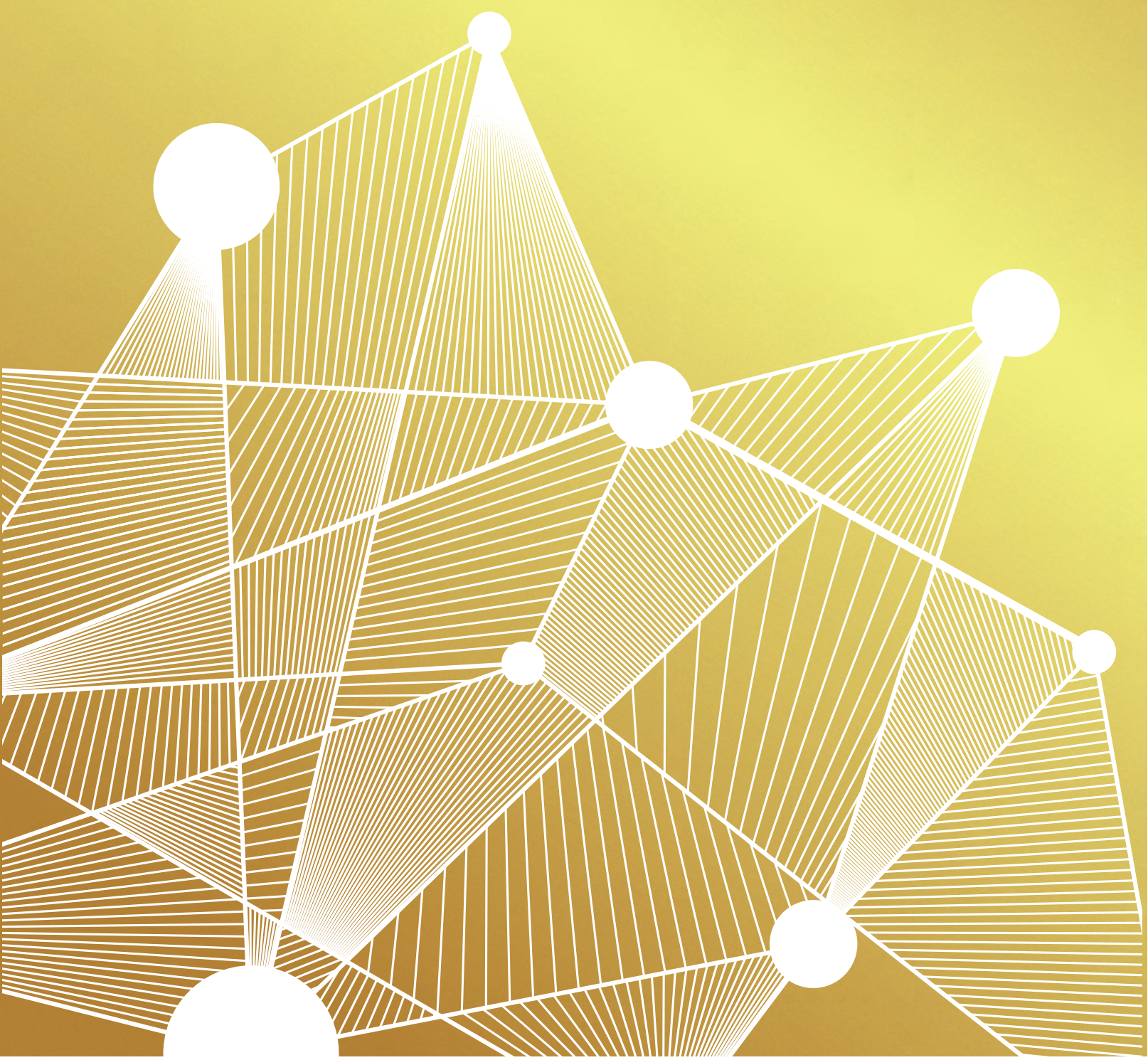
Mathematics with industry: driving innovation

Annual Report 2016



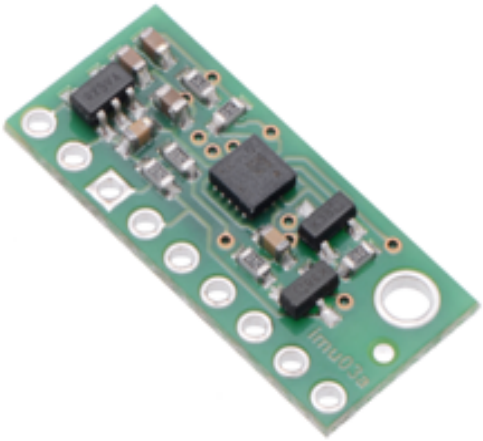
ECMI EUROPEAN CONSORTIUM FOR MATHEMATICS IN INDUSTRY

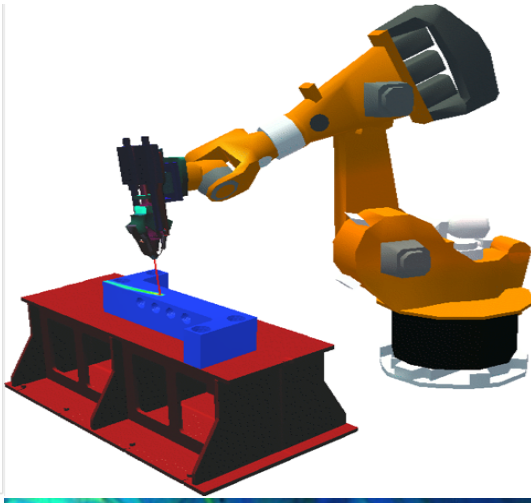
Mathematics with industry: driving innovation

Annual Report 2016

EUROPEAN CONSORTIUM FOR
MATHEMATICS IN **INDUSTRY**


ECMI 2016
June 13-17, 2016 - Santiago de Compostela



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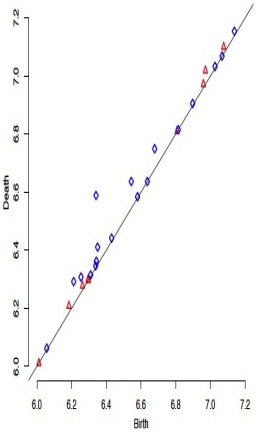
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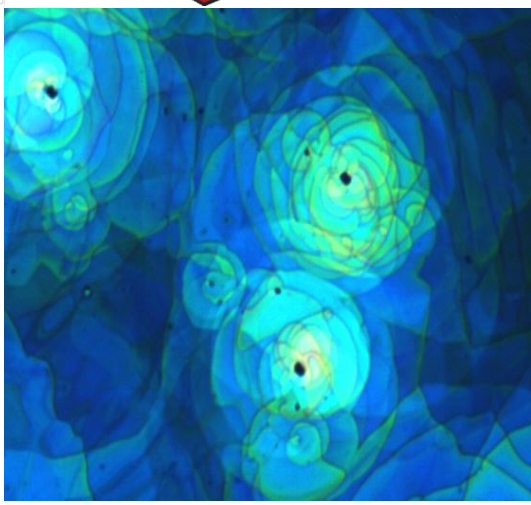
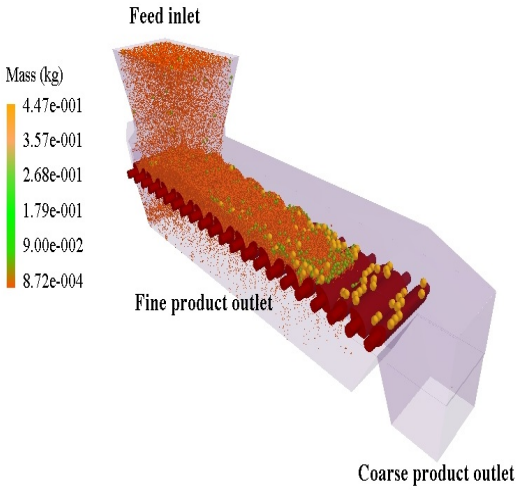
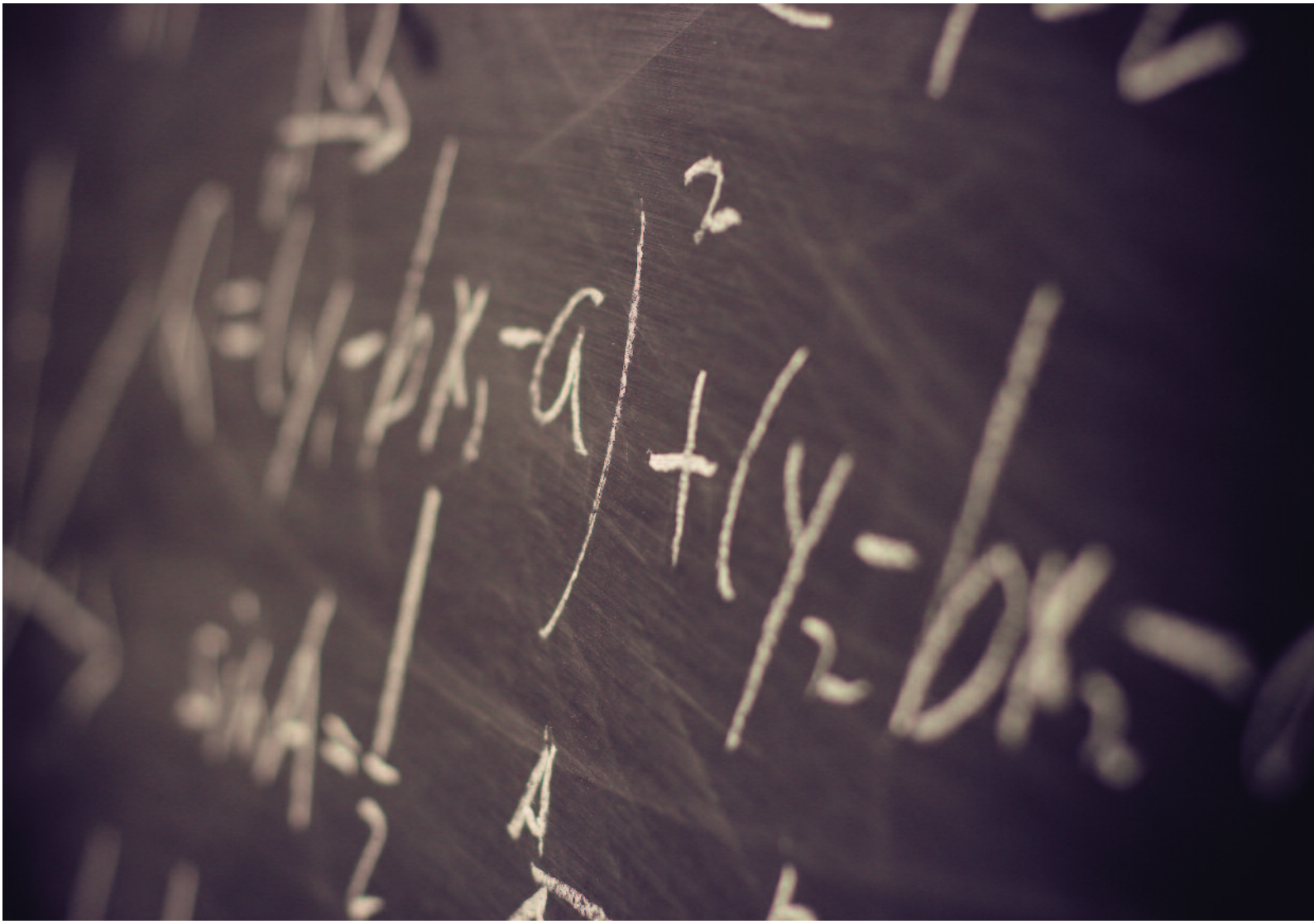


