Thibaut Lery - Mario Primicerio Maria J. Esteban - Magnus Fontes Yvon Maday - Volker Mehrmann Gonçalo Quadros - Wil Schilders Andreas Schuppert - Heather Tewkesbury Editors

## European Success Stories in Industrial Mathematics







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# European Success Stories in Industrial Mathematics







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ISBN 978-3-642-23847-5 c DOI 10.1007/978-3-642-23848-2 Springer Heidelberg Dordrecht London New York

e-ISBN 978-3-642-23848-2

Library of Congress Control Number: 2011938138

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Cover design: WMXDesign GmbH, Heidelberg

Printed on acid-free paper

Springer is part of Springer Science+Business Media (www.springer.com)

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# Foreword

# By Sean Sherlock T.D., Minister for Research and innovation, Ireland.

It is impossible to look at the world today and not be amazed at the mathematics knowledge which has enabled us to get here. As the complexity of the challenges which are faced by society and industry increases so does the mathematical skill required to understand and solve them.

This publication of Mathematics and Industry Success Stories has been developed from the recognition that the mathematical sciences, and in particular European mathematics, have delivered great innovations to society and industry and have the potential to deliver far more. In order to fully realise this potential, the collaborations between mathematics and industry must be expanded and improved. The expertise in mathematics is extremely high in Europe both in variety and quality and similarly these networks of European mathematics must be further grown, nurtured and sustained.

The Forward Look Mathematics and Industry Report separately published by the European Science Foundation and the European Mathematical Society outlines recommendations to bridge the gaps between mathematics in academia and industry, in particular our SMEs, and reduce the fragmentation within the European Research Area. This has involved the input and experiences of a wide range of stakeholders, from academic and industrial researchers, to engineers and policy makers. Both industry and academia are challenged to come together and realise the opportunities involved.

Groups working at the interface between mathematics and industry were invited to submit examples of problems and challenges successfully overcome with the application of mathematics. The collection of success stories in this book shows the wide range of problems and challenges industry face on a daily basis and which can be addressed in collaboration with the mathematical scientists. From early cancer detection and optimising satellite coverage, or modelling of rogue ocean waves to understanding customer needs and behaviours, these success stories demonstrate what is achievable for companies of all sizes.

The development of mathematics education followed by attractive careers for young researchers is a vital element to help Europe reach its potential as a knowledge leader. It is recognised worldwide that attracting young people to mathematics as a path of learning and a career is very difficult. Many European countries, including Ireland, are evolving their own mathematics curricula at a primary and secondary level. Building on these initiatives with European Masters and PhD level programmes should then enable greater recognition of careers for industrial mathematics.

Dublin will host the Euroscience Open Forum (ESOF) from 11-15 July 2012. ESOF is an interdisciplinary, pan-European meeting, held under the auspices of Euroscience, which aims to:

- Showcase the latest advances in science and technology,
- Promote a dialogue on the role of science and technology in society and public policy,
- Stimulate and provoke public interest, excitement and debate about science and technology.

I believe this event will provide an opportunity also to showcase the value of mathematics to science and society. The event will bring together 6,000 scientists, business leaders, government officials and international media to discuss the best of European science and to address all of the major global challenges, including energy, climate change, food and health.

The publication of this volume presents us all with excellent examples of European industry and mathematical sciences coming together to overcome the complex challenges our industries face. This is of particular importance in these tough economic times for many European countries.

In conclusion, I commend the European Science Foundation and the European Mathematical Society for their work in producing this volume of Mathematics and Industry Success Stories and we in Ireland are proud to be part of what we hope will be a new era of collaboration in industrial mathematics with our European partners.

# Preface

# By Máire Geoghegan-Quinn, the European Commissioner for Research, Innovation and Science.

The mathematical sciences have been central to our civilisation for centuries. The global economy and Europe's knowledge society have placed information and communication technologies at the forefront, and these technologies are increasingly dependent on scientific research driven by mathematics.

Mathematics also provides the tools to help us understand and interpret the world around us. It also helps us predict trends in the economy, the environment and demography that are essential to tackling many of the grand challenges faced by our society.

This is especially true in areas where innovation is contributing to a better society, such as health, security, communications, and environmental stewardship. The search for new life-saving drugs, the development of high-performance materials, continued miniaturisation in electronics, and the protection of sensitive ecosystems - all of these activities, and many others, are strongly dependent on fundamental research, and that research is inextricably linked to mathematics.

Europe has some of the world's best mathematicians, and in many European universities and research centres, they are often organised in research communities along national lines. In collaboration with industry, they have developed great expertise at the forefront of maths research. They are also participating in a number of research centre networks, exchanging students in joint training programs in industrial mathematics. This is a European scientific community in the making, and the diversity of approaches and cultural differences is an important factor in the cross-fertilisation of ideas produced by European cooperation.

This book presents a number of success stories that demonstrate the crucial contribution of mathematics to innovation in products and technologies. Each story describes the challenge that led to industrial cooperation, how the challenge was tackled and how the solutions were achieved and implemented. Taken together, these stories illustrate the extensive European landscape of projects in almost all areas of applied mathematics and across all business sectors. Close collaboration between industry experts and academia was both crucial to the success of the projects and highly valued by all the participants.

We are increasingly reliant on science, engineering and technology to help boost innovation and economic growth and to improve our quality of life. With this reliance comes a growing need for improved education and training in mathematics and statistics, both for the scientific and technical workforce and for the general public in an increasingly technological and digital world.

