real time information on the current height of the tip of the bucket for accurate digging or grading. This system consists of portable sensors to be attached to the different segments of the excavator arm providing orientation information. To determine the bucket height, the exact lengths of the arm segments as well as information on the mounting positions of the sensors are needed in addition to the actual sensor data.

Conventional solutions for the calibration problem rely on specialised equipment and a time-consuming and error-prone direct measurement of the required lengths and positions. To allow for a true portability of the system, AGATEC aimed for a simplified procedure and contacted the Institute for Industrial Mathematics (IFIM) at the University of Paderborn, Germany, to develop a simple calibration procedure which can be carried out by the operator of the excavator within a short period of time and with little or no additional equipment.

Implementation of the initiative

The IFIM entered into a research and development contract with AGATEC to design the calibration procedure, to analyse the resulting accuracy of the system and to develop the algorithm for the computation of the necessary calibration data. The implementation of the algorithm had to take into account restrictions due to the specific software and hardware environment of the system. The algorithm design was therefore carried out in close collaboration with AGATEC and its third party contractors responsible for the actual implementation. Following the successful execution of this first project a second contract between the partners was concluded in order to extend the calibration procedure to cover further use cases.



The Problem

From a mathematical point of view the calibration problem is a parameter estimation problem. The unknown segment lengths and mounting positions need to be determined from different measurements using the orientation information of the sensors. The main challenge within this project was to find an appropriate mathematical model as well as a corresponding measurement procedure which on the one hand leads to a well-posed system and on the other hand can be easily carried out by the operator of the excavator at any construction site.

Results and achievements

It was possible to develop a suitable calibration procedure and an associated solver for the parameter estimation problem satisfying all requirements of AGATEC. It is fully integrated into their new product EZDigPro (www.ezdigpro.com) and a patent is filed for this system including its simple calibration procedure.

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Crew rostering at *EuskoTren*

Executive summary

This project entailed designing and resolving a procedure for fair annual rostering of shift work for train crews at *EuskoTren*, based on chain resolution of various binary programming problems.

Challenge overview

Following a basic study commissioned by Metro Bilbao into optimal shift rostering using mathematical tools, *EuskoTren* approached us to request a full project along similar lines.
EuskoTren has been drawing up shift rosters "by hand" for many years. The core idea of this project was to design a procedure which was not too different from the conventional one (so that there would be no problems in workers accepting it), but made use of all the degrees of freedom of rostering and all the capabilities for undertaking extra shifts on the part of the workforce, to produce an annual roster that fairly shared out the full workload.

Implementation of the initiative

The full scheme was developed in the form of three consecutive one-year projects. The final result was reached by means of successive approximations starting from a basic rostering assignation for winter and summer, and resulting in a roster that includes all the increases in services scheduled to cater for festivities and special events in all the geographical areas where *EuskoTren* operates. The work was carried out by three tenured lecturers at the University of the Basque Country, and was funded entirely by the company.

The problem

The main challenge lay in breaking down the rostering process into linear sub-problems capable of reflecting all the complexity arising from the demands and preferences of employees without those problems thus becoming too big to solve.

Results and achievements

It is very important for the company to have an annual work roster that covers all the services envisaged for the coming year and is acceptable to employees. The workload required and the preferences of employees may change from year to year, so *EuskoTren* intends to continue working with us so as to adapt to new situations.

Universidad del País Vasco Euskal Herriko Unibertsitatea

For the university, these projects have provided a source of funding and have given rise to scientific publications. There is no problem in publishing the results because, as was made clear from the outset, the Metro in Barcelona (for instance) does not compete for passengers with Metro Bilbao.

Lessons learned and replicability

This scheme could be exported to many other similar companies. In fact, Metro Bilbao is considering taking a similar path, and we have also carried out a preliminary project for narrow gauge rail operator Ferrocarriles Españoles de Vía Estrecha. However, given the specific organisational features of the work of each company, individual studies and tailor-made solutions are required in each case. In general, to maintain ongoing technology transfers, we at the Mathematics Department usually have to take the initiative and seek out companies: we cannot just wait for them to come to us with significant mathematical problems. The driving force must always be to adapt ourselves so as to meet the needs of businesses rather than sitting back and waiting for them to suggest problems that we may wish to investigate.

EuskoTren

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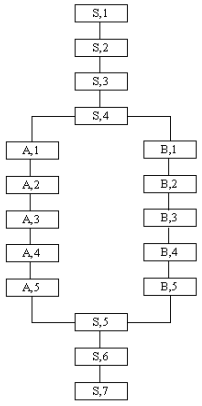
Preventive Maintenance optimization of trains air conditioning systems

Executive summary

The purpose of this project was to propose some preventive maintenance policy for air conditioning (AC) systems used in French regional trains, in order to reduce their mean number of failures without increasing their mean functioning cost.

Challenge overview

Failures of AC systems imply client dissatisfaction, which is damaging to the image of the French national railway society (SNCF). They also imply high repair costs and hence should be prevented. Within the context of a traditional cooperation between the SNCF and academic researchers, a PhD thesis has been initiated on the subject, which is accompanied by a financial contract between the partners. A first challenge for the study of the AC system was to correctly understand its operating mode, which includes a special redundant structure. Discussions with experts from the SNCF were necessary on this point.



Structure of the air conditioning system

Implementation of the initiative

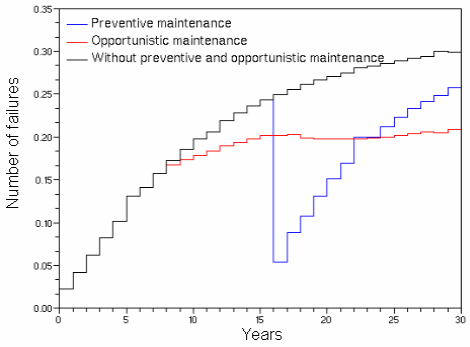
The subject has been treated by the student at the beginning of its PhD studies, using modern techniques previously developed in an academic context. A first problem for him has been to overcome difficulties in the practical implementation of the theoretical methods, which has resulted in his development of new approximations. A next problem has been to convince the head of the SNCF research department that such approximations were adequate and that they were providing accurate results. The support of the contact person at the SNCF on this point has been crucial.

The problem

The AC system is a small but complex system, with 17 aging components and a special redundant structure. The numerical assessment of such systems is usually performed through Monte-Carlo (MC) simulations. However, the preventive maintenance policies envisioned for the AC system have about a dozen parameters which all had to be optimized. In this context, MC simulations are not very well adapted, first because of long computation times, secondly because of the randomness of the results they provide. An alternate method has therefore been used, which relies on the modeling of the AC system by an emerging class of stochastic processes: the piecewise deterministic Markov processes, and on their numerical assessment by finite volume methods.

Results and achievements

Two types of preventive maintenance policies have been envisioned and optimized: a classical one with a global revision of the system and an opportunistic one, which takes advantage of a system failure. In each case, components which are too old are replaced. Both strategies lead to about 20% fewer failures with a clear decrease of the cost (about 10%). Based on that, the SNCF has decided to make effective use of this research and the recommended preventive maintenance policy with the general revision is now in use.



Mean number of failures for the AC system under different maintenance strategies

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Optimization in Sea Logistics

Executive summary

The initiative refers to the integration of optimization methods in an Italian logistics company. The working framework was that of modelling a sea transportation problem in which the main goal was to define the number, the type of containers and the freight to be loaded in each container.

Challenge overview

The initiative was taken by the company (Felian S.p.A.), which contacted the Institute with the aim of improving the direct costs deriving from relevant issues associated with their business. Their main problem was how to migrate from a non-automated management of the freight shipment definition to an automated and optimized one. First, the company tried to understand what kind of benefits would have been obtained if an optimization strategy was implemented within their working framework. Next, they tried to understand whether the optimization tool was compatible with the interfaces existing among the firm managers responsible for the process. Finally, they tried to see whether the methodology to be applied to their decision problem was compliant with the size of the application data.

Implementation of the initiative

The contract lasted two years. The personnel involved into the project were mainly permanent staff. The industrial partner played a very collaborative role in giving data, testing the models and trying to come up with an end-product embedding all the requirements defined in the briefing phase of the project. The initiative did not produce relevant shortcomings.

The problem

Operations research techniques were used to manage the problem. Two mathematical programs were defined and implemented: one to optimize the cost of the containers to be shipped daily, the second one to optimize the used volume of the cheapest container. The first mathematical program is NP-hard from the complexity point of view, and therefore the major challenge was in its experimentation; indeed, for some datasets we defined a time limit for the execution and tried to post-optimize by means of a heuristic algorithm, in particular in those scenarios in which the solutions were not feasible. The second model was linear and therefore no particular difficulties emerged during its definition and resolution.

Results and achievements

The results obtained were sufficient to release to the company a program implemented in the C and AMPL languages with a graphical user interface implemented in the Visual Basic language in order to be used at all levels in the firm. The program has been tested on real data by the company and the results showed improved solutions compared to the past records in very fast computing times. From the beginning the initiative was designed to provide a definite solution.

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Control of navigable rivers

Executive summary

The problem of regulating levels and flow rates in open channels is of primary importance for the management of navigable rivers (as well as for irrigation canals). The regulation is achieved through the design of feedback controllers that use level measurements at the control gates. The position of the gates is computed using a Lyapunov approach on the basis of a mathematical model described by Saint-Venant equations. The method is applied to Sambre and Meuse rivers in Wallonia (Belgium).

Challenge overview

Navigable rivers are made up of hydraulic pools separated by gates (see Fig. 2) for real time control. In order to improve the management, it is important to accurately regulate the water levels allowing the operators to maximize the transported loads, and to guarantee the water supply of electrical power plants and industries located on the river banks. Moreover, the control must attenuate perturbations due to meteorological hazards or to external water uptakes.

Implementation of the initiative

Generally, set point water levels are delivered by the public administration (SPW-Service Public de Wallonie). The aim of the local regulators is then to maintain in each pool, the desired water level. This has been implemented on parts of Sambre and Meuse rivers.

The problem

It is difficult to obtain accurate models of such systems, taking into account the geometry of the channels, the slope, the friction etc. It is therefore important to elaborate robust controllers dealing with such uncertainties. The only available information on the system is the height of the water at each gate. The water dynamics in each pool are described by one-dimensional shallow water equations (Saint-Venant; see Fig. 1) and the controller is designed using an energy-based approach (Lyapunov method).

Results and achievements

The new controls have given rise to significant performance improvements: the amplitude of water levels variations has been half reduced and the damping of the flow rate disturbances is twice as fast as previously.

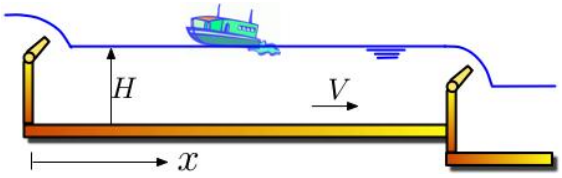

Fig.1. **The Saint-Venant equations** are (hyperbolic) partial differential equations which describe the time variations of the water depth H and the water (horizontal) velocity V in a pool, as a function of the derivatives of H and V with respect to the abscissa x along the pool. All the points on the same vertical are supposed to move with the same horizontal speed V.