Contents





1

Editorial

Dear Colleagues!

As many of you may have noticed, the former biannual newsletter has been replaced by the annual ECMI report. After the complete redesign of the layout for the first issue which appeared last year, Peter Flynn from Silmaril consultants has now reimplemented the layout into LaTeX classes. As those of you who have contributed to this report have noticed, authors can now utilise the full power of the standard typographic tools that they also use for their daily scientific work.

The second issue closely follows the structure of the first report: The first comprehensive chapter is on recent and upcoming initiatives and activities – this time, we have several articles on the ECMI conference in Santiago de Compostela as well as the modelling week and the ESGI in Bulgaria last year. I want to seize the opportunity to remind you that the next ECMI conference is now less than a year ahead (22 June 2018), and Budapest promises to be a wonderful setting for this highlight in the industrial mathematics academic calendar – see András Bátkai's announcement on p. 21.

People are central to all industrial mathematics – and mathematics in general – so we will have a chapter where we introduce personalities who are active in fields that are important to ECMI, as researchers, networkers or students. I hope you will read the interviews with Aviv Gibali and Joanna Jordan, and Marcin's testimony as as a recent graduate of the ECMI Master programme at Wroclaw University. Moreover, we have a chapter with several articles on a host of interesting projects and case studies which present a small but interesting selection of the wide range of research covered by industrial mathematics today.

About two years ago, the first ECMI special interest groups (SIGs) were founded, and their number has now grown to ten. Do take a look at the reports for each of the current groups, and choose one to network with, or consider starting your own!

As we go through further issues of the report, we will continue to develop its design and content, so please do not hesitate to provide us with feedback, ideas for improvments, and keep on sending us your contributions. We are looking forward to hearing from you!

Andreas Münch, University of Oxford, July 2017

2

Welcome from the President

Dear colleagues,

time flies quickly. While writing these lines I am already in the second part of my term as ECMI president. I took over this duty from Stephen o'Brien in January 2016 and I would like to express my sincere gratitude to Stephen for his work. During his presidency he initiated a number of activities, which helped to shape the future of ECMI, just to mention the new ECMI branding and our new reporting structure with a blog as service to the community of applied and industrial mathematicians in Europe and the new annual report.

In January 2016 Poul Hjorth from Technical University of Denmark started his four year term as ECMI Executive Director. Poul is a well-respected researcher in applied and industrial mathematics and an experienced organizer of study groups. I am really happy that he has accepted our offer. Moreover, Cláudia Nunes Philippart is a new board member. She followed Agnieszka Jurlewicz as head of the ECMI Educational Committee.

Clearly, the most important ECMI event in 2016 was the 19th European Conference on Mathematics for Industry in Santiago di Compostela. You'll find a detailed report by the chair of the organizing committee, Peregrina Quintela in this volume. I would like to thank Peregrina and her team for their excellent organization of a very successful event. In an impressive way ECMI 2016 highlighted the important role of mathematics in strengthening the innovative potential and competitiveness of European industry and economy. I am already looking forward to the 20th conference, which will take place in Budapest from 18 to 22 June 2018. And I am confident that this attractive location will provide an excellent meeting place for applied and industrial maths in Europe.

In 2016 two new and timely *Special Interest Groups (SIGs)* have been initiated. Alessandra Micheletti and Natasa Krejic started a new SIG on *Mathematics for Big Data*. On the interface

between education and research Thomas Götz and Matti Heiliö organize a new SIG on *Virtual Education*. Tim Myers has taken over the burden of coordinating *European Study Groups with Industry (ESGIs)* and keeping track of their numbering. We profit tremendously from close collaboration and financial support by the *Cost Action "Mathematics for Industry Network" (MI-NET)*.

In addition, there were many activities throughout the year, which would deserve mentioning, modelling weeks and further teaching events organized and overseen by the *Educational Committee*, SIG workshops, and a number of European Study Groups with Industry, proving that ECMI indeed is a vibrant organization.

In the second half of my presidency I would like to further strengthen the bond with our institutional members. It seems ECMI is in a sensitive phase of expansion and re-interpretation of the spirit in which it was originally created. We very much welcome new ideas and new initiatives and I would like to encourage you to contact me or any other board member if you have any suggestion, question, ideas, praise or criticism.

Dietmar Hömberg
Weierstraß-Institut and Technische Universität Berlin
July 2017

3

Activities and Initiatives

19th European Conference on Mathematics for Industry (ECMI 2016)

Some highlights of the nineteenth edition of ECMI conferences.

The European Conference on Mathematics for Industry is organized every two years with the aim to reinforce the interaction between academy and industry, leading to innovation in both fields. ECMI conferences also encourage industrial sectors to propose challenging problems where mathematicians can provide insight and new ideas. These conferences are one of the main forums where significant advances in industrial mathematics are presented, bringing together prominent figures from business, science and academia to promote the use of innovative mathematics to industry.

Some outstanding names

The 19th edition of these conferences (ECMI 2016) was held from 13 to 17 June in Santiago de Compostela (Spain), ant it was jointly organized by the Department of Applied Mathematics at the Universidade de Santiago de Compostela (USC) and the Spanish Network for Mathematics & Industry (math-in). The chair of the Scientific Committee was Alfredo Bermúdez (USC, Spain). Co-chairs were, Dietmar Hömberg (President of ECMI, Weierstrass Institute, Germany) and Stephen OBrien (University of Limerik, Ireland). This Committee was also formed by András Bátkai (Eötvös Loránd University, Hungary), Alexander K. Belyaev (Institute of Problems of Mechanical Engineering, Russia), Andrea L. Bertozzi (University of California, USA), Luis Bonilla (Universidad Carlos III de Madrid, Spain), Emilio Carrizosa (Universidad de Sevilla, Spain), L. Pamela Cook (University of Delaware, USA), Patrick Joly (INRIA/CNRS, France), Tuomo Kauranne (Lappeenranta University of Technology, Finland), Tim Myers (Centre de Recerca Matemática, Spain), John Ockendon (University of Oxford, UK), Alfio Quarteroni (EPFL, Switzerland and Politecnico di Milano, Italy), Giovanni Russo (University of Catania, Italy), Otmar Scherzer (Universität Wien, Austria), Barbara Wagner (Weierstrass Institute, Germany) and Graeme Wake (Massey University, New Zealand).

The Organizing Committee would like to address our warmest thanks to the invited speakers: T. Abboud (IMACS, XTEC, École Polytechnique, France), S. J. Chapman (University of Oxford, UK), L. J. Cummings (New Jersey Institute of Technology, USA), L. Formaggia (Politecnico di Milano, Italy), W. González (USC, Spain), M.A. Herrero (Complutense University of Madrid, Spain), B. Kaltenbacher (Alpen-Adria Universität, Austria), P. M. Pardalos (University of Florida, USA), K. Rubinstein (Technion, Israel & Indiana University, USA), and J. M. Teran (University of California, USA) for coming to Santiago de Compostela and contributing to the success of the conference with the high quality of their presentations. We are also greatly indebted to the Scientific Committee for their efforts to select the excellent invited speakers of ECMI 2016.

Group photo at the Gala dinner (forecourt of Hostal dos Reis Católicos).

The program

The ECMI 2016 scientific program consisted of 10 plenary talks by above invited speakers, 40 mini symposia in specific areas covering a wide variety of recent developments, and 19 sessions of contributed talks. In short, it had a total of 306 presentations distributed along 5 days with 8 parallel sessions per day. In these presentations there were, directly or indirectly, involved 49 companies that, in one way or another, have funded the research presented to meet their specific demands. In many cases, success stories from established collaborations with industry were also presented. Special mention must be made to the dissemination event "The mathematical way to the Oscars" which was held in the Auditorium of Abanca, and featured the participation of an invited speaker from academia and two representatives from companies familiar with the use of mathematical technology in movie production. The conference program has also paid special attention to establishing discussion forums in various fields, such as mathematics in the H2020 programme, Master's programmes related with Industrial Mathematics, or Study Groups as a tool for dissemination and promotion of mathematical technology.

Finally, it should be noted that there also was time for relaxing, with a wide social program, which included a welcome reception at Pazo de Fonseca hosted by the Rector of the USC, an excursion to the coast (Rías Baixas), a guided tour of Santiago de Compostela, a gala dinner at the Hostal dos Reis Católicos, and an additional excursion consisting on a hike as part of the Pilgrim's Way to Santiago.