There are great benefits to be gained from a dynamic mathematics community working actively with industry and business. I hope that the examples included in this publication will serve as inspiration for the development of a coordinated and dynamic community of industrial and applied mathematicians in Europe. They have an important role to play in helping to foster Europe's competitiveness and prosperity.

Maine Geogheepen Qui

# Introduction

This book of success stories shows the impact of collaborations between mathematics and industry. It has its origin in the Forward Look about Mathematics and Industry that was funded by the European Science Foundation (ESF) and coordinated by the Applied Mathematics Committee of the European Mathematical Society (EMS). This Forward Look aimed to compare the state of the art at the mathematics-industry interface and the needs for the future development of science and technology in Europe.

One of the key factors in this respect is the use of mathematics as a driving factor for innovation. Only via mathematics can the complex processes and products in current key technologies and short innovation cycles be managed in an efficient, robust and sustainable way.

Although the mathematics-industry interaction has reached a satisfactory level in some countries of the European Union, it is far from being equally developed in others. This fragmentation is a source of imbalance and inhomogeneity at the European level. Even in the countries where this interface is functional, it needs to be improved and extended. The conclusion of the analysis of the different scenarios was that unless important measures are taken by the various actors, since Europe is using a too small amount of its potentialities, it risks losing its position in the global competition.

The White Paper produced within this Forward Look has been written taking into account past analyses made in various contexts (the reports produced by the OECD and various national initiatives), and the experiences from not only Europe but also other countries. It also took into account the results of an online survey, launched within this project, of more than a thousand participants in academia and industry throughout Europe. Its conclusions are summarised in a list of recommendations on measures to be implemented (they can be found as the Annex to this book, while the White Paper can be downloaded from the website http://www.ceremade.dauphine.fr/FLMI/). The key recommendation is the creation of a European Institute of Mathematics for Innovation (EIMI) that should stimulate, coordinate and implement cooperation between mathematicians and companies at the continental level.

The Forward Look was coordinated by a Scientific Organising Committee (SOC) composed of Maria J. Esteban (CNRS, France), Magnus Fontes (Univ. of Lund, Sweden), Thibaut Lery (ESF), Yvon Maday (Univ. P. et M. Curie), Volker Mehrmann (TU Berlin and Matheon), Mario Primicerio (Univ. of Firenze, Italy), Gonçalo Quadros (Critical Software, Portugal), Wil Schilders (NXP, The Netherlands), Andreas Schuppert (Bayer Technologies, Germany), and Heather Tewkesbury (Industrial Mathematics Knowledge Transfer Network, UK).

To demonstrate the importance of mathematics in innovation, it was decided to publish a collection of success stories on the impact of the collaboration between mathematics and industry. This volume shows the wide spectrum of industrial sectors where the use of mathematics is the decisive factor for success. It also shows the variety of mathematical areas involved in this activity. The Mathematics-Industry collaboration is a two-way transfer of knowhow, providing industry with solutions and mathematics with new research topics and stimulating new methodologies.

The editorial board and members of the Scientific Organising Committee of the Forward Look "Mathematics and Industry"

> Thibaut Lery Mario Primicerio Maria J. Esteban Magnus Fontes Yvon Maday Volker Mehrmann Gonçalo Quadros Wil Schilders Andreas Schuppert Heather Tewkesbury

# **Health & Biology**

# Optimisation of Radiation Therapy

#### **Executive summary**

The project concerns new optimisation 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 Optimisation 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 optimisation models and optimisation 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 duties at RavSearch, 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 optimisation problem arising in intensitymodulated 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 tumour cells whereas sensitive organs must be spared. A major challenge is how to formulate the optimisation problem so that the solution obtained is clinically acceptable while it at the same time best fulfils the given requirements. The PhD student project was aimed at utilising problem structure to analyse and design methods for solving the optimisation problem in order to achieve these goals.

#### **Results and achievements**

The PhD student project led to significantly deepened understanding of the optimisation problems that arise. The interaction between problem structure and behaviour 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 behaviour of methods required a deep understanding of properties of the optimisation problems. Conversely, practical aspects of the optimisation problems led to new interesting fundamental research questions on optimisation 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 modelling 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 modelling and computational analysis of canine atrial action potentials. Having previous experience of mathematical modelling, 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 realised 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 was 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 co-worker 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 modelling and simulation of electro-chemical activity in large scale cell networks. A geometric model of the canine atria has been constructed utilising ultra sound imaging data and a realistic fibre 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. Colour 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 behaviour 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 predicting 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 Modelling of Human Head Tissues Exposure to Electromagnetic Waves

This research project is concerned with the numerical modelling 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 modelling 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 discretised, 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 modelling (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 specialised 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 modelled 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 discretisation of interfaces between tissues suffer from the so-called staircasing effect, which affects the accuracy of the calculations. This problem is only partially solved thanks to the use of highly refined discretised models and more elaborated numerical methods are required if a realistic modelling is the objective.

#### **Results and achievements**

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



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## 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 support 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.





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## Mathematical Modelling of an Ultrasound Sensor for Bioprocesses

#### **Executive summary**

The focus of this project was to develop further the acoustic component of the mathematical modelling 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 bioprocessing, 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 working in a multi-disciplinary environment involving engineering, bio-processing, mathematical modelling 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 involving 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 employed the second Intern to continue this modelling work and this further underlines the success of the internship.



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