Fig.2. Gates on the Meuse river.

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Liner Network Modeling

Executive summary

For large container shipping liners, properly designing the network is a highly complex task, but also a process with a critical impact both on the bottom line and the fossil fuel consumption. In the liner business, a decision support tool allowing a proper design of the network is considered a strategical differentiator.

Challenge overview

Ange Optimization is a mathematical optimization company with half a decade of experience in the container liner business. Knowing several liner companies from within, we anticipated a need for a decision support tool to assist in the network design process, were able to get traction for the concept among specialists in the respective organizations and finally managed to get top management committed to the idea.

Implementation of the initiative

The development and implementation of the system was done in an agile way, i.e. by gradually implementing prototypes of increasing complexity, continuously keeping the users, the domain experts, in the loop an integrating their feedback. The first prototype was delivered after 2 months, and today, 3 years later, development is still ongoing. On the technical side, the main challenge was to get execution time below an acceptable level (15 minutes), which was done by gradually improvin g the algorithms and profiling the code. On the change management side, the main problem was that the early adopters, critical for the succeeding with the user acceptance, were 1) rare and 2) got continuously relocated.

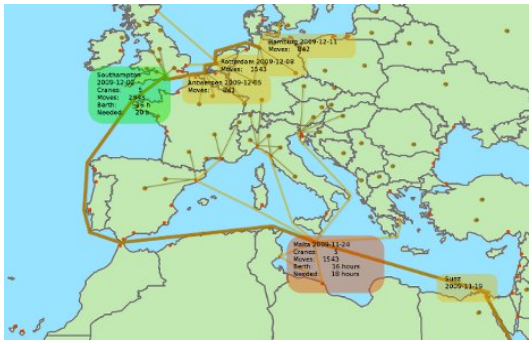
The problem

Tens to hundreds of thousands of containers transit on the network every week, on cyclic, periodic “strings” of vessels. The network is represented as a graph, on which a constrained multi-commodity flow problem is solved using LP with column generation. The particularity of the problem is that empty containers have to be returned to their origin at the lowest cost, that parts of the network is considered scheduled while other parts do not have a fixed schedule and finally that fuel consumption curves (as a function of speed and draft) need to be modeled.

Results and achievements

The system is currently being used for several tasks, ranging from the originally intended string design, over vessel procurement, demand forecasting and operational container flow management.

Some of these can be quantitatively assessed, example KPIs being «how many containers, relatively, are being routed via the optimal route?» or «what is the profitablity of a given network given a demand configuration? «
But the perhaps most important success indicator is that the specialists, who have decades of experience with the problem and who need to take into account a large number of factors that cannot reasonably be modeled, actually see the system as an asset to their work and use it on a daily basis.



Lessons learned and replicability

Mathematical modeling can be an essential component in a decision support tool. However, one unavoidable constraint on the output of the tool, is that a human being will eventually have to take responsibility for the decision. In consequence, the human has to trust the output, generally requiring that he has to understand the solution to some extent. This in practice tends to cap the complexity of model.
Also, the adoption of the technology in the organization will often be a question of social engineering, user training and stakeholder management, rather than the pure technical merits of the system.
Finally, most of the value often comes from the functional description of the problem rather than the optimization *per se* of the function. Again, this would seem to be a question of assessability (simplicity) of the output.

Ange Optimization
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Building the digital society

Executive summary

The past few decades have seen the rapid growth of digital technology in every area of life, enhancing our society in ways that were previously impossible. Now that we've all come to rely on ultra-fast communication, instant access to the world's information, online shopping and more, our digital infrastructure that aids business, government, and the public is as essential as our waterworks or roads.

Challenge overview

Digital data sets the new society apart from the old, and it comes in many forms. Social networks, supermarket loyalty cards and energy smart meters are just some of the mechanisms for capturing vast amounts of data, but turning this data into information involves more than just recording it. Peter Grindrod, as part of the Horizon Research Institute, is currently developing a new mathematical discipline to handle and interpret this wealth of data, and while it is currently in an early phase, the study of mathematics for the digital society is expected to be commonplace within the next ten years.

Modelling interactions between people and information are complicated, and we need to develop new concepts and models to understand and predict behaviour in the new digital society.

Networks are a key component of this new society, as illustrated by the rise of mobile phones, email, and social networking websites, and Grindrod's research aims to develop an understanding of evolving, rather than static, networks.

Studying evolving networks enables the evaluation of how different people use communication tools. Some individuals might be good at broadcasting information, reaching out to lots of circles, while others might be good listeners, receiving messages from a variety of sources. Network operators could also monitor for any patterns that don't match the model's predictions, which could indicate a traffic spike or unusual behaviour. These theories could be applied to network management, surveillance, consumer behaviour or even viral marketing.

Businesses already use this data to segment their customers into different groups, but as with networks, these models are static. A bank might place customers in a particular group based on their age or location and target them with certain products. A more intelligent model could learn over time, shifting customers into different groups as the bank builds up their data profile and ultimately leading to more successful businesses.

This kind of customer analysis has grown over the last twenty years in the retail and banking industries, but it's now being adopted in other sectors as usable data becomes available. The roll-out of smart meters across the UK will for the first time give energy providers real-time details of individual household consumption, allowing them to manage and predict demand based on customer behaviour. This will require a new mathematical understanding of how electricity is used, especially in a world of electric vehicles, micro-generation and renewable energy, all of which introduce new complexities into the power networks.

To capture evolving behaviour, Grindrod's research models networks a sequence of graphs that changes in a probabilistic way. In this model the connecting edges between vertices are either “alive” or “dead”, indicating whether communication between the two vertices is taking place, and at each point in time a new edge can be “born” or an old one can “die”. Edges can also be “immortal” or “extinct”, reflecting constant and no communication, respectively.

This model displays four long-term behaviours, depending on the rate of edge births and deaths. The resulting network graph can be one in which each vertex is linked to all the others, or one in which there are no links at all. Alternatively, each edge in the graph can become either immortal or extinct, leading to a static graph, or the edges can continue to change, leading to a graph of random connections.

Results

Applying the model to real-world data from a Chinese social network shows that the longer two vertices remain disconnected, the less likely it is that they will connect in the next week. In other words, if two individuals don't make a connection when they first join the network, it becomes increasingly unlikely that they ever will as time goes by.

The University of Nottingham

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Other domains

Optimal Financial Portfolios

Executive summary

The challenge is to select the portfolio of financial securities which is optimal under given criteria.

Challenge overview

The Financial Mathematics Group at the University of Warsaw was contacted by executives of The Central Bank of Poland to solve the optimal tactical asset allocation problem for the currency reserve of the Bank. The problem definition was complex and combined primary and secondary objectives for the Bank. The first stage of the project analysed the problem and identified the primary goals.

Implementation of the initiative

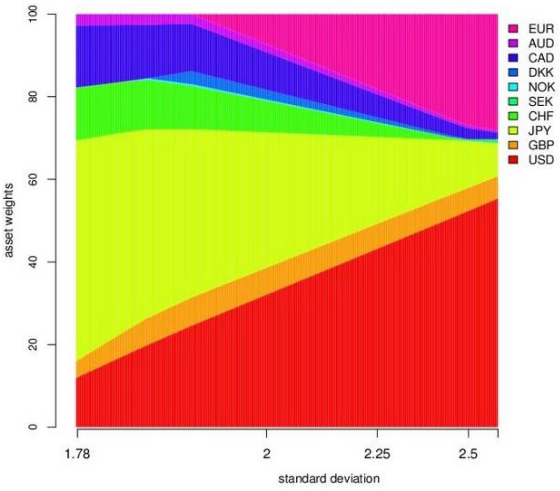
The duration of the contract was 15 months (then extended to 18 months). During the first stage (analysis of the problem) it was a constant cooperation between both sides (4 people from each side). Once the mathematical model was designed, it was worked on by 6-8 people from the permanent staff of the Group with a support of 5-7 graduate and Ph.D. students. After preliminary results were obtained, the staff of the Bank was able to see the potential of the final product and gave strong support to design it in the form most desirable for its future use.

The problem

The construction of a good combination of financial instruments involves a multi-goal optimization problem which is usually formulated as a risk-return trade-off. To solve this problem, it is necessary to know the distribution of random returns of risky assets. The solution procedure is then executed under the implicit assumption that we know both the mean and the covariance matrix. In fact the estimation of the mean and covariance is an important part of the solution of the optimization problem. The difficulty in estimating mean returns has been overcome by the use of Bayes estimators incorporating the Bank experts' forecasts. Since our experiments have shown that standard estimators of the covariance matrix lead to unstable portfolios, we have improved the portfolio stability by applying sophisticated robust estimators and implementing methods that account for a memory effect in the data.

Results and achievements

The result of the contract was the design of an optimization method that uses a reasonable set of market data and produces 'good' optimal portfolios, i.e. portfolios that are well diversified and have asset shares that are stable with respect to estimation errors. A typical example of a multicurrency portfolio obtained by our approach is presented on the illustration below. The developed methodology was accompanied by appropriate software. The product has been in use for some time and is evaluated by the Bank managers very positively. During the contract we have discovered a number of unsolved mathematical problems. These problems are presumably well known to practitioners but not discussed in the literature. We worked out some of these problems in our academic research preparing a number of scientific publications.



Optimal 10 currency bond portfolios. Picture shows asset weights as a function of portfolio risk measured by standard deviation (in percent).

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Financial derivatives pricing

Executive summary

The need of specific software to price complex financial derivatives and structured products by Caixa Galicia requires the expertise in quantitative finance models and rigorous mathematical tools provided by academics.

Challenge overview

The accurate pricing of the financial products contained in a financial institution portfolio is crucial for its management, especially in the case of the so called complex financial instruments. It allows the optimization of not only the assets management but also of the associated risk management. Moreover, it is essential to evaluate the balance sheet real situation, thus helping to prevent losses due to incorrect pricing and accounting of transactions in financial markets. The first project proposal arises at the Treasury and Markets Area of Caixa Galicia, from the necessity to develop autonomous capabilities to price increasingly complex and non-standard financial products, the valuation of which is not supported by conventional professional software. In this setting, the development of specific pricing software requires not only the practical knowledge of the financial products but also the mathematical modeling tools and the statistical and numerical methods to solve the models and simulate the prices. Taking this into account, a joint project with researchers from the universities of A Coruña, Santiago and Vigo has been developed in order to incorporate all the theoretical knowledge, software development skills and research capacities.So far, the valuation of these complex products had to be purchased from specialized firms, thus leading to substantial cost and, in addition, preventing from the control of the calculations and valuations by the financial institution staff.

Implementation of the initiative

The project has been entirely funded by the financial institutions and a continuation project is now being developed. Although the confidence in the scientists has been absolute and the objectives were covered within the time schedule, a constant review of all developments has been carried out by Caixa Galicia, partly motivated by the large financial impact of valuations in the general ledger and partly by the interest on the knowledge transfer from academics to practicioners. The working team combines analytical capabilities of researchers with experience in the business of Caixa Galicia members.