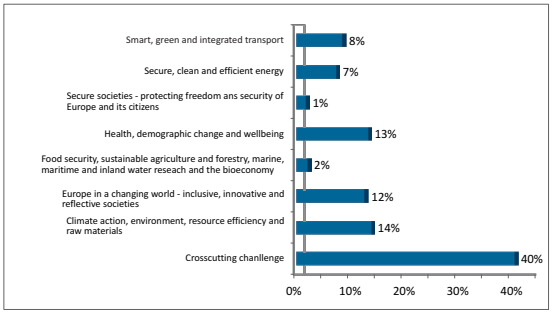

Awards Anile-ECMI (left) and Hansjörg Wacker Memorial (right).

Some numbers

In this 19th edition a wide variety of applications were presented ranging from problems in Electronics (15%), Energy and Environment (14%), Mechanics and Mechatronics (12%), among industrial sectors with the highest number of talks. When classifying the talks according to the societal challenges of the EU Framework Program for Research and Innovation H2020

(see bar chart on the right), 14% of them fell into the challenge Climate action, environment, resource efficiency and raw materials; 13% to the Health, demographic change and wellbeing; while a 12% belonged to the Europe in a changing world - inclusive, innovative and reflective societies.

This edition has counted with 350 participants from 40 countries, involving the five continents. The majority of the attendees came from 26 European Countries but there were also representatives from Australia, America (Canada, Mexico and USA), Africa (Niger, Tanzania and Uganda) and Asia (China, India, Israel, The Philippines and Japan). The European Consortium for Mathematics in Industry (ECMI) has allocated 6 grants covering the cost of registration of participants from third-world countries. These grants were combined with the corresponding Campus Housing grant, funded by the Organizing Committee. Furthermore, the Organizing Committee has assigned three additional grants for students, covering the cost of registration and also the Campus Housing.



Distribution of scientific contributions per societal challenges H2020.

Acknowledgements

ECMI 2016 received generous support from the ECMI, the Universidade de Santiago de Compostela, the Spanish Network for Mathematics & Industry , the Spanish Ministry of Economy and competitiveness, the Naval Research Office of United States of America, the Thematic Network of Mathematics & Industry, the Technological Institute of Industrial Mathematics, and the Galician Network of Industrial Mathematics. It also have had the collaboration of several institutions or companies like GDI, Iberia, Renfe, Springer, Xacobeo Galicia, and Santiago Turismo.

Peregrina Quintela, Patricia Barral, Dolores Gómez, Francisco Pena, Jerónimo Rodríguez, Pilar Salgado and Miguel E. Vázquez-Méndez

Universidade de Santiago de Compostela
Spanish Network for Mathematics & Industry

The Mathematical Way to the Oscars

This article summarizes the outreach event *The Mathematical Way to the Oscars* **held in the framework of the ECMI2016 Conference**

Within the 19*th European Conference on Mathematics for Industry (ECMI 2016)* a dissemination event opened to the general public was organized, under the suggestive title *The Mathematical Way to the Oscars*. This event, held on 14th June at the Abanca Auditorium of Santiago de Compostela, had simultaneous translation. The aim was to show that mathematics is behind the special effects in many films and video games we know.

Picture of the roundtable of the event.

Program of the event

The main conference of this event, *Snow business: scientific computing in the movies and the classroom*, was given by Joseph Teran, Professor of Applied Mathematics at the University of California, and invited speaker of ECMI 2016 conference. Professor Teran showed various mathematical models and the corresponding numerical simulations made by his team in the Frozen film. In particular, how they recreated the movement of snowflakes and the spectacular effects achieved on the film. This research is conducted within the framework of a stable collaboration with the Walt Disney Studios. In his statement to the El País newspaper, Professor Teran indicated that he visited every Thursday the Studios, and met with some of his phd students who work performing simulations of actual behavior of different materials, simulations that recreate virtually after in the movies.

In 2013, Frozen was awarded with the Oscar for *Best Animated Feature* for its adaptation of the story of Hans Christian Andersen, *The Snow Queen*. Snow is an element that combines properties of solids and liquids. As Professor Teran explained in his magnificent conference, the snow is modelled as an elastoplastic, rigid and deformable material at a time, which behaves differently if it is powder or it is compacted, if it is a ball that collides, or it is rolling down a slope. Snow changes when stepping on crunchy ice or sinking into its virgin and fluffy condition; it is not the same the trail that skies leave than the beam left by a snowplow; neither is the destructive weight of an avalanche, nor the snow flakes that freeze again once they have started to melt, nor the way they melt because of the heat. Professor Teran said to the El País newspaper.

In Disney Studios, his team uses polyhedral discretizations which are colored to allow a visual realism, which is greater the smaller they are. Thus, millions of polyhedra are needed to recreate an extreme elasticity as gelatin, the fragility of glass, the drop of cloths, or the movement of each hair in a mane.

As Professor Teran explained to the newspaper La Voz de Galicia, thanks to all the research for the Frozen film, his team created a prototype that Walt Disney uses to recreate mud or sticky substances in their new movies. Professor Teran began these research lines in his thesis stage where he worked for Industrial Light & Magic, the special effects company of George Lucas. They used some of the elements of his work to develop the tentacles of the beard of the fictional villain Davy Jones in the second film of the Pirates of the Caribbean: *Dead Man's Chest*.

After the main conference, a round table was organized in which, besides Professor Teran, Ignacio Vargas and Xenxo Álvarez also participated. Ignacio Vargas is co-founder of the Spanish company Next Limit Technology. He spoke about the *High quality physics in game cinematics*. In his speech he showed some applications made by his company, in particular, to recreate the movement of large bodies of water that appear in films such as *Ice Age*, and the lava of Mount Doom in *The Lord of the Rings*.

Meanwhile, Xenxo Álvarez spoke on behalf of two Galician companies, The Gearing and Ottiplanet, the latter being the responsible for the first 3D feature animation made in Europe, *The Living Forest*, which was awarded with two Goyas. Xenxo Álvarez focused his speech on *Trends in character development for animation and videogames*. *The Mathematical Way to the Oscars* was moderated by the excellent science communicator, Professor of Electromagnetism at the University of Santiago de Compostela, Jorge Mira Pérez.

The event aroused great interest in both the researchers involved in ECMI 2016, as in the rest of the public, being the subject of numerous articles in the media.

Participants at the Abanca auditorium.

Peregrina Quintela

Universidade de Santiago de Compostela

Spanish Network for Mathematics & Industry

30th ECMI Modelling Week: Sofia, Bulgaria, July 17-24, 2016

The 30th ECMI Modelling Week took place in Sofia, Bulgaria, July 17-24, 2016 and was organized by the Faculty of Mathematics and Informatics of the Sofia University.

The event gathered together 54 participants from 14 countries. On the first day, students formed international teams of 5-6 persons each to work intensively during the week on the challenging problems that were posed by instructors from all over Europe. This year, students worked on the following projects:

- Denoising and feature extraction of 2D CT radiographic images;
- Computation of free surface in electromagnetic shaping of liquid metals;
- Design optimization of an electric motor;
- Drug delivery from polymeric contact lenses;
- Investment decisions under uncertainty;
- Modelling an optical tweezers setup;
- Modelling species transport through membrane in haemodialysis;
- Red deer import;
- S-box analysis;
- Volatility stripping in fixed income derivatives.

Then, on Saturday, July 23, each group presented the results from its work in front of all participants, as well as members of the ECMI Educational Committee, who had arrived in Sofia for their traditional meeting. The final reports that the groups submitted after the event can be found on the website of the Modelling Week [1]. As can be seen from them, the collaborations, established during the Modelling Week, were very fruitful and led to some very good results.

Figure 3.1. *Group work during the MW2016.*

A particularly nice example is the fact that

students from Project 1 continued working with their instructor after the event and one of them is expected to present the results at the BGSIAM'16 conference in Sofia in the end of December. Also, a paper is about to be submitted.

Figure 3.2. *Final presentations.*

Besides intensive work, though, there was also time for relaxation and getting to know a little about the Bulgarian culture. On Wednesday evening, everybody was invited to join a traditional Bulgarian line dance, called Horo. Professional dancers led the Horo, while the others were trying to follow the steps.

Horo, a traditional Bulgarian line dance.

On Saturday afternoon, after work was finished, it was time to take the bus and visit the old city of Plovdiv, where after a long walk for sightseeing, the closing reception took place. As in every ECMI Modelling Week, all participants were asked to present their country. Songs, dances, jokes, and games, typical for each country, brought a lot of enjoyment to everybody.

Tour to Plovdiv.

The local organizing committee would like to thank everybody who was involved in the Modelling Week and hopes to welcome again the ECMI Community in Sofia.

Tihomir Ivanov[1]

[1] Sofia University, Bulgaria

References

1. Modelling week 2016. http://ecmimw2016.fmi.uni-sofia.bg/Problems.html.

A Success Story from the Bulgarian ESGIs

The 120th European Study Groups with Industry took place in Sofia, Bulgaria, July 25-29, 2016. This was the fourth consecutive year, in which a Study Group was held in Bulgaria, following ESGI'95 (2013), ESGI'104 (2014), and ESGI'113 (2015).

At the 120th ESGI the participants worked on 7 projects:

1. Multi-frame denoising of still images
2. Optimal cutting problem
3. Authenticity Management Algorithm for Digital Images
4. Laboratory calibration of MEMS rate sensors
5. Future Cyber Attacks Modelling and Forecasting
6. Post-Processing for Beam Elements: Calculating the Second Order Work and Strain Energy
7. Mathematical Model of Residential Storage Water-heating System.

One of the projects, "Laboratory calibration of MEMS rate sensors", happened to be a particularly nice success story, connected with the development of the Bulgarian ESGIs. The background behind this project goes back to the first ESGI in Bulgaria. At ESGI'95, a company, developing software for the cameras of mobile devices, posed a problem connected with three-axial MEMS accelerometer sensors. Those are miniature devices, measuring linear acceleration in three (ideally) orthogonal directions. Because of their low cost, they are widely used for many different applications. In particular, the company was interested in measuring the acceleration of the mobile device, so that the movements can be compensated and video stabilization can be achieved.

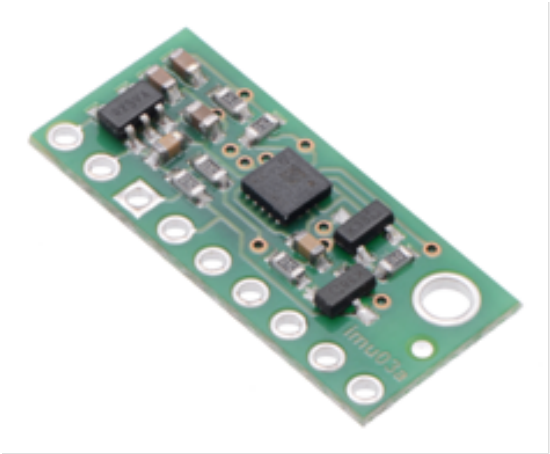


Figure 3.1. *A MEMS accelerometer.*

It is well-known, however, that MEMS accelerometers are subject to different sources of error that should be accounted for, before they can be used in practice.

There are two main types of errors—deterministic and random. The deterministic error sources include the bias (offset) and the scale factor errors as well as non-orthogonality of the axes. The random errors include bias-drifts or scale factor drifts, and the rate at which these errors change with time. Furthermore, all the errors are sensitive to different environmental factors, especially to temperature variations. Thus, the device should be calibrated before it can be used.

The company was interested in an initial calibration to compensate for the deterministic errors. Taking into account the fact that when in still position, the sensor measures only the gravitational acceleration g, the following approach was used.
i) A relation between the raw and calibrated data, depending on several parameters, is defined. Two approaches were tried—a simple linear relation and a physically derived model.
ii) A least squares fit gives the values of the calibration parameters so that the calibrated data is as close to the gravitational acceleration as possible. Details can be found in [1]. The representative of the company expressed his satisfaction of the achieved results and said he is going to incorporate them in the practice of the company.

Even though the project from ESGI'95 did not result in a long-term collaboration, it led to a very unexpected success story. Three years later, in the spring of 2016, a specialist from the borehole drilling industry was facing a very similar problem. In his company, they were trying to build a device, able to measure three angles, determining the orientation of the borehole—toolface, inclination, and azimuth angle. For this purpose, they equipped the device with MEMS accelerometers, magnetometers, and gyroscopes. When facing the issue of calibrating the sensors, they made a search of the literature, that led them to the report from ESGI'95. Thus, a contact was established and the problem was posed at ESGI'120.

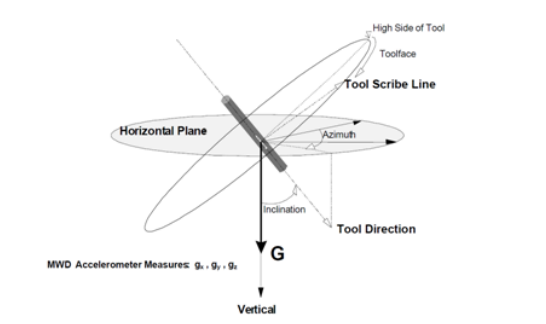


Figure 3.2. *Drilling co-ordinate system.*

During the week, the experience from ESGI'95 was used to calibrate the accelerometer sensors. Adjustments in the algorithm were made, so that accurate results for the toolface and inclination measurements can be achieved. Also, a plan for further development of software for calibrating the device were suggested. The results obtained during the meeting seemed promising to the company, which led to further work. This collaboration is ongoing and involves members of the team that worked on the project during ESGI'120.

Tihomir Ivanov

University of Sofia, Bulgaria

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1. I. Georgieva, C. Hofreither, T. Ilieva, T. Ivanov, and S. Nakov. Laboratory calibration of a mems accelerometer sensor. In *ESGI'95 Problems and Final Reports*, ISBN 978-954-9526-84-4, 2013.

ECMI-Springer cooperation: Mathematics in Industry

ECMI has a longstanding cooperation with Springer, established by our past-president Vincenzo Capasso. This short article aims at providing ECMI members with information on how to exploit this relation when realizing book projects and/or publishing high-quality peer-review research articles.

The ECMI book sub series of *Mathematics in Industry*

15 years ago ECMI has established a cooperation with Springer by creating a sub series of the Springer book series on *Mathematics in Industry*, which focuses on the research and educational aspects of mathematics used in industry and other business enterprises. Relevance to the actual practical use of mathematics in industry is the distinguishing feature of the books in the *Mathematics in Industry* series. It should be mentioned that the overwhelming majority of books in the *Mathematics in Industry series* has been published within our ECMI sub series.

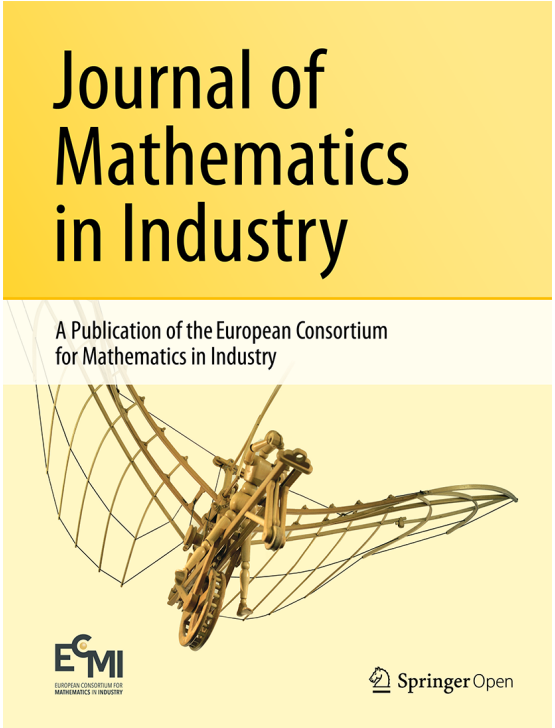
You might know the series only from the ECMI conference proceedings. However, the series has been used quite often to publish monographs of ECMI colleagues reporting on the outcome of huge European projects such as CoMSON (Coupled Multiscale Simulation and Optimization in Nanoelectronics, volume 21) or on recent advances in research topics such as *Meteorological Modelling* (volume 24). In the next months a bunch of books will be published by ECMI colleagues on recent problems in Mathematics in and for industry, for example *Mathematics for the Digital Factory*, *Nanoelectronics Coupled Problems Solutions* or *Novel Methods in Computational Finance*.

If you have a book project in mind, do not hesitate to contact one of the series editors of ECMI: Louis Bonilla, Otmar Scherzer, Wil Schilders or myself.

The ECMI journal on *Mathematics in Industry*

Five years ago ECMI has extended the cooperation with Springer by establishing an ECMI-journal on *Mathematics in Industry*. In terms of theory, and in contrast to

journals with a similar name aiming mainly at case studies, our journal seeks articles with demonstrable mathematical developments motivated by problems of modern industry. With regard to computational aspects, it publishes works introducing new methods and algorithms that represent significant improvements on the existing state of the art of modern numerical and simulations methods.



In 2016, 17 papers have been published. Up to now, the journal is abstracted/indexed in SCOPUS, Zentralblatt Math, Chemical Abstracts Service (CAS), Google Scholar, DOAJ, EI-Compendex, Mathematical Reviews, OCLC, SCImago, Summon by ProQuest and ESCI (Emerging Sources Citation Index). The latter has been especially introduced to cover new journals such as ours before being mature enough to be listed in SCI.

According to the new politics of publishing houses, the journal is based on the open-access paradigm, i.e., publishing costs are realized by article processing charges (APC), while reading is free of charge. Though the open-access policy is strongly supported (or even demanded) by most public funding agencies on a national and European level — and increases the accessibility and possibly number of citations, it is quite new to the (applied) mathematics community. To overcome the possible hesitation to publish within our journal due to its open access policy, the ECMI board is currently negotiating with Springer to find an easy way to waive the APCs for ECMI members. Until this agreement has not been reached, please contact me as editor-in-chief to get the APC waived for you as ECMI member, if the APC is not waived anyway: it might not be commonly known that for many authors the APCs are waived through their home institution being a SpringerOpen member or are covered by the public funding agencies as part of the funding.

Michael Günther

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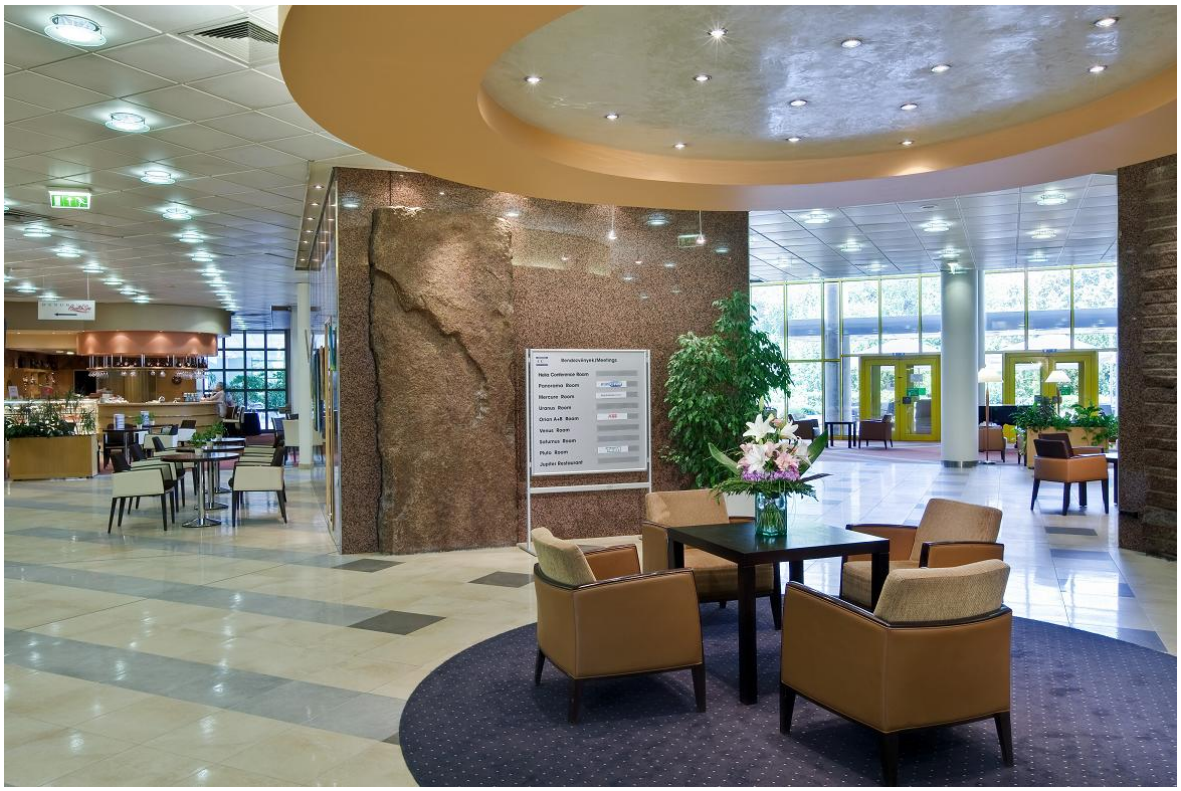
Coming up soon: ECMI 2018!