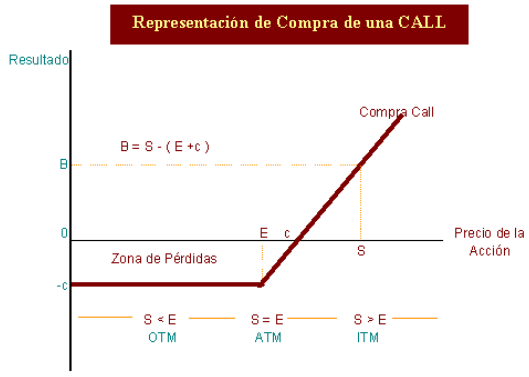
The problem

The main data of the pricing problems are contained in the forms that detail the specifications of each complex financial product. Several mathematical techniques have been combined, such as Monte Carlo simulation or geometric Brownian process, or newer techniques such as copula techniques for multidimensional distributions, Markov Switching for volatility, and Brownian bridge for barrier options. Generally, each pricing problem includes the following steps:

1. **Determine the pricing models:** Understanding each product and their associated cash flows and payoff
2. **Calculate the inputs of the pricing models:** by predicting the assets volatility and/or correlations involving complex predictive techniques
3. **Define the simulation methodology:** statistical and numerical tools such as stochastic processes, Monte Carlo simulation, antithetic variables, or Cholesky factorization.
4. **Optimize the computing time and software integration:** efficiency of the software toolbox.

Results and achievements

The project results provided Caixa Galicia of a flexible and robust software toolbox that allows: to have their own valuations for complex financial products, allowing an optimization of accounting control and risk management, and to reach the ability to quote prices for these products, thus giving a new business dimension. Both targets represent a relevant differential factor with respect to financial institutions of the same size. Also partial results have been presented in congress publications.



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Pricing model of catastrophe bonds with complete calibration procedure

Executive summary

Pricing formulae for zero-coupon and coupon CAT bonds in the compound doubly stochastic Poisson model framework have been derived. Complete fitting procedure of the compound non-homogeneous Poisson process has been described.

Challenge overview

Catastrophe (CAT) bonds are one of the more recent financial derivatives to be traded on the world markets. They are more specifically referred to as insurance-linked securities. The distinguishing feature of these bonds is that the ultimate repayment of principal depends on the outcome of an insured event.

The creation of CAT bonds, along with allied financial products such as catastrophe insurance options, was motivated in part by the need to cover the massive property insurance industry payouts of the early- to mid-1990s. They also represent a ``new asset class'' in that they provide a mechanism for hedging against natural disasters, a risk which is essentially uncorrelated with the capital market indices. Subsequent to the development of the CAT bond, the class of disaster referenced has grown considerably. As yet, there is almost no secondary market for CAT bonds which hampers using arbitrage-free pricing models for the derivative.

Implementation of the initiative

The research has been conducted at Hugo Steinhaus Center with co-operation with Professor David Taylor, University of the Witwatersrand (South Africa) and Grzegorz Kukla, Towarzystwo Ubezpieczeń EUROPA SA (Polish non-life insurance company). It has been a part of Scientific and Technological Cooperation Joint Project for Years: 2004-2005 between Poland and South Africa.

The problem

Catastrophe bonds are insurance-linked securities that enable insurers to transfer the risk of natural disasters like earthquakes or hurricanes to the capital markets. They are sold to large institutions.

For insurers the deals create a pool of money that can be tapped immediately into a disaster. CAT bonds appeal to professional money managers because catastrophe risk is a new asset class that is uncorrelated with the stocks and traditional bonds. They are growing in importance also because insurance capacities worldwide have been severely reduced by the events of 11 September 2001.

We have modelled the catastrophe process as a compound doubly stochastic Poisson process. The underlying assumption is that there is a Poisson point process (of some intensity, in general varying over time) of potentially catastrophic events. We assume the economic losses associated with each of the potentially catastrophic events to be independent and to have a certain common probability distribution. This is justifiable for the Property Claim Loss (PCS) indices used as the triggers for the CAT bonds.

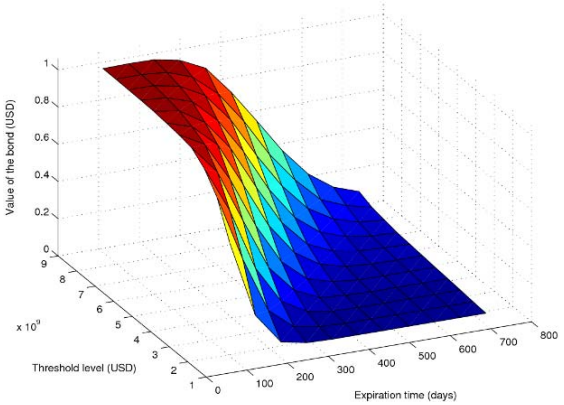

Fig. 1. The zero-coupon CAT bond price with respect to the threshold level (left axis) and time to expiry (right axis)

Results and achievements

We have investigated the pricing of CAT Bonds. The developed methodology in the compound doubly stochastic Poisson model framework can be extended to most other catastrophe related instruments.

We have presented a calibration procedure and illustrated it on the PCS loss data, We have found a distribution function which fits the observed claims in a satisfactory manner and estimated the intensity of the non-homogeneous Poisson process governing the flow of the natural events. We calculated the values of different CAT bonds associated with PCS loss data with respect to the threshold level and maturity time, and preformed sensitivity analysis. To this end we have applied Monte Carlo simulations.

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Quantifying the liquidity premium in bond spreads for insurance liability valuation

Executive summary

This project has provided important insights into the existence of liquidity premiums in corporate bond spreads and helped identify the best methods for quantifying the size of the liquidity premium. The reports produced have been widely referenced by the industry and have had an impact on practice: the CFO Forum updated its Market Consistent Embedded Value (MCEV) principles to allow the inclusion of a liquidity premium in liability valuation; CEIOPS now includes an allowance for liquidity premium in their QIS5 study – an important step towards Solvency II regulation.

Challenge overview

It is generally accepted in financial theory that illiquid assets will have lower prices than equivalent liquid ones. These liquidity effects may be observed in many asset markets, including equities and corporate bonds, and the additional compensation that an investor receives for holding a less liquid asset is known as a liquidity premium. The issue of liquidity premiums in bond markets has recently become very important in the European insurance industry because of the emphasis that is now being placed on market-consistent valuation in financial reporting (the MCEV - Market Consistent Embedded Value - standard) and regulatory capital assessment (the Solvency II regime). The effect of this in periods of illiquidity is that liabilities appear much more costly than assets that would typically be used to fund the liability cashflows, and this has an obvious effect on capital requirements.

There has been a clamour from insurance companies for liquidity premiums to be taken into account when valuing liabilities. The industry would like to be able to lower the market consistent value of liabilities by increasing the risk-free interest rates that are used in the discounting of liabilities. In order to do this, a reliable method of quantifying the size of the liquidity premium in bond spreads is required so that the adjustments can be made in a way that is acceptable to regulatory bodies.

Barrie & Hibbert conducted research looking into the evidence for liquidity premiums and the various methods by which these premiums could be measured.

Implementation of the initiative

A team was put together involving researchers from Barrie & Hibbert, Heriot-Watt University's Department of Actuarial Mathematics and Statistics, and Edinburgh University Business School. The work stream was divided into two components: (1) a literature review; (2) a comparative study of liquidity premium estimation methodology. The academic researchers were closely involved in these components and carried out part of the work with the assistance of MSc students on the Maxwell Institute's MSc in Financial Mathematics.

Challenge overview

The comparative study looked at three main methods of quantifying a liquidity premium: the method based on the so-called CDS basis; the structural method based on a firm-value model such as Merton's model; and a direct approach based on the observation of covered bond spreads.

The CDS basis method involves the comparison of CDS premiums with corporate bond spreads. The existence of a negative basis, particularly in crisis periods, is taken as evidence of other components priced in the corporate bond spread including a liquidity premium. Empirical work using Bloomberg data was carried out to quantify this premium and corrections for counterparty risk premiums were considered. The firm-value approach derives a theoretical value for the credit spread of a bond by calibrating a model of the default of a firm using equity market information. The difference between the theoretical spreads and true spread is taken as a liquidity premium. The approach considered extended Merton's original model by allowing for bankruptcy costs. The covered bond method simply compares spreads for appropriate pairs of instruments referencing the same underlying firm but where one bond (the covered bond) has a priority claim on collateral assets. For this method the effort goes into identifying appropriate pairs of instruments and collecting the data.

Challenge overview

The comparative study has helped to show the methods that are most reliable for extracting a robust and meaningful measure of the liquidity premium and these insights have entered practice. The covered bond method is the simplest and most direct method, although data is often limited. The CDS basis method is also appealing and robust, whereas the firm-value approach can give somewhat more volatile results. There is strong evidence of a premium and combined liquidity score using more than one method gives good results.

The CFO Forum has updated its Market Consistent Embedded Value (MCEV) principles to allow the inclusion of a liquidity premium in liability valuation and CEIOPS have included an allowance for liquidity premium in their QIS5 study – an important step towards Solvency II regulation.

barrie+hibbert

Modelling and Forecasting Stock Price Behaviour in High Frequency Trading

Executive summary

In cooperation with Dresdner Kleinwort Ltd London, a model for short time prediction of the price process at equity markets is developed and tested. The price process is described by a stochastic partial differential equation. The drift and volatility parameters are estimated in a way that is consistent with the nature of hig frequency trading.

Challenge overview

Dresdner Kleinwort Algorithmic Trading Department contacted the Department of Mathematics at Faculty of Science University of Novi Sad proposing a research project on modelling stock price behaviour with the emphasizes on short-time period and application in algorithmic trading. The industrial partner posed very general guidelines and was clearly interested in a fresh approach to the problem of price modelling with specific properties arising from short time horizon.

Algorithmic trading is a profitable arm of many investment banks and hence a new model might provide a significant edge. Applicability of the results in algorithmic trading was the main goal hence the real time solvability of the model was important. The problem was computationally demanding and the testing phase took a lot of time and effort.

Implementation of the initiative

The research was carried out as a research project payed by the industrial partner during one year by permanent staff of the Department (Center for Mathematical Research of Nonlinear Phenomena - CMINF). Several master and PhD students were involved in coding and testing of the proposed model. The industrial gave support through regular weekly contacts and provided the trading data for modelling and testing. Difficulties arising from time constraints and industrial requirement for parameters that are good enough but perhaps not optimal were overcame after some weeks of work.

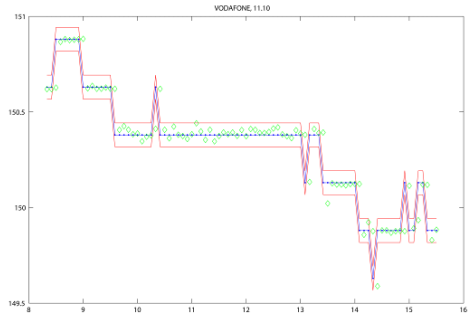
The problem

Main properties of high frequency financial data (HFFD) are irregular temporal spacing, discreteness, diurnal patterns and temporal dependence. Multiple transactions occur within a second with different transaction prices and trading volumes. These properties make HFFD difficult to analyse and built reliable forecasting models. They are also an extremely rich source of information for understanding market dynamics. The main idea was to capture the dynamics of intraday market and form a good model for short time prediction. The model we considered was based on a stochastic partial differential equation with two parameters - drift and volatility. The main challenge was to estimate these two parameters such that HFFD behaviour is captured and that the model is solvable in real time.