We are proud to announce the 20th European Conference on Mathematics for Industry, to be held in Budapest, 18–22 June 2018.



The series of ECMI conferences are devoted to enforce the interaction between academy and industry, leading to innovation in both fields. These events attract leading experts from business, science and academia, and promote the application of innovative mathematics to industry. They also encourage industrial sectors to propose challenging problems where mathematicians can provide insight and new ideas.

The 20th ECMI conference will be jointly organized by the János Bolyai Matheamtical Society, the Institute of Mathematics at Eötvös Loránd University and the Hungarian Academy of Sciences Institute for Computer Science and Control. It follows tremendously successful conferences in Santiago de Compostela 2016 (notice the articles in this report), Taormina 2014, Lund 2012, Wuppertal 2010, and London 2008. The conference will focus on various fields of industrial and applied mathematics, including

- Applied Physics
- Biology and Medicine
- Cybersecurity
- Data Science
- Economy, Finance and Insurance
- Energy
- Production Systems
- Social Challenges
- Vehicles and Transportation

The conference venue will be at the Danubius Health And Spa Resort Hotel Helia, which is a conference hotel with spa and wellness complex on the bank of the Danube, opposite Margaret Island offering world-class facilities and services.

Participating in the conference will give a great opportunity to visit Budapest, one of the world's great capitals, a magnificent city on the Danube that combines past-century charm with modern comfort and vitality.

The conference registration will open in the fall 2017.

András Bátkai

Eötvös Loránd University

4

Featured People

Interview: Aviv Gibali

Tell us about yourself: what is your background and training?

My name is Aviv Gibali and I define myself as an industrial mathematician. I finished my PhD in 2012 (Department of Mathematics, The Technion - Israel Institute of Technology, Haifa, Israel) under the supervision of Prof. Simeon Reich and Yair Censor.

My Dissertation: Algorithms for Solving Variational Inequalities and Applications Afterward, between 2012-2014, I did my postdoctoral studies with the Optimization Department of The Fraunhofer Institute for Industrial Mathematics (ITWM), Kaiserslautern, Germany. There I received the opportunity to be involved in industrial projects in fields such as Radiation Therapy, Gemstones Cutting, and Image reconstruction.

My research area is devoted to Mathematical theory and the development of iterative algorithms for solving systems of nonlinear equations and inequalities. I am mainly focused in applying my techniques in Radiation Therapy Treatment Planning and Image Processing.

Where are you currently employed?

I am a Senior Lecturer (starting my third year) with the Mathematics Department of ORT Braude College in Karmiel, Israel. I am also a research associate with the Center for Computational Mathematics and Scientific Computation (CCMSC), University of Haifa, Haifa, Israel.

How did you get involved in doing industrial mathematics?

While completing my master degree at the Mathematics Department of the University of Haifa, I was introduced to the field of Intensity-Modulated Radiation Therapy (IMRT) treatment planning by my supervisor, Prof. Yair Censor who is one of the leading experts in this field. This already proved to me the strength and abilities of mathematics to real-world problem. Later, in Fraunhofer ITWM, I was given the chance to work on real industrial problems guided by the head of the Optimization Department Prof. Dr. Karl Heinz Küfer.

How did you get in touch with ECMI?

While still in Fraunhofer ITWM, I had the great pleasure to meet in person Prof. Dr. Helmut Neunzert who told me about the ECMI activities and also encouraged me to publish in one of its journals, Journal of Mathematics in Industry. In 2013 I also organized a workshop titled: "Projection methods, Theory & Practice" in which I brought together industrial and mathematician to collaborate.

Since 2015 I am a management committee member of the COST Action TD1409 Mathematics for industry network (MI-NET). While attending the annual meetings I was given the opportunity to meet various persons who play active roles within the ECMI. These are also the reasons I decided to represent ORT Braude and become a ECMI member.

What are current and upcoming activities for Industrial Mathematics in Israel?

My agenda is that mathematics is the key to any solution and is not a luxury, but a vital necessity in the industry and in general. I am trying to promote mathematical education and its strength on all levels, from elementary school to higher education. I give lectures in schools regarding the important role mathematics has in everyday life and how it can be found anywhere. I show that there is such an occupation called mathematician. I am working on establishing a mathematical club in Braude for elementary pupils in which we'll try to show them helpful mathematical things "beyond the numbers".

For high-school mathematics teachers, I am organizing a workshop on November 21, 2017, in which we'll emphasize the importance of mathematics and all the things that it can do in real life. My belief is that if we'll convince these teachers that mathematics is a very important tool for solving real-world problems, then, they will train their pupils in a better way to become aware of the need of mathematics and its applications to Industry.

I am co-organizing with Dr. Yirmeyahu Kaminski an Industrial Workshop at the Holon Institute of Technology (HIT) on June 29, 2017. Between 2-6 of July, 2017, I am organizing a Modelling Week for the first time in Israel.

These two activities are sponsored by the MI-NET and other European and Israeli companies and organizations.

What special opportunities, and challenges, do you see for industrial mathematics in Israel?

In Israel, the big challenge is to convince people from all sectors that as industrial problems become more and more sophisticated, there is a necessity to rely heavily on mathematical modeling and understanding, and that mathematics is not just for teaching! Organizing joint events between mathematicians and industrials creates internships for mathematics and have better marketing, are all essential tools to increase the awareness for the applications of mathematics to industry!

Interviewed by Prof. Poul G. Hjorth

Technical University of Denmark, Lyngby, Denmark

Interview: Joanna Jordan

Describe your role (manager of Bath IMI/ Chair of MI-NET) in three words.

Enabling industrial mathematics.

What are the key projects you're involved with at the moment with the Mathematics for Industry Network?

A key goal of MI-NET is to share best practice of academic-industrial interaction (e.g. Study Groups with Industry) more widely among mathematicians across Europe. I was thrilled that MI-NET could enable the first ever Study Groups in Italy and Cyprus in 2016, and the first ever Israeli Modelling Week for postgraduate students is taking place this week (July 2017).

What excites you about your current role with Bath IMI?

The thing that most excites me about my current role in Bath IMI is our ability to react quickly and flexibly to a wide range of new opportunities. I've built a team of experienced mathematical and statistical modellers, whom we call Commercial Research Associates, who work on small-to-medium projects - from industry and other disciplines - with the intellectual support of academics from different departments across campus.

What does an 'average day' look like for you?

In leading IMI's commercial activities and day-to-day operations, no two projects are alike, so my role changes daily. I am very fortunate to work with a wide variety of different people, including a very talented team, and there is no average day!

Your role sits between academia and industry – what attracts you about this area?

What excited me about this area is the opportunity: mathematics can address problems of real social and economic value. I love working with people, and working at the interface is all about building and developing strong relationships.

What challenges do you face? Can you give any specific examples?

I think one major challenge facing industrial mathematics, and anyone who works in the area, is recognition and respect within the academic community. I recall one colleague, who shall remain nameless, saying he felt sorry for me because industrial mathematics was a bit like cleaning the toilet: very worthy, but he didn't want to do it!

In 2011, you finished a post-doctoral position and moved to a managerial position at the University of Limerick – what prompted the move? Do you miss being a researcher?

In 2011, I paused a two-year fellowship from the Irish government to take up a short-term role as manager of MACSI, the Mathematics Applications Consortium for Science and Industry, as I firmly believed that I could make a positive difference in this type of outward-facing role. Within a few days, I was hooked. Six months rapidly turned into three years, during which I led a major effort to strengthen and formalise relationships with industry partners, creating a culture of Knowledge Exchange, and securing several million Euros of grants for MACSI. I do not miss being a researcher - I never returned to my fellowship! Instead, the experience I gained in MACSI has inspired the kind of work I want to do for the rest of my career. I draw on my mathematical training and research experience every day, and by enabling new projects I can personally make a bigger impact.

What would you say is the most interesting/ enjoyable research you have been involved with and why?

I've been fortunate to be involved in a wide range of projects from brewing a better cup of coffee to improving modelling of typhoons. I think the most rewarding project I've been involved with to date is the collaboration between MACSI and Aughinish Alumina. As the first industrial project I set up, it will always hold a special place in my heart, and it was fantastic that MACSI was able to develop an algorithm – now in daily use - which resulted in a 200% increase in the accuracy of product quality predictions. This initial piece of work has also led to a long-term relationship, and several projects involving different aspects of the manufacturing process.

What do you look for when deciding whether to get involved in a new project or engagement with industry?

I look for the benefit that mathematics can bring to the project, as well as the potential for a long-term mutually-beneficial relationship. Some people are really supportive of the role that mathematics can play in industry. Having a champion within the company makes a real difference.

How do you see the future of Applied Mathematics in Europe?

I would like to see the future of Applied Mathematics in Europe as less silo-ed and more joined up. Real-world problems are frequently multi-faceted, and require an interdisciplinary approach often including both modelling and statistics.

What changes would you like to see in the culture of applied mathematics in academia?

I would like to see industrial mathematics become a more widely respected field.

It's not for everyone and that's fine, but it's nice to see people who haven't done any before when they work on their first project, really get stuck in and get a bit of a taste for it.

In my experience, successful industrial mathematics requires a wide breadth of knowledge. Unfortunately, the current academic promotion system rewards tightly-focused research portfolios. In my opinion, polymaths are integral in connecting different areas of mathematics to tackle important challenges; new reward schemes are needed to encourage these talented individuals to engage in knowledge exchange activities and remain in academia. There's more now than there has been, but not as many as there's room for. I would also like to see structured career paths for mathematics knowledge exchange professionals!

...and in industry?

I frequently encounter potential partners who are pleasantly surprised that their problems can be cast precisely and solved using mathematics. Despite successes in fields such as engineering, there are others in which the mathematical approach has yet to be fully developed, including agriculture and some areas of social science. I would like to see more of an understanding of the process of mathematics generally; as a logical approach to be applied to problems. It would be wonderful if industrialists thought of mathematicians as their first port of call when tackling new challenges.

What do you mean when you say 'knowledge exchange professionals'?

They go by lots of names; technology translator, industry liaison, business development... A role that bridges the gap between industry and academia.

And finally... if you could do any (other!) job for a day, what would it be?

Vice Chancellor of a major research intensive university - in a day I could meet all Pro-Vice chancellors and Deans to extol the benefits of working with mathematicians! I wouldn't want to be VC for any longer than a day!

Interviewed by Melanie Beckerleg

University of Oxford, UK

Master in Techno-mathematics: A testimony

Marcin Michałowski recently completed his studies in the ECMI educational programme at Wrocław University of Technology. Here is what he has to say about the experience.

After I had finished my first degree studies in Mathematics at Wrocław University of Technology (WUT) I faced a choice: what to study as my master degree. My faculty offered two options – Mathematics (in Polish), which was believed to be more theoretical, or studies according to the ECMI educational programme (in English), more focused on applications of mathematics. My decision to go for the ECMI studies was based on my interest in applied mathematics, the positive feedback from older colleagues, as well as on the fact that the studies were led in English. Facing the same decision now, my choice would not be different.

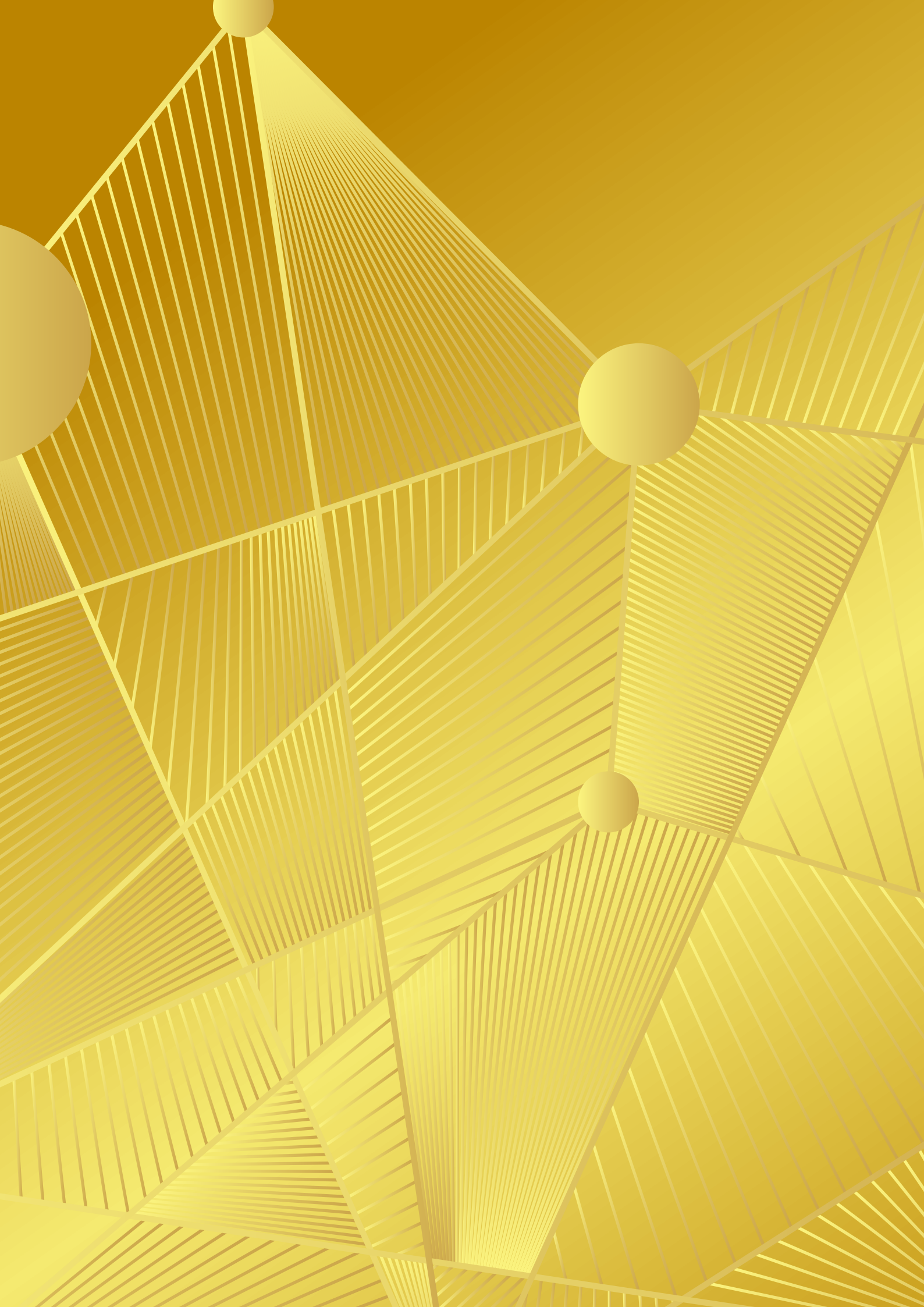
In addition to the above, the studies in ECMI programme made it easier to go on an Erasmus exchange. Due to the collaboration between ECMI centres I found out about Lappeenranta University of Technology (LUT) and that it could be an exciting Erasmus destination. As the programmes on both Universities are more or less aligned, the exchange did not delay the completion of my studies and proved to give a very interesting insight on how the same subjects may be taught differently around the world.

Another opportunity I had, and took, during my studies was to participate in a MODCLIM. The Modelling Clinic for Industrial Mathematics was a program consisting of 2 weeks of intensive courses held at the University of Las Palmas, followed by a remote project I worked on with people from Spain, Poland, Germany and Russia. The last part of the programme – a Modelling Week – was held in LUT, during my Erasmus exchange there. MODCLIM was a great chance to broaden the specialist knowledge and to get to know people working in the same field around the world. On top of that, it allowed me to see interesting places in the world.

My two years ECMI master degree studies were full of exciting courses spread across 3 Universities, full of remarkable people – both academia staff and my fellow students – and left me with great knowledge and memories. On top of that, having such studies in your curriculum opens up a lot of career perspectives.

Marcin Michałowski

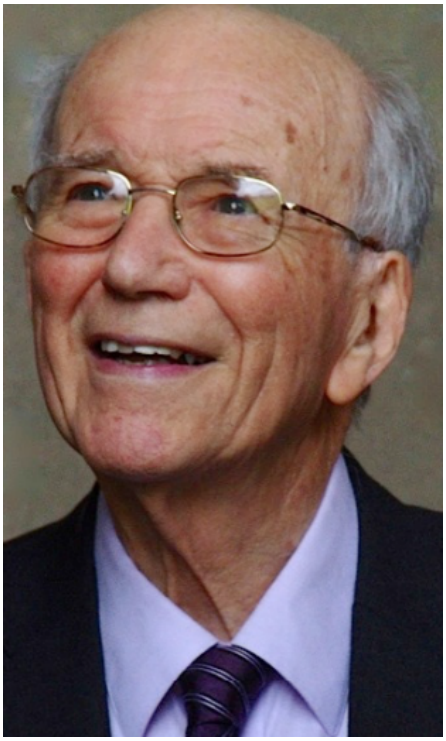
Wrocław University of Technology, Poland



5

Orbituary

Donald Cecil Pack



14 April 1920 – 3 December 2016

On the instigation of Professor Helmut Neunzert, and by the unanimous decision of the British and Irish contingent of the ECMI Board, Professor Donald Pack was awarded the first Honorary Membership of ECMI during the European Conference for Mathematics in Industry in 1988, held at his old university in Glasgow, the University of Strathclyde.

During and soon after the war, Donald carried out pioneering research on acoustic waves in metals that have been deformed well-beyond their yield strengths and his work is gaining increasing recognition in this century.

After 1945, Donald was given the rank of Captain and, as a prominent member of a group, he was tasked with finding out what he could about German Science. He recalled flying from the Royal Aircraft Establishment in a Savoia Marchetti, a three-engined Italian medium bomber, that had been part of Mussolini's fleet. This made a big impression on him as it was his first flight. With his kindly manner and his ability to speak German, he not only learned a great deal about German Science but he also struck up genuine friendships; this experience made him a convinced European and a great Europhile. His first contact with German Mathematicians was with Professor Erhard Meister at TU Darmstadt whom he met in 1963: this led to annual visits; another of his collaborators was Professor Frank Speck, currently professor Emeritus at the University of Lisbon. In the 1970s he met Helmut Neunzert and Kaiserslautern became his second "home" with annual visits thereafter. His long collaboration with Professor Neunzert led to the organisation of five conferences on transport theory and the kinetic theory of gases at the Mathematisches Forschungsinstitut in Oberwolfach. Throughout his career, Donald received many invitations to visit leading universities (particularly in Germany and Italy) where he gave plenary lectures related to his research.

As the celebration of his life by his colleague, Professor Adam McBride, makes clear, (https://www.rse.org.uk/wp-content/uploads/2017/02/Pack_DC.pdf), he was an archetypal Industrial Mathematician long before the foundation of ECMI. Indeed, Alan Tayler, who was one of the founders of ECMI, often stressed how important Donald's encouragement had been when he was setting up the Oxford Study Groups with Industry programme in 1968; these study groups later evolved into ESGI.

Sean McKee
University of Strathclyde
Founder Member of ECMI

6

Projects and Case Studies

Drug delivery from ophthalmic lenses

This article aims to contribute to the mathematical modelling of drug release from a device - the therapeutic lens - to the anterior chamber in the presence of a glaucoma. A brief description of the physiology of the anterior segment of the eye as well as the dynamics of the aqueous humor, the main contributor in the open-angle glaucoma, will be presented. Recent advances in therapeutic strategies to treat the open-angle glaucoma are also presented focusing on ophthalmic therapeutic lenses. The mathematical description of the drug release from a lens containing drug in different states and its transport until the target tissue, is established. Some results illustrating the drug distribution are also included.