Results and achievements

Starting from the assumption that only a short-time history (1 minute) is important we introduced two liquidity measures (potential volume imbalance and trading volume imbalance). The drift and volatility parameters were estimated "together" i.e. no clear distinction between stochastic and deterministic parameter existed in the model since the liquidity measures captured stochastic behaviour to some extent. The model was tested on a large set of trading HFFD counting the win/loss and missed opportunity situation of the proposed prediction. The results indicated that the model is able to predict the price movement on a short time scale to an extent that can provide an informational edge in trading.

This research project has a follow up with research conducted at CMINF. Several master thesis were developed in the area of mathematical models for HFFD. Furthermore a research project regarding optimal trading trajectories in algorithmic trading is ongoing and the present industrial partner in this research is a London based hedge fund. A number of scientifically challenging problems is under consideration, in particular in the area of stochastic optimization.



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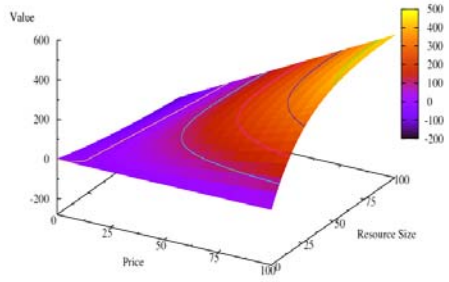
The Resource Valuation and Optimisation Model



Executive summary

This project is providing a way for the mining industry to optimize their decision making in the presence of economic and geological uncertainty. Rigorous, cross-disciplinary and industry-focused mathematical analysis has been carried out in the development of this project. Consequently, the algorithms underpinning the project are being turned into a computer software package to be licensed for commercial use.

Challenge overview

Mining companies operate in an uncertain world. Commodity prices can vary dramatically, and geological uncertainties mean that physical extraction amounts regularly differ from initial predictions. Within this unpredictable climate, the mine operators must make decisions, such as whether to expand the current mine operation, or whether to abandon the operation altogether. These decisions are costly to take, and hard to reverse. Making such decisions defensible, transparent and optimal is therefore highly desirable to the economic success of this global industry.

Implementation of the initiative

The University of Manchester was awarded a grant by the Engineering and Physical Sciences Research Council to investigate the Sustainability of Nuclear Power (the SPRING project). The grant allowed for a mathematical investigation into the usage of uranium over its lifetime. At an early stage, it became apparent that very little mathematical analysis had been conducted into the first stage of the commercial lifetime of uranium: its extraction phase. By digging deeper into this problem, it rapidly became apparent that there was an immediate industry need for the solutions the University of Manchester was creating, to help with the many challenges faced in this uncertain world. The University of Manchester then contacted several companies who operated in mining industry solutions, about the possibility of creating a joint commercial venture. From these early dialogues, a preferred partner was selected, Gemcom Software International. Next, research material was patented (where appropriate) and then openly published where all algorithms and assumptions are laid bare for robust criticism. With these algorithms, a C++ library and user interface has been created to tackle this class of problem. Finally, trials of the model by real users are about to commence, in which feedback from these users will be incorporated into the model.

The problem

To create a model determining the maximum expected valuation of an extraction project, one must first know which decisions are possible for a company to take, and the operating constraints to which they must adhere. Decisions can be one-off, such as setting the extraction and processing capacity, or can be dynamic, such as deciding whether to expand, mothball or abandon the mine at any point during the extraction process. Once these decisions are defined, one can construct the underpinning mathematical model. From this, one can derive feasible operating solutions, determine the optimal strategy, and calculate the sensitivity of the model, including calculating the likelihood of taking each decision. By utilising a diverse array of tools, one is able to select the most appropriate technique to arrive at the solution without having to resort to over-simplification.

Results and achievements

The research utilises a broad array of modern mathematical techniques to solve a technically difficult real-world problem. The team went far beyond simply publishing academic papers and filed a US patent upon their algorithms, gained an engineering award, worked in partnership with a world-leading company and showed how mathematics can produce real economic gains to both academia and the private sector.

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Realistic assessment of financial products

Executive summary

Appropriate mathematical treatment to realistic assessment of complex financial products and their risk.

Challenge overview

One of the causes of the recent financial crisis is considered to be the misspecification of credit derivatives and their risk. In general, a false assessment of financial products may be partially traced back to wrong choices of mathematical models describing such products, wrong calibration of such models, or both. The financial mathematicians at WIAS tackle these issues in close cooperation with financial institutes.

Implementation of the initiative

The finance group at WIAS consists of Matheon members and members of the permanent WIAS staff. The research advances within an active interplay with industrial partners (LBB Berlin, HSH Nordbank, WGZ bank and others).

The problem

The general problem of validating and assessing risk of financial products typically involves the development of realistic mathematical models in high-dimensional environments. Of equal importance, efficient calibration procedures for these models are called for.

Results and achievements

Advanced financial models for quantifying complex products in a realistic way are developed. By incorporating jumps and stochastic volatilities the models take into account various stylized facts observed in the market. On the other hand they are designed in such a way that they allow for feasible and robust calibration to market data. In this setting, new simulation based algorithms are developed for evaluating complex structured products. In particular, rather than providing a single price value, these methods provide lower and upper bounds for prices, confidence intervals for their risk etc.. From a mathematical point of view the achievements in this context are related to the theory of (Ito-Levy type) stochastic differential equations, theory of optimal stopping and control, mathematical statistics, and other topics.

Figure 1 General interplay in financial modeling

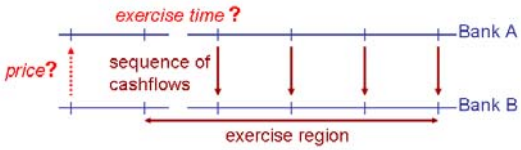

Figure 2 Payment scheme example of a callable interest rate swap

$$\widehat{V}^{up} = \frac{1}{N}\sum_{n=1}^{N} \max_{0\le j\le k} \left[{}_nZ_j - \sum_{t_i\in\pi;0\le t_i<T_j} \widehat{h}^{\pi}(t_i, {}_nL_j)\cdot\Delta_n^{\pi}W_i \right]$$

Figure 3 Efficient Monte Carlo estimator for price upper bounds

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Model based optimum design of experiments

Executive summary

New methods and software for model based optimum design of experiments and their application in industry open up the potential of gaining more information about processes and significantly improving models at drastically lower experimental cost.

Challenge overview

In chemical industry there is a high demand for the understanding and for quantitative simulations of dynamic chemical processes and for the scale-up of processes. This requires the description of processes by validated models based on physical and chemical laws of nature. The interdisciplinary cooperation in the field of Scientific Computing presented here brings together two partners with different profiles: BASF deals with real-world problems, describes them by mathematical models and has demand of state-of-the-art numerical tools. Heidelberg University is researching on application-driven development of mathematical methods and software tools.

Implementation of the initiative

The collaboration has started 1996 as a Dechema initiative funded by the German Federal Ministry of Education and Research. Currently, a Junior Research Group at Heidelberg University is funded by BASF.

The problem

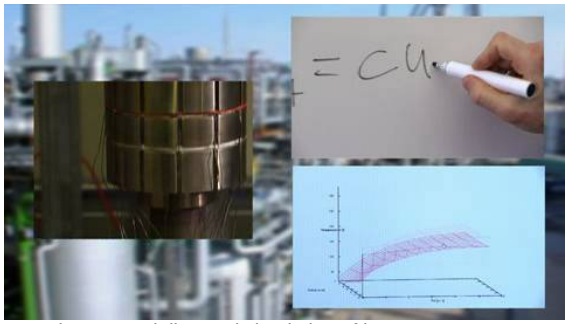
The standard approach of statistical design of experiments is insufficient for highly nonlinear dynamic processes, e.g. reaction kinetics, catalysis, thermodynamics, separation processes. Appropriate is the description of the processes by nonlinear differential equation systems. Such models have to be calibrated from experimental data. The main question in model based optimum design of experiments is: What experiments should be performed to obtain a fast and reliable calibration? This results in optimization of layout, setup, operation, selection of measurement devices, sampling subject to restrictions to cost, safety, time, model validity. Highly nonlinear non-standard mixed-integer optimal control problems with state and control constraints have to be solved.

Results

A new mathematical methodology for the treatment of problems of model based optimum design of experiments has been developed. It comprises:

1. the description of processes by nonlinear differential equation models,
2. parameter estimation including statistical analysis,
3. the formulation of intricate non-standard nonlinear optimal control problems,
4. tailored methods for the numerical solution,
5. the implementation in the software package VPLAN,
6. the demonstration of efficiency by treating benchmark problems,
7. the application to practical problems in industry.

The new methods are now routinely used by 4 staff members at BASF.



Experiment, modeling and simulation of heat transport.

Achievements

The application of model based optimum design of experiments yields information about processes much more reliable, much faster and at significantly lower cost than other (trial-and-error or black-box) approaches. Quantitative information from the simulation of processes can be improved drastically. Due to BASF, up to 80% of the experimental effort can be saved. Validated models allow scale-up of process simulations from laboratory to production plant scale and from short term experiments to long time behavior.

Lessons learned and replicability

The results of the collaboration give rise to new mathematical challenges, e.g. the optimum design of experiments with robustification, in real-time, for spatially distributed processes. Further application fields for the methodology are mechanics and bio-mechanics, systems biology and life sciences, chemical and mechanical engineering. As an ongoing cooperation, BASF is investing in further university research.

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The Chemical Company

Integral Equation Method

Executive summary

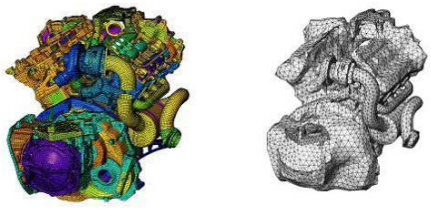
The Center of Applied Mathematics (CMAP) at École Polytechnique has a long tradition of collaboration with the industry. That led to the creation of several successful spin-offs which demonstrate the existence of a strong need in knowledge transfer from academic laboratories to industry. IMACS has been working for more than fifteen years in mathematical modeling and scientific computing and has clients in aerospace, aeronautic, automotive, energy and electronic industries.

Challenge overview

Integral equation method is a powerful mathematical theory to study equations arising from physics. A long standing challenge was its practical applicability to solve time domain problems, such as electromagnetic or acoustic wave problems. IEEE literature is full of papers desperately trying to overcome instability problems. Building on research at CMAP under the supervision of Prof. Jean-Claude Nédélec, IMACS has been the first company to develop and propose a robust solution to this challenge, providing a new tool SONATE© used in industry for time domain simulations in acoustics, and which proves to be much more efficient and precise for multi-frequency problems than existing tools.