Introduction

Glaucoma is one of the most common diseases and is a consequence of disorders in the anterior segment of the eye. It is the result of anomalies in the aqueous humor dynamics that lead to increasing intraocular pressure (IOP). This pressure pushes the lens and consequently, the vitreous humor, inducing a pressure on the retina. It can lead to damaging of the optical nerve with subsequent vision loss. In extreme situations, it can even lead to blindness.

The mathematical modelling of drug delivery from a device and its transport until the target tissue requires the knowledge of the physiology of the eye, mainly (i) the anterior segment (ii) the dynamics of the aqueous humor, responsible for such anomalous pressure. The increase in IOP is due to an increase of the resistance to the fluid outflow, an increase of the aqueous humor production or even both. It is necessary to identify the physiologic processes involved in aqueous humor production and in its drainage.

Therapeutical contact lenses is one of the drug delivery devices used to treat high IOP. Different drugs have been considered depending on the pathology that leads to IOP increasing: (i) *beta blockers* and *carbonic anhydrase inhibitors* reduce eye pressure by decreasing the production of intraocular fluid; (ii) *prostaglandin analogs* induce a reduction of IOP, diminishing the resistance to aqueous humor outflow; (iii) *alpha agonists* induce a decrease in the production of fluid and also increase the aqueous humor drainage.

This article aims to contribute to the mathematical modelling of drug delivery from therapeutical contact lenses to treat glaucoma. We start by presenting the

anterior segment of the eye and the dynamics of aqueous humor. The set of anomalous situations that lead to increasing intraocular pressure is then described. An overview on some therapeutic strategies that can be used to treat open-angle glaucoma is presented. The main part of this work concerns a mathematical model that describes the drug release from therapeutic lenses and its evolution in the cornea and anterior chamber. To simplify, the model is built under some assumptions on the phenomena involved as well as on the geometry of the anterior chamber.

Anterior segment of the eye and aqueous humor dynamics

Glaucoma is a group of diseases that lead to the damage of the optical nerve and it is usually associated with an increase of the IOP. This increase is due to pathological modifications of the physiology of the anterior segment of the eye, see Figure 1. This part of the eye is composed by the cornea (the outer boundary), the anterior chamber, the iris, the lens and the ciliary body that define the anterior boundary of the anterior chamber. The cornea is composed by several layers: (i) the epithelium (the outer layer); (ii) the stroma; (iii) the endothelium (the inner layer). It is coated by a tear film known as precorneal film, see Figure 1 (source: `theeyecenter.com`).

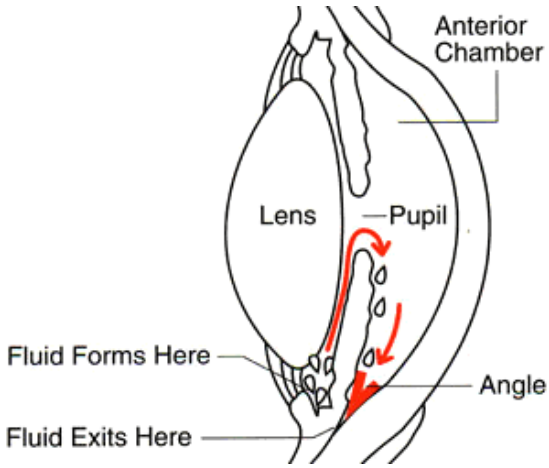


Figure 6.1. *Anatomy of the eye*

The anterior segment of the eye is filled with the aqueous humor. This clear watery fluid is produced by the ciliary epithelium of the ciliary processes located in the ciliary body. It flows from the posterior chamber to the anterior chamber by the narrow space between the posterior iris and the anterior lens and enters in the anterior chamber by the pupil. The aqueous humor leaves the anterior chamber mainly through the trabecular meshwork. It reaches the episcleral venous system via Schlemm's canal. It is also drained from the anterior chamber by the uveoscleral route. The aqueous humor has a multi-purpose nature, see [1]: (i) provides nutrients to the avascular tissues of the anterior segment; (ii) removes metabolic excretory products; (iii) stabilizes the ocular structure; (iv) contributes to the homeostasis of these tissues.

Two main factors contribute to aqueous humor flow: (i) the pressure difference between the trabecular meshwork, that induces a resistance to the outflow (porous structure), and the end of Schlemm's canal, which is similar to the blood pressure (8-10 mmHg); (ii) the temperature difference near the cornea and lens. Two convective flows are then induced that are driven by a pressure gradient and a temperature gradient. The balance between the aqueous humor production and its drainage maintains the IOP stable. The drainage through the uveoscleral route appears to be pressure independent, see [2].

Glaucoma

Optical nerve damaging is usually induced by an increase of the IOP. Such increase can be induced by several physiological modifications of the anterior chamber: (i) the blockage of the flow canal defined by the lens and the iris tissue; (ii) an anomalous production of the aqueous humor; (iii) the damage of the trabecular meshwork tissue

or Schlemm's canal structure, that increase the resistance to the aqueous humor outflow. While in the first case the pathology is usually called *closed-angle glaucoma*, in the second and third cases this pathology is usually called *open-angle glaucoma*. The *closed-angle glaucoma* can be induced by different causes that influence an iris dilation and its adheration to the lens.

The aqueous humor is produced in the ciliary body involving complex phenomena that include ultrafiltration, diffusion and active transport (active secretion). The ultrafiltration occurs in the capillaries of the ciliary processes and it is a passive movement of water and water soluble substances across cell membranes, diffusion of solute takes place in the tissue between the capillaries and the posterior chamber in response to concentration gradient. Active transport occurs in nonpigmented epithelial cells and it is the main responsible for the aqueous humor formation, see [2, 3]. An abnormal production of the aqueous humor can lead to increased IOP.

In the human eye, 75% of the resistance to the fluid outflow is due to the trabecular meshwork and 25% occurs beyond the Schlemm's canal. Trabecular meshwork's resistance to the drainage of aqueous humor is due to the hydration of the trabecular meshwork structure that can cause obstruction of its structure. Such obstruction is also associated with the formation of deposits within this tissue. Recently, the region of the trabecular meshwork that is responsible by the IOP regulation was identified: the *juxtacanalicular tissue*, which is adjacent to Schlemm's canal. To keep the aqueous humor flow channels open in the juxtacanalicular tissue, the extracellular matrix of this tissue presents a continuous remodelling. An interference in this remodelling process compromises the aqueous humor drainage and increases the IOP, see [4].

The hypothesis that the biomechanical properties of Schlemm's canal contribute to the aqueous humor outflow was studied, for instance, in [5, 6]. It was observed that the pore formation is a mechanosensitive process: an increase of the biomechanical strain induces an increase of the porous density. Changing this biomechanical behaviour, it was observed that the porous formation decreases, leading to increased IOP.

Therapeutics strategies to open-angle glaucoma

To decrease the IOP it is necessary to attack the anterior segment of the eye fortress and introduce drugs in the anterior chamber. This fortress is defended by the *tear fluid barrier*, the tear film that coats the corneal epithelium, the permanent blink, the cornea (lower impermeable structure) and the blood-aqueous barrier. Eye drops are the most used ocular route to administer drugs. However the drug bioavailability in the anterior chamber is very low. The tear film turnover is one of the main contributors to this fact. The drug residence time in the corneal epithelium is equal to 5-6min before being completely washed way. The permanent continuous blinking removes the mixture of drug solution with tear fluid from the corneal epithelium to the nasolacrimal ducts.

The low permeability of the corneal layers also contributes to the reduced amount of drug that reaches the anterior chamber. Less than 5% of the drug present in the eye drops reaches the ocular tissue. The use of the systemic rout to delivery drug into the anterior segment of the eye is also very inefficient. In fact, the blood-aqueous barrier restricts the entry of drugs from the blood stream into the posterior segment and consequently, to the anterior chamber.

The poor eye drug absorption requires repeated applications during long periods to achieve drug concentrations in the anterior chamber within the therapeutic window.

Different drugs have been used to decrease the IOP and they depend on the specific pathology. For instance, if the increased IOP is due to an anomalous production of aqueous humor, β-blockers, α-agonists and carbonic anhydrase inhibitors lead to decreasing of aqueous humor inflow. Other approaches use prostaglandin analogs to enhance the uveoscleral outflow or muscarinic agonists to enhance the trabecular outflow, see [7].

Several approaches have been followed to avoid the limitations of classical topical administration, like, for instance, the use of viscosity enhancers, mucoadhesive and lens which aim at increasing the drug corneal residence time. Other strategies, like the use of penetration enhancers, prodrugs and colloidal systems aim to increase the corneal permeability, see [8]. The purpose of such strategies is to delivery drug into the anterior chamber at a sustained and controlled rate complying the drug concentration in the target tissue to therapeutic window .

Since the nineties, several types of therapeutical contact lenses have been proposed by researchers to increase the drug residence time in the cornea. Without being exhaustive we mention

- (i) soaked contact lenses, see [9];
- (ii) compound contact lenses with a hollow cavity, see [10];
- (iii) entrapment of proteins, cells and drugs by polymerization of hydrogel monomers, see [11];
- (iv) biodegradable contact lenses, see [12].

We remark that the corneal drug residence time for soaked lenses increases (it is around 30 minutes) by increasing the drug bioavailability. However, such increase is not significantly high because there are no barriers to the delivery and the loading is limited by the drug solubility. Compound lenses with hollow cavities as drug reservoirs present lower permeability to oxygen and carbone dioxide. In the polymerization process the drug can loose its therapeutic characteristics, see [13].

To delay the drug delivery process such that the corneal drug residence time and loading increases, several authors propose to encapsulate the drug in polymeric particles that are dispersed in the lens, see [14, 15, 16, 17]. In this case, the drug can also be dispersed in the polymeric structure leading to increasing drug loading. Such drug can be in three states in the polymer: free, bounded or encapsulated. The dispersed drug, when in contact with the tear fluid, is immediately released followed by the delivery of the bounded drug. The release on the encapsulated drug is delayed by the particles structure and the corneal drug residence time increases significantly. One of the main advantages of such devices is the possibility to build lenses that deliver the drug with a pre-defined profile.