Implementation of the initiative

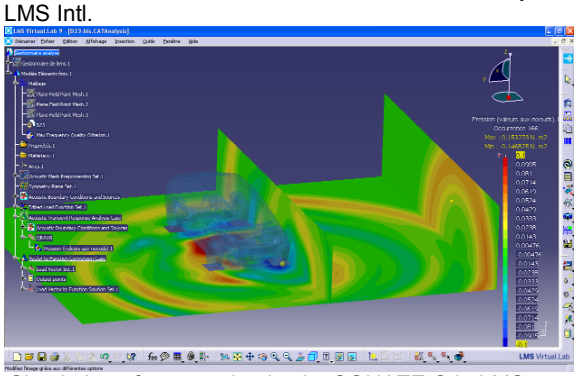
This transfer started with two PhD theses at IMACS and CMAP which set up the mathematical foundations of a stable numerical method and lead to a first software prototype. In a second phase, thanks to fruitful collaborations with domain experts in industry, we learned about practical industrial problems that could be solved with this method, and we worked hard (and we still do) to achieve this goal. We had to broaden our scope and learn about the use cases, CAD/CAE link, parallel computing…



The surface mesh for the integral equation cannot always be generated from a CAD model. In this example, the acoustical mesh of the engine (right) is built from the envelop of its structural mesh (left).

Results and achievements

Following the success of SONATE© in automotive applications (PSA Peugeot-Citroën and Renault), a partnership has been signed with LMS International, the world leader in acoustic simulations. SONATE© is now integrated in the CATIA V5 based platform LMS Virtual.Lab®, and distributed worldwide by LMS Intl.



Simulation of tyre-road noise by SONATE © in LMS Virtual.Lab ®: time domain transfer function.

Furthermore, in the framework of a partnership, IMACCS collaborates with EADS Innovation Works, on integral equations and their coupling with other methods (FEM, TLM, rays...) with many applications in aircraft and aerospace: Radar Cross Section computations for Defence, Electromagnetic Compatibility analysis and indirect effects of lightning on composite aircrafts, electrostatics discharge prediction. In partnership with EDF R&D, IMACS also applies integral equations to non-destructive testing based on eddy currents for crack detection.

Lessons learned and replicability

A team work where mathematicians, computer specialists, domain experts and engineers collaborate is mandatory to transform ideas, theorems and software prototypes developed in academic laboratories into tools and methodologies for everyday use in the design process in industry. The key of the success is the cover the full spectrum from mathematical modeling to very practical end users' concerns. Software maintenance and user support proved to be a rich source of new challenging problems which stimulate upstream research.

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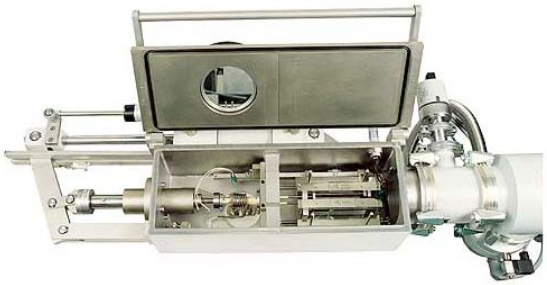
Evaluation of dilatometer experiments

Executive summary

A mathematical result paved the way to a joint project with engineers and a producer of dilatometer equipment to develop a new approach towards the evaluation of dilatometer experiments.

Challenge overview

Starting point for this project was a mathematical result. In a joint fundamental research project with the Department of Ferrous Metallurgy of RWTH Aachen University funded by the German Science Foundation (DFG) we were able to prove that the complete phase transition kinetics for two growing phases can be uniquely identified from dilatometer measurements.



Such a dilatometer (see Fig. above) is a device to measure the deformation and temperature evolution subject to controlled heating and cooling.

State of the art in dilatometer data analysis is that it is used solely to detect the transformation temperatures for the onset and end of phase transitions. In the case of more than one phase transition the detection of the final phase fractions up to now requires costly micrograph section analysis.

Implementation of the initiative

Since we were able to confirm our results also numerically, we approached the market leader in producing dilatometer equipment, a German SME. Together with that company and the Aachen group we set up a two year project supported financially by ZIM, a funding agency for the German Ministry of Economics and Technology to support SMEs.

The problem

Since induction heating is not only used in the heating stage but also to realize slow cooling rates the mathematical model includes thermo-mechanics and an eddy current formulation of Maxwell's equations.

The phase kinetics can be computed from an inverse problem using a Gauss-Newton method.

To obtain reasonable computing time it is indispensable to reduce the resulting model exploiting especially the symmetries of the problem.

Results and achievements

After one year an identification algorithm for the case of fast cooling has been developed and implemented. Our engineering partner is conducting experiments to validate the numerical approach. In cooperation with the company we have started to investigate ways to enhance the reliability of the solution to the inverse problem by a consequential use of all available experimental data.

Lessons learned and replicability

Scientific cooperation with engineers may be a convenient way to initiate industrial cooperations.

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Solution and model appraisal in reservoir inverse problems using global optimization methods

Executive summary

This story describes a multidisciplinary project in reservoir optimization using stochastic global approaches. This research is done within the Stanford Smart Fields and Stanford Center for Reservoir Forecasting, two industrial consortia held at Stanford University to perform research in subjects of interest in the oil industry, both in exploration and production. The industrial partners in these consortia fund and share the developments made at the Department of Energy Resources of Stanford University on different areas of research. In this case the example that we will describe concerns the use of global optimization methods in reservoir engineering. The research groups are formed by geophysicists, reservoir engineers, mathematicians, and computer scientists.

Challenge overview

The oil production history matching problem is highly ill-posed because the production data alone does not contain enough information to obtain the porosity and permeability of oil reservoirs. The knowledge of these two rock physics properties is very important for reservoir engineers to correctly manage and forecast production of a real oil field during its life. The forward problems involved have a very high computational cost because to match adequately the reservoir heterogeneities the number of cells in the three dimensional reservoir models has to be very high. This increases the dimensions of the inverse problem. The challenge is to solve the inverse problem in a robust manner accounting at the same time for uncertainty on the reservoir properties, that is, the ensemble of reservoir models that equally fit the observed data.

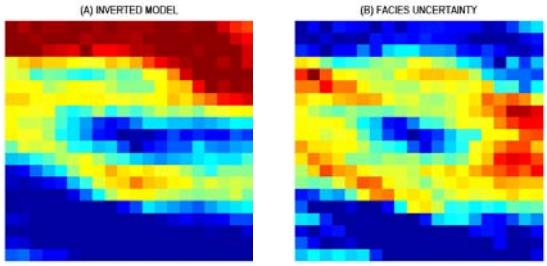
Implementation of the initiative

The initiative was carried out by a close collaboration between the Stanford Smart Fields and Stanford Center for Reservoir Forecasting consortia. The Stanford Center for Reservoir Forecasting is focused on creating geostatistical techniques to spatially describe the highly heterogeneous character of the oil reservoirs. The Smart Field consortium deals with mathematical models describing the multiphase flow in highly heterogeneous media and with all the inverse and optimization problems related to those: history matching inverse modeling, well placement, production optimization, etc. The aim is to model iteratively the oil reservoir following what has been name a closed-loop methodology. Both consortiums funded jointly the research at Stanford University during one year.

The problem

Inverse problems and numerical models are very important in reservoir characterization to increase future oil production. The production history matching problem provides to the reservoir engineers with some physical properties to be used in later stages in the field management. The ill-posed character of the history matching problem increases with the reservoir complexity, causing the optimization problem to be highly non-convex. These features cause traditional optimization methods to be highly dependent on the initial guess used and on the regularization criteria used to stabilize the inverse solution. In our methodology the ill-conditioned character of this history matching inverse problem is attenuated by model reduction techniques and by combining different kind of observables: production and time lag seismic data. The inverse problem is solved in a stochastic framework by searching for the set of reservoir models that fit the data (model uncertainty).

Results and achievements



We have applied these algorithms to the Stanford VI synthetic reservoir, showing that the PSO optimizers have a very reasonable convergence rate and provide approximate measures of uncertainty around the optimum reservoir model. The uncertainty estimation, although it is a proxy for the true posterior distribution of model parameters, allow us to perform risk analysis on the reservoir properties. This feature makes our algorithms more robust in presence of noise, which is always the case for real data.

Contact

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The Fastest Arithmetic in the World

Executive summary

GMP, a widely used and already very fast and highly mature software package for high-speed large integer arithmetic (used in cryptography and computer algebra systems), has been sped up by factors ranging from two to six.

Challenge overview

Shortly after the start of the Center for Industrial and Applied Mathematics (CIAM) at KTH, Torbjörn Granlund, the principal architect and creator of GMP, was recruited to CIAM. GMP, developed by the company SWOX, was already the most widely used library for large integer arithmetic. However, even though GMP was already very mature and sophisticated, it seemed likely that developing and implementing more mathematically advanced algorithms would result in significant performance improvements.

Implementation of the initiative

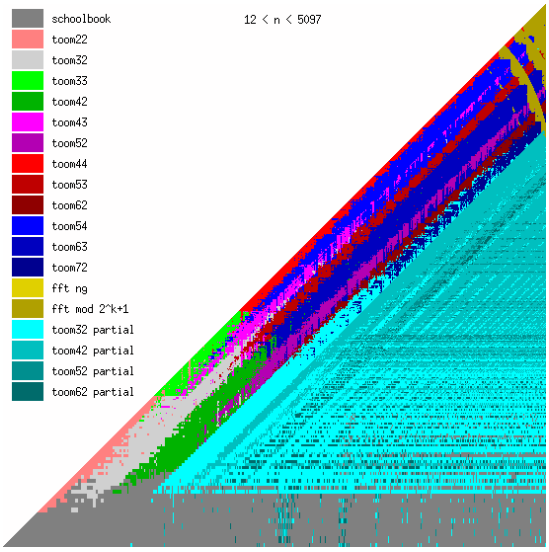
Torbjörn Granlund was recruited as a CIAM PhD student under the supervision of Johan Håstad (Professor, theoretical computer science) and Pär Kurlberg (Professor, number theory). So far the project has also involved a postdoc (Niels Möller), and two MSc students who are writing their theses under supervision of the group.

The problem

The major challenge is to develop new algorithms with improved asymptotic runtime, *and* to implement these in an efficient manner on the many popular CPU architectures currently in use. For further improvements, ever more mathematically sophisticated and subtle algorithm are needed, but implementing these efficiently is then a major challenge. Due to the large ranges of operand sizes, many different algorithms (see figure) are needed for good performance across all situations. To do this, one must exploit all available synergies between computer science and mathematics, and a major challenge is finding and synthesising a very wide spectrum of skills, ranging from advanced mathematics to a high-level ability to overcome subtle engineering challenges.

Results and achievements

Public key cryptography, as well as most computer algebra systems (*e.g.*, Maple, Mathematica, Sage) in widespread use today, are all highly reliant on high-speed integer arithmetic. Since the inception of the project within CIAM, speedups of factors between two and six have been obtained – a quite remarkable result for such a mature project.



Lessons learned and replicability

A key insight is that software engineers, even extremely good ones, reap tremendous benefits from learning more advanced mathematics. Another realization is the huge value in using more sophisticated models of algorithm runtimes, and then analyzing these with traditional mathematical tools (i.e., rather than relying on benchmarks) when developing better algorithms in this setting.

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Modeling and assessment of maintenance efficiency of repairable systems

Executive summary

Laboratory Jean Kuntzmann (LJK) and EDF R&D collaborate from 2003 until now on the joint modelling and assessment of ageing and maintenance efficiency of complex repairable systems.

Challenge overview

The contact was taken when LJK and EDF members met in research groups and conferences on reliability modeling. The initiative was taken by EDF's department on Industrial Risk Management, which has a strong tradition of cooperation with mathematicians. This research is a part of a large strategic project on plants ageing and durability. Throughout their operational life, industrial systems are subjected to preventive and corrective maintenances. Efficient maintenance allows extending the service life of an equipment, which is a crucial industrial issue. It is therefore important to build models of the effects of maintenance of complex repairable systems and develop methods to assess their efficiency.

Implementation of the initiative

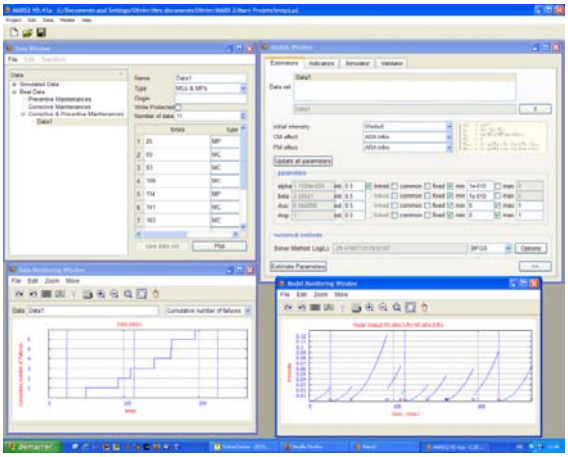
LJK and EDF have signed 8 successive contracts on this topic, one each year since 2003. The total financial contribution of EDF is 185000 €. It supported 2 PhD thesis and 2 internships. 4 people from the permanent staff of LJK and 8 people from the permanent staff of EDF were involved in the contracts. No real problems were encountered in the collaboration.

The problem

Basically, it is assumed that either maintenance is perfect (As Good As New), or maintenance is minimal (As Bad As Old). The reality is of course between these two extreme cases. This is called imperfect maintenance. In this project, several stochastic models have been developed for this situation. The first challenge of this work is modeling. Maintenance effect is supposed to reduce either system age or system failure intensity. A global modeling of the joint effect of preventive and corrective maintenance have been proposed, using mutually excited random point processes. The dependency between both kinds of maintenances have been studied using generalized competing risks. The second challenge of this work is the statistical analysis of the proposed models. Frequentist and Bayesian methods have been used. Algorithms have been implemented for the computation of the parameter estimates and the assessment of reliability indicators.

Results and achievements

This collaboration led to the development of a free software tool, which aims to implement the models developed and to estimate jointly the effects of ageing and maintenance (preventive and/or corrective). This software, called MARS (Maintenance Assessment of Repairable Systems), is now used in several companies (EDF, SNCF, HP, Dassault Aviation) and universities (Bordeaux, Littoral, Magdebourg, Karaghpur).



From the company point of view, the main result of the project it that it helps to forecast the future behavior of the maintenance process and then to update the Reliability Centered Maintenance process, through preventive maintenance planning. It is of great interest as regards the problem of extending the operating lifetime of complex systems such as electricity plants.

From the laboratory point of view, the main result is the development of new stochastic models, which are now used in the international research community on this field. The diffusion of the software is also a good showcase for the company and laboratory expertise. This collaboration has lasted several years and it is expected to be continued in the future

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Optimization of electricity production

Executive summary

Every day, EDF (French Electricity Board) has to compute production schedules of its power plants for the next day. This is a difficult, large-scale, heterogeneous optimization problem.

Challenge overview

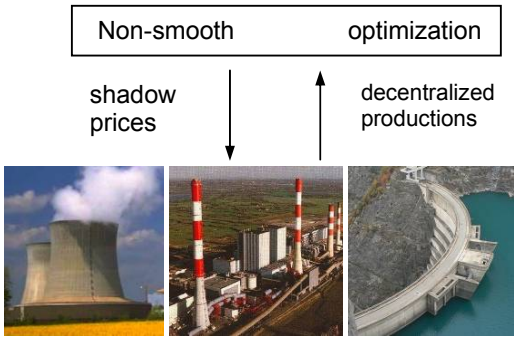
In the mid eighties, a meeting was organized between INRIA and EDF R&D. The idea was to let EDF present some of their applications, to explore possible collaborations. Indeed, EDF has a long tradition of scientific work, in particular with academics. Their production optimization problem was presented among others. Its mathematical model was clearly established; even the relevant software existed, but the solution approach needed improvement. The mathematics at stake turned out to perfectly fit with INRIA competences.

Implementation of the initiative

Collaborative work therefore started immediately. No difficulty appeared with administrative issues such as intellectual property or industrial confidentiality. It was a long-term research, so deadlines posed no problem either.

The problem

The solution approach is by decomposition: each power plant (EDF software) optimizes its own production on the basis of ``shadow prices'' remunerating it; these prices are iteratively updated (INRIA software) so as to satisfy the balance equation. The working horse to compute the prices is a non-smooth optimization algorithm.



The difficulty was to join the EDF and INRIA-software. This turned out to be harder than expected. The model appeared as not mature enough and significant bugs were revealed. The project was basically abandoned and it is only in the mid nineties that intensive collaboration could resume on a renewed model.

Results and achievements

This time, the collaboration was successful and the new software became operational a few years later. This relatively long delay was due to necessary industrial requirements (mainly aimed at achieving reasonable reliability). Substantial improvements in cost and robustness were achieved. EDF is highly satisfied with this collaboration, which continues and will probably continue for many years.

Current research focuses on developing more accurate models of the power plants, entailing more delicate price optimization.

Several academic outcomes resulted from this operation:
• to understand better and to improve highly sophisticated optimization methods;
• to assess these methods in the “real world”, thereby introducing them for new applications;
• to exhibit the practical merits of a mathematical theory (convex analysis, duality), generally considered so far as highly abstract (and taught as such in the university curriculum).
Lessons learned
Beyond science and techniques, a lesson of this “success story” is that any academic-industrial collaboration should be undertaken with strong mutual esteem and confidence.

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Optimized needle boards based on simulations of needle punch patterns

Executive summary

The development of evaluation criteria for needle punch patterns based on simulations is the key of success for a innovative construction-method of optimized needle board designs adjusted to customer specific process settings.

Challenge overview

In spring 2008 the Fraunhofer ITWM followed an invitation of Oerlikon Neumag Austria. At that time Oerlikon Neumag Austria developed an new generation of needle machines. The long-lasting successful partnership between its sister company Oerlikon Neumag and Fraunhofer ITWM led to their wish to optimize the needle boards of the new needle machines using mathematical methods. A contract was closed to solve this challenging problem. For a duration of 13 months two scientists of Fraunhofer ITWM and one engineer of Oerlikon Neumag Austria have been working together on this research project.

Implementation of the initiative

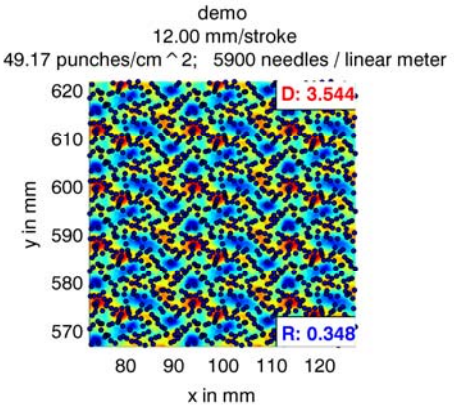
The dream of Oerlikon Neumag Austria was to find a needle board that produces for all customer specific process settings an optimal nonwoven. Needle punching is a well-established method to bond nonwovens mechanically. Thousands of barbed needles penetrate simultaneously into the nonwoven and solidify it. The resulting properties depend significantly on the machine and process parameters, in particular the feed per stroke has a tremendous effect on the nonwoven. Typically, the feed per stroke is tiny compared to the needle board length, i.e., the material is penetrated up to 30 times before it leaves the needle zone, and therefore the needle punch patterns interfere with each other. Due to this complexity it is impossible without computer to predict the effect of modified needle arrangements on the product.

The problem

The first idea of developing an optimal needle board was to transfer methods from number theory on the needle arrangement in order to gain homogeneous nonwovens. But are homogenous needle punch patterns really the aim we have to look for? Actually, a homogeneous distribution of the needle punches is only one criterion of a good nonwoven. Furthermore, there should be no patterns like stripes, and humans tend to identify everywhere structures. Hence, the strategy to optimize needle boards was changed and the project extended.

Results and achievements

The simulation of the needle punch patterns combined with the development of evaluation criteria for quantifying the quality of the simulated nonwovens was the key to success. Hereby, one difficulty of the simulations is the modelling of the shape distortion. Since the nonwoven is transported by rollers the material is stretched out in production direction while penetrating the material leads to a shortening in cross direction. These effects have to be included by a shape distortion model based on ordinary differential equations and validated by measurements. The development of the evaluation criteria was carried out in close cooperation with Oerlikon Neumag Austria. From mathematical point of view a wide variety of different fields came together: radial functions, Fourier analysis, projection methods, and statistics. With these evaluation criteria the design process of needle boards can be automated. Needles can be placed step by step by judging all resulting needle punch patterns for all remaining free positions and choosing the best one.
The results of the project are a great success for Oerlikon Neumag Austria. Using the automatic design process the time duration of new needle board constructions can be effectively reduced and simultaneously the quality of the nonwoven improved.



Density distribution of a needle punch pattern

Contact

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Fraunhofer ITWM

From satellite antenna design to piano modelling

Executive summary

As a consequence to our work on satellite antenna design, we succeeded to create the first virtual piano based on mathematical modelling.

Challenge overview

Thales Alenia Space (TAS, formerly Alcatel Espace) took contact with us because it had some difficulties in designing the repartitor of a new complex antenna. A repartitor is the radio-electrical feeding device located at the focus of the antenna reflector and is a network of elementary waveguides. We succeeded in solving this problem and the solution has been protected by a patent. It was the first time that TAS in Toulouse, France, worked with mathematicians. The natural extension to this project is to calculate the electromagnetic field in the repartitor and to find its optimal design.

Implementation of the initiative

This project has been carried out in the frame of a contract with the IMT (Institute of Mathematics of Toulouse). A prototype has been implemented in the laboratory with the help of my colleague Philippe Guillaume. To validate our approach, we had the geometry of a waveguide and measurements of its electromagnetic response (transmission coefficient) in a given frequency range. There was a large discrepancy between our computation and the measured response. We realized that we had wrong information on the geometry description, and we succeeded in finding the real geometry thanks to parameterization. This ended the initial scepticism and opened new collaboration opportunities. Industrial software implementing this technique has been developed by the company CADOE (see below). In the frame of these collaborations, three from our students in mathematics have been hired by TAS.

The problem

The basic problem is to calculate the solution of elementary waveguides which must be expressed as a function of shape and excitation parameters. Then we solve the global problem at the repartitor level by using these waveguide solutions as basis functions. For this purpose, we considered higher order derivatives of the waveguide solutions with respect to parameters. In fact we discovered that in linear algebra, the Jacobi, Gauss-Seidel, and relaxation methods can be seen as a Taylor approximation of the solution with respect to a hidden parameter. We pointed out that Krylov subspaces are generated by vectors obtained by derivating with respect to a parameter. By making the connection between our problem and advanced linear algebra methods, we pushed forward the state of the art in the field of reduced order models.

Results and achievements

We continued the collaboration with TAS, and no less than ten collaboration projects have been carried out. Thanks to this success story and the support of TAS, a start-up called CADOE (Adaptive Computation by Higher Order Derivatives) has been created. This company has 40 employees and is today an R&D centre of Ansys. Quite a few employees were students in mathematics at our university. Parameterization techniques could be seen as a way to store computing. Thanks to the know-how that we acquired in the frame of these projects, Philippe Guillaume succeeded in introducing the very first model for piano that generates the sound in real time. This innovation is seen, at the international level, as the state of the art and the future of virtual pianos (see http://www.pianoteq.fr/references).

Lessons learned and replicability

To listen and not to give lessons.

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Secure communication for automatic teller machines

Executive summary

Automatic teller machines (ATM) are widely used in the banking sector. Due to their popularity, ATMs are the frequent target of attacks, both by outsiders and insiders. The goal of this project was to prevent insider attacks on ATMs by securing the communication channels between the various components of an ATM.

Challenge overview

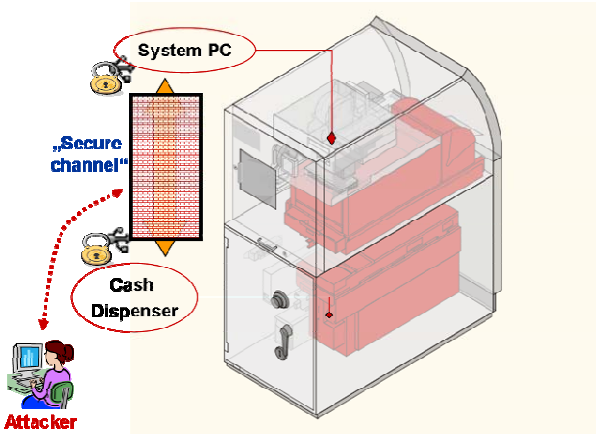
Wincor Nixdorf is one of the world's largest manufacturers of self-service transaction systems, such as ATMs. Outside and inside attacks on ATMs not only cause significant financial damage, they also threaten to destroy the trust of customers in self-service systems.

While mechanical countermeasures against outside attacks have been intensively studied for decades and are employed in almost all current ATMs, security measures against insider attacks are often still in their infancy.

The goal of the collaboration between Wincor Nixdorf and the Institute for Industrial Mathematics was to secure by cryptographic means the internal communication between the different components of an ATM, such as the system PC and the cash dispenser. This was intended as a first step in the development of a system wide security concept for automatic teller machines.

The problem

To design and implement secure and efficient communication channels in an ATM, first a precise model of attack scenarios had to be developed. Based on this model, appropriate cryptographic tools had to be identified and implemented on the various communication devices of an ATM.
As an additional challenge, the cryptographic tools had to be implemented on various, often computationally limited hardware platforms.



Implementation of the initiative

In a year-long project, funded by Wincor Nixdorf, a member of the Institute for Industrial Mathematics designed a cryptographic protocol securing the communication channels in an ATM. Together with a student from the University of Paderborn and with several staff members from Wincor Nixdorf a prototype of this protocol was implemented on the main communication components of an ATM.

Results and achievements

The cryptographic protocol satisfied all requirements set at the start of the project; it provides efficient, authenticated, and confidential communication in an ATM. Furthermore, Wincor Nixdorf applied for a patent for the cryptographic protocol and the main features of its implementation.

Contact

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Uncertainty assessment in high-dimensional nonlinear inverse problems

Executive summary

This story describes a multidisciplinary collaboration with the Schlumberger-EMI Technology Center located in Richmond (California). By combining different expertise, skills and experiences we were able to put together a methodology to assess uncertainty for high-dimensional nonlinear inverse problems, a very challenging and long-standing problem in geophysics that interests the oil and gas industry as a way to perform risk analysis for exploration. Although the invention of this methodology has been motivated by the oil industry, it is completely general. This technique has the potential to be applied to other fields such as mining, hydrogeology, biomedical engineering, finance, weather prediction, earthquake modelling and many other scientific, technological and industrial inverse problems.

Challenge overview

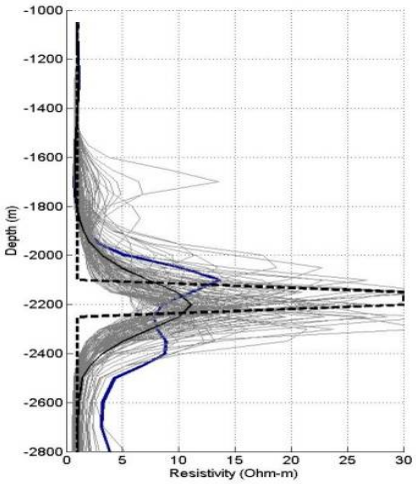
The main objective of this research was to produce a simple and robust methodology to perform uncertainty analysis for high-dimensional nonlinear inverse problems to accomplish risk analysis in oil exploration. Another requirement was that the methodology should be (if possible) agnostic to the physics of the problem, that is, it could be applicable to other kinds of inverse problems coming from any other field of engineering and technology.

Implementation of the initiative

The initiative was carried out by a tight collaboration with the Schlumberger-EMI Technology Center in Richmond (California).

The problem

An important trait of nonlinear inverse problems is that they have a wide range of non-unique solutions, which contributes significantly to the uncertainty of any one inverse solution. Linear analysis techniques, to estimate solution uncertainty, have a limited range of validity due to the nonlinear character of the inverse problem. Also, the dimensionality of typical geophysical problems and high cost of forward solutions hamper the use of Monte Carlo sampling techniques and Bayesian approaches. These methods are highly inefficient and computationally expensive (even for low dimensional problem) due to the random character of the sampling procedure. The solution that we have proposed is based in a combined use of model reduction techniques (principal component analysis, singular value decomposition, discrete cosine transform, discrete wavelet transform), parameter constraint mapping to the model reduced space, and very sparse adaptive sampling. This is possible due to the algebraic structure of uncertainties in inverse problems: equivalent models are located along flat elongated valleys of the cost function landscape. The beauty of this methodology is that it allows us to sample and classify different kinds of solutions prior to computationally intensive forward evaluations. This method has been named Geometric Sampling.



Results and achievements

The main achievement is to be able to perform uncertainty estimation in high-dimensional nonlinear inverse problems with real cases from oil exploration and production where inverse problems are often used coupled with complex forward mathematical models. Electromagnetic example: ninety nine sparsely sampled equi-feasible models representing the non-uniqueness of our solution. We show the true model (dotted black), the deterministic inverse solution (bold black), and an example of multi-resistor model (blue) found by our sampling methodology. This model fits the observed data within the prescribed error tolerance and is compatible with our prior. Knowledge of these models is very important to quantify risk.

Lessons learned

One of the most important lessons learnt from this experience is that problems cannot be solved by means of dogma and we can do things otherwise. The second lesson is that original ideas always come from putting together at work different kinds of knowledge. Engineering and technology need mathematics and physics, and mathematics and physics need real engineering challenges. Problems from the real world make us humble and show that the distinction between pure and applied mathematics is false.

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A long lasting success story: Oxford study groups with industry

Executive summary

Here the story and the philosophy of Oxford study groups with industry is briefly outlined. It is an experience that started back in 1968 and has given origin to many similar events around the world

How it all began

In the 1960's, the Royal Society of London issued a report that suggested that UK applied mathematics was not realizing its potential in terms of societal benefit. The cause was identified as being that academics were focusing too narrowly, especially in the then-fashionable area of theoretical mechanics. Two Oxford mathematicians, Alan Tayler (see photograph) and Leslie Fox, studied the report and came up with the inspirational idea of proposing week long interactive workshops, each initiated by a group of industrial researchers posing open problems of current relevance. One or two tutorial-style lectures were then interposed in 3 days of informal brainstorming by both the industrialists and interested applied mathematicians, before executive summaries were presented on the final morning.

Implementation of the initiative

With generous support from the government to supplement the registration fee charged to industry, these "Study Groups" ran annually in Oxford from 1968 to 1989. In 1984, the idea caught on in the US and Australia and now there are a dozen annual events of this kind around the world, and a similar number less regularly. It is no exaggeration to say that these events have been one of the foundation stones of maths-in-industry as it is in 2010. Evidence of their impact can be provided by the hundreds of industries around the world that have used Study Groups to benefit from the unique framework that mathematics can provide for understanding and improving industrial processes; moreover and the thousands of novel mathematical papers that have been driven by the Study Group formula for bridging the interdisciplinary divide. Indeed this formula is now regularly adopted by large industries for "in-house" Study Groups and by academic scientists for interdisciplinary research between departments. And ample evidence for the success of the concept is provided by the surprisingly high percentage of companies that repeatedly present new problems.

Study groups today

As an example of how a study group might work we look at the 68th European Study Group with Industry which was held in Southampton in 2009. There were 5 problems considered:

- Reaction Diffusion Models of Contamination (DSTL)
- Human Decompression Modelling (VR Technology)
- Chauffeur braking (Jaguar Land Rover) Oil Price Cycle and Sensitivity Model (EPRasheed)
- Underreamer Mechanics (SmartReamer Ltd)

The outcomes

Since the meeting, internships have been set up on the first two problems, through the Industrial Mathematics KTN (www.ktn-internships.net). This involves a postgraduate student working within a company for 3-6 months on a specific problem: in both these cases the student will be developing software based on the ideas that came out of the study group. Other possible outcomes after a study group might be industrial sponsorship of a postgraduate student or a post doctoral researcher, consultancy agreements or further academic work leading to publication in a learned journal (see two case studies on next page). Problems can also be used as a basis for training students via modelling weeks or books on case studies.

http://www.math-in-industry.org/

Modeling and Detection of Realistic Human Actions in Video

Executive summary

Video has evolved into a vibrant, live cultural heritage of our society providing rich resources for education, entertainment and sociology studies. Automatic video analysis is crucial to enable access to information in huge and rapidly growing video archives. This research project is concerned with the robust modeling and recognition of human actions in archive videos based on the recent progress in computer vision and machine learning.

Challenge overview

One of the major challenges in automatic video understanding is to overcome large variations in video data due to individual differences of people in expression, posture, motion and clothing; perspective effects and camera motions; illumination variations and other factors. To handle this problem, we use local invariant video descriptors in combination with statistical learning techniques. We deploy weakly supervised learning to reduce or to eliminate completely the need of costly manual annotation of training data. Compared to the state of the art, this project is among the first to consider human action recognition outside previously addressed constrained domains such as surveillance and sports.

Implementation of the initiative

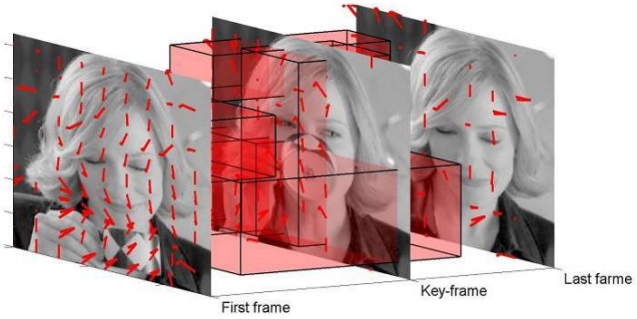
This project is currently being realized within the on-going collaboration between Microsoft Research and INRIA in the joint INRIA-Microsoft Research Centre. The work in the project has been carried out by INRIA teams LEAR, VISTA and WILLOW involving several permanent researchers (F.Bach, I.Laptev, P. Pérez, J.Ponce, C.Schmid and J.Sivic) as well as three PhD students (O.Duchenne, A.Gaidon and M.Marszałek). The collaboration has also involved Institut National de l'Audiovisuel (INA, L.Laborelli and D.Teruggi) providing access to the large video archives.

The problem

From the mathematical viewpoint, this project is based on statistical learning theory providing a principled way of predicting unknown properties based on the current and previous observations. Predicting the class and location of human actions in video requires estimation of complex decision functions which can be resolved by formulating and solving convex optimization problems.

Results and achievements

The main achievement of this project has been to demonstrate and to quantify the performance of action recognition in realistic video data. In the follow-up collaborations we plan to develop prototypes of on-line interactive video browsing and search for the end-users.



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Real-time Video Distortion Correction for the MyHome Embedded System

Executive summary

In this project several image distortion correction methods are adapted in order to add real-time video processing capabilities to an embedded system.

Challenge overview

In 2009, M2M Solution and R&D Bulgaria posed the problem to add fisheye lens distortion correction to their emerging camera-enabled embedded device: the MyHome home security gateway. By that time the hardware has already been fixed, so an efficient solution, utilizing just the main processor of the embedded system, must have been found. After the implementation of the distortion correction, the request to add digital zoom and pan capabilities was made.

Figure 1: Distorted original

Implementation of the initiative

R&D Bulgaria recruited me – a graduate student at the Faculty of Mathematics and Informatics, University of Sofia – to implement the project. The contract lasted for 6 months. The project was supported by the lens manufacturer (Sunex), the image sensor manufacturer (Atpina) and both R&D and M2M software teams. Test hardware was provided by M2M. Financial resources were provided by R&D.

The problem

Most of the distortions, caused by fisheye lenses, are captured by a radial model (only the radial component in a polar coordinate system is distorted). Due to the essential stretching effect of the distortion correction and since we are working with digital images (which are discrete in nature), in addition to the model distortion function, an interpolation scheme is needed to fill-in the missing values. To find the distortion model and to estimate its parameters were relatively not complicated tasks. The tricky part was to design an algorithm that could implement undistortion and interpolation without hogging the embedded processor – the most systems, described in the literature, were either non-real time, or dependent on customized hardware, or requiring desktop processors.

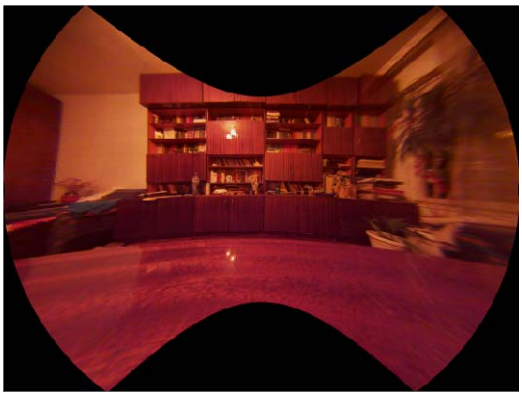

Figure 2: Fisheye distortion correction

Results and achievements

The outcomes of this initiative were several distortion correction algorithms carrying out undistorted image, interpolation and digital zoom in a single processing step. As a result, company performance requirements were more than satisfied: we were able to process up to 16 frames per second 640x480 video using only 25% processor time. For the digital zoom, we took advantage of the different image sensor modes supported, so we were able to achieve detailed output even at high zoom levels.
The contacts with R&D were continued in the frame of the Mathematical Modeling Seminar at FMI.

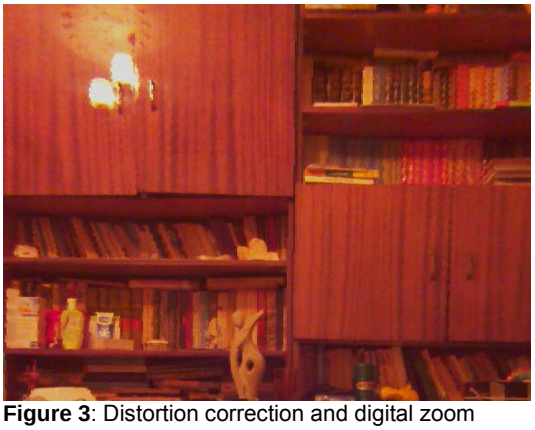

Figure 3: Distortion correction and digital zoom

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Cognitive Vision

Executive summary

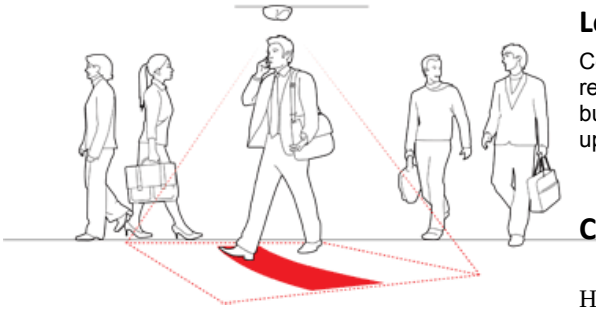
The story is about research in algorithms for automatic detection and classification in images and image streams and a spin-off company formed in 2003.

Challenge overview

The project was initiated internally at the research group for computer vision within the centre for mathematical sciences. Experiences from a previous startup, Decuma, had shown that there was some interest for cognitive vision applications within mobile telephones and surveillance cameras. The business case within mobile telephones was less clear and based on entertainment products such as facewarp and caricatures; whereas the case was more clear within consumer behaviour analysis.

Implementation of the initiative

Using results from their research in computer vision, the group of inventors developed first products for the mobile telephone market and later for Intelligent Surveillance. Previous experience with the spin-off company Decuma, was useful when a new joint-stock company Cognimatics was formed. After a couple of years, there were roughly 10 employees. The company has had positive cash flow and has not needed to attract external financing through venture capital.

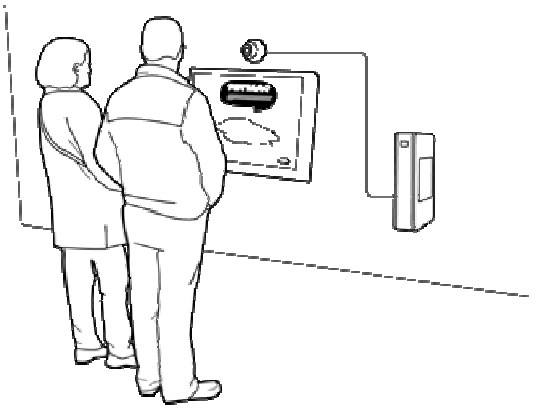


The problem

Detecting objects such as faces, eyes, mouth, humans, cars, bicycles etc in still images is a considerable challenge. The major difficulty lies In the large variability of the signal over time, viewpoint, etc. Efficient algorithms for solving such problems are based on novel research e g within mathematics, statistical machine learning, optimization etc. Similarly automatic analysis of scene and action content in images streams is difficult because of the large variability in data.

Results and achievements

The research within cognitive vision has resulted in various products within mobile communications (FaceWarp, MakeOver) and within intelligent surveillance (People Counter - Counts persons passing through in a predefined area, Zone Counter - Counts number of persons standing in a predefined area in still images, Parking - Counting and showing traffic to and from parking facilities, Dwell Time - Counts faces and how long they are watching into a camera.) The customers for the mobile communication products are fewer and larger companies, whereas the sales of intelligent surveillance are based on a network of more than 100 partners worldwide.



Lessons learned

Certain business segments have shorter time from research to products. By combining a few different business alternatives it has been possible to build up the company without the need for venture capital.

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Handwriting recognition

Executive summary

The story is about the development of a system that transfers handwritten text on a pressure sensitive screen to ascii-code, and the forming of a spin-off company around this.

Challenge overview

All started as a cooperation between the Mathematical Imaging Group at Lund University and the mobile phone manufacturer Ericsson. The company saw a future need for input alternatives to keyboards. In particular, they were interested in the use of pressure sensitive screens, where the existing technologies at that time were not very well developed.

Implementation of the initiative

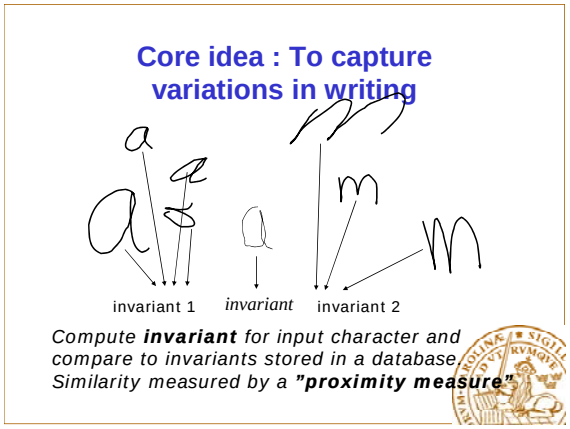
Using results from their research in computer vision, the group of inventors developed methods solving the task. Encouraged by Ericsson, they prepared a patent application around the mathematical concepts of “invariance” and “proximity measures”. After its approval in 1999, they founded the joint-stock company Decuma. After a while, not only Latin letters but also Chinese and Japanese were handled. The company grew, recruiting also expertise in linguistics and marketing. After a couple of years, there were 28 employees, of which 8 were doctors in mathematical subjects. Financing was obtained through venture capital companies.

The problem

Obvious complications in handwriting recognition are the facts that the appearance of a letter varies from person to person, and over time even for a single person. By modeling such variations by some class of transformations, e.g. affine or similarities, geometric invariants could be used as identifiers for the different characters.

Results and achievements

The systems developed performed very well, and Decuma received a lot of attention, e.g. the very prestigious Grand Prize 2003 from the EC Information Society Technologies, for "groundbreaking products and services that represent the best of European innovation in information society technologies". A prominent customer became Sony Inc., with whom contracts were signed for recognition of Latin, Chinese and Japanese writing. In 2003 Sony even became the largest shareholder of Decuma, before they, during the then ongoing IT-crisis, unfortunately decided to shut down their division for handheld computers. After losing Sony as a customer, Decuma was sold to Zi-Corporation (Canada), and then later on to Nuance (US). Today Decuma’s products are part of a bigger portfolio of mobile services and sold on a global market, with customers like Nintendo.



Lessons learned

It is hard for a small company with a niche product, even if very good, to act together with very big global players, and to be dependent also on venture capital with short time perspectives.

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