Mathematical modelling of drug delivery from therapeutic lenses

Building a mathematical model that describes the drug delivery process from a specific device and its transport to the target tissue is a complex work that requires different tasks. Let us consider the case of a therapeutic lens used to treat open-angle glaucoma, that is to deliver a specific drug in the anterior chamber to decrease IOP. Different tasks can be identified in the mathematical modelling of this drug delivery process.

The drug release and transport involves a set of complex phenomena presented before:

- the drug release from the polymeric structure;
- its clearance by the tear turnover;
- the drug transport through the different layers of the cornea;
- the drug transport and its drainage by the aqueous humor;
- the dynamics of the fluid, which includes the aqueous humor production in the ciliary body, its transport in the posterior chamber and in the anterior chamber, its drainage through the trabecular meshwork and uveoscleral route, and its transport in the Schlemm's canal.

It should be remarked that a mathematical model describing all phenomena taking place will be very complex and its numerical simulation will be a very difficult task. Therefore it is necessary to identify the main phenomena involved and the spatial domains were they occur.

The drug delivery from a lens and its transport in the anterior chamber is naturally a three dimensional problem. However, to simplify the geometry of the domain we reduce the domain to a two dimensional one using the symmetry of the anterior segment of the eye and lens. We remark that in [18] the mathematical model is defined in bounded intervals for the lens and cornea and the anterior chamber was considered as a sac with passive role in the process. The mathematical models introduced in [19, 20] were defined in a two dimensional domain and the influence of the aqueous humour motion was taken into account. It is assumed that the fluid enters the anterior chamber through the space between the iris and the lens that we denote by $\Gamma_{ac,i}$, see Figure 2, and it is drained through the trabecular meshwork.

The tear turnover and the uveoscleral drainage were neglected, the aqueous humor production is not explicitly considered as well as its transport through the trabecular mesh until the Schlemm's canal. The last transport is described by a condition on the flux that leaves the anterior chamber through $\Gamma_{ac,tm}$. The aqueous humor production is described by a boundary source term specified at the fluid entrance $\Gamma_{ac,i}$. These assumptions allow us to consider the domain plotted in Figure 2.

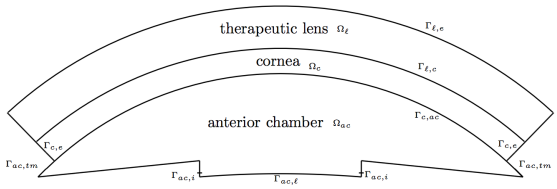


Figure 6.2. *Spatial domain*

We point out that the properties of the polymer used to construct the lens and particles entrapping the drug should be provided. We assume that the drug is dispersed in the polymeric lens presenting three different states, free, bounded and entrapped, while the cornea is composed by a single layer.

Let Ω_ℓ, Ω_c and Ω_{ac} denote the lens, the cornea and the anterior chamber, respectively. By c_f, c_b and c_e we denote the free, bound and entrapped drug concentrations (g/m^3). In what follows we specify the phenomena and their mathematical laws in each domain:

- Ω_ℓ - In the lens three different phenomena occur: the links between the polymeric chains and the drug molecules break and the bounded drug is converted in free drug that diffuses. Let $\lambda_{b,f}, \lambda_{e,f}$ be the transference coefficients ($1/s$) between bounded and free drug and entrapped and free drug, respectively, and $\mathbf{D}_{f,\ell}$ denote the free drug diffusion tensor (m^2/s). Then the

behaviour of the free and bound drugs is described by the diffusion equations

$$\begin{cases} \dfrac{\partial c_f}{\partial t} = \nabla \cdot (\mathbf{D}_{f,\ell} \nabla c_f) + \lambda_{b,f}(c_b - c_f) \\ \qquad\qquad + \lambda_{e,f}(c_e - c_f), \\ \dfrac{\partial c_b}{\partial t} = -\lambda_{b,f}(c_b - c_f), \\ \dfrac{\partial c_e}{\partial t} = -\lambda_{e,f}(c_e - c_f), \end{cases} \tag{6.1}$$

in $\Omega_\ell \times (0, T]$, where $T > 0$ denotes a fixed time.

- Ω_c - Only the free drug is released from the lens and enters in the cornea where it diffuses. If $\mathbf{D}_{f,c}$ represents the free drug diffusion tensor in the the cornea then

$$\frac{\partial c_f}{\partial t} = \nabla.(\mathbf{D}_{f,c} \nabla c_f) - \lambda_c c_f \tag{6.2}$$

in $\Omega_c \times (0, T]$. Equation (6.2) is established assuming that the clearance of the drug occurs here being λ_c the clearance rate $(1/s)$.

- Ω_{ac} - In the anterior chamber the free drug diffuses and its transported by the aqueous humor to the trabecular meshwork. The evolution of c_f is described by the following convection-diffusion-reaction equation

$$\frac{\partial c_f}{\partial t} + \nabla(\mathbf{v} c_f) = \nabla.(\mathbf{D}_{f,ac} \nabla c_f) - \lambda_{ac} c_f \tag{6.3}$$

in $\Omega_{ac} \times (0, T]$. In equation (6.3), $\mathbf{D}_{f,ac}$ and λ_{ac} $(1/s)$ represent the drug diffusion tensor and the drug clearance rate in the aqueous humor. As the aqueous humor is mainly composed by water, and its dynamics is mainly driven by the IOP, the velocity field $\mathbf{v}$ can be described by the incompressible Navier-Stokes equations

$$\begin{cases} \rho \dfrac{\partial \mathbf{v}}{\partial t} + \rho(\mathbf{v} \cdot \boldsymbol{\nabla})\mathbf{v} - \nu \boldsymbol{\Delta} \mathbf{v} + \nabla p = \mathbf{0}, \\ \qquad\qquad\qquad\qquad\qquad\qquad \nabla \cdot \mathbf{v} = 0, \end{cases} \tag{6.4}$$

in $\Omega_{ac} \times (0, T]$. In system (6.4), p represents the intraocular pressure, ρ the density of the aqueous humor and ν its kinematic viscosity.
The velocity field $\mathbf{v}$ is time and space dependent if the drug molecules have a therapeutic effect in the trabecular meshwork. Otherwise the velocity does not change in time and then the system of equations (6.4) should be replaced by steady Navier-Stokes equations.

The boundary conditions are specified now. We start by defining the boundary conditions for drug concentration:

- Let $\Gamma_{\ell,e}$ be the exterior boundary of Ω_ℓ, see Figure 2. We assume that this surface is isolated, meaning that the drug mass flux is zero. Then

$$\mathbf{D}_{f,\ell} \nabla c_f \cdot \boldsymbol{\eta} = 0 \text{ on } \Gamma_{\ell,e} \times (0, T], \tag{6.5}$$

where $\boldsymbol{\eta}$ denotes the outward unit normal to Ω_ℓ on $\Gamma_{\ell,e}$.

- By $\Gamma_{c,e}$ we represent the exterior boundary of Ω_c, see Figure 2. As no drug mass flux occur on $\Gamma_{c,e}$ we have

$$\mathbf{D}_{f,c} \nabla c_f \cdot \boldsymbol{\eta} = 0 \text{ on } \Gamma_{c,e} \times (0, T], \tag{6.6}$$

where $\boldsymbol{\eta}$ denotes the outward unit normal to Ω_c on $\Gamma_{c,e}$.

- On the fluid outflow boundary $\Gamma ac, tm$ (see Figure 2) we assume that the drug mass flux depends on a function $A_c(c_f)$ that reflects the drug effect in the increasing of the porosity of the trabecular mesh. This function should increase as c_f increases reaching a maximum threshold. Therefore we assume that

$$\mathbf{J} \cdot \boldsymbol{\eta} = A_c(c_f) c_f \text{ on } \Gamma_{ac,tm} \times (0, T], \tag{6.7}$$

where $\mathbf{J} = -\mathbf{D}_{f,ac} \nabla c_f + \mathbf{v} c_f$, and $\boldsymbol{\eta}$ denotes the outward unit normal to Ω_c on $\Gamma_{ac,tm}$.

- In the boundary $\Gamma_{ac,\ell} \cup \Gamma_{ac,i}$ (see Figure 2) we take

$$\mathbf{J} \cdot \boldsymbol{\eta} = 0 \text{ on } (\Gamma_{ac,e} \cup \Gamma_{ac,i}) \times (0, T], \tag{6.8}$$

where $\boldsymbol{\eta}$ denotes the outward unit normal to this portion of the boundary.

The boundary conditions for the Navier-Stokes equations are specified in what follows:

- In the inflow boundary $\Gamma_{ac,i}$ we assume that the normal component of the velocity is known

$$\mathbf{v} \cdot \boldsymbol{\eta} = v_{in} \text{ on } \Gamma_{ac,i} \times (0,T]. \tag{6.9}$$

- There are several approaches to define the boundary condition when the pressure is known. One of them is to consider

$$(\nu \boldsymbol{\nabla} \mathbf{v} - p\boldsymbol{I})\boldsymbol{\eta} = -p_0 \boldsymbol{\eta} \text{ on } \Gamma_{ac,tm} \times (0,T], \tag{6.10}$$

  where p_0 denotes the pressure in Schlemm's canal which is taken equal to the blood pressure and $\boldsymbol{I}$ is the identity matrix.
- On $\partial\Omega_{ac} \backslash (\Gamma_{ac,i} \cup \Gamma_{ac,tm})$ the normal component of the velocity is null

$$\mathbf{v} \cdot \boldsymbol{\eta} = 0 \tag{6.11}$$

  on $(\Gamma_{c,ac} \cup \Gamma_{ac,e}) \times (0,T]$.

For interface boundaries we assume the next conditions for the free drug concentration.

- Interface between the lens and cornea:

$$\begin{cases} \mathbf{D}_{f,\ell} \nabla c_{f,\ell} \cdot \boldsymbol{\eta} = \mathbf{D}_{f,c} \nabla c_{f,c} \cdot \boldsymbol{\eta} \\ -\mathbf{D}_{f,\ell} \nabla c_{f,\ell} \cdot \boldsymbol{\eta} = A_{\ell,c}(c_{f,\ell} - c_{f,c}) \end{cases} \tag{6.12}$$

  on $\Gamma_{\ell,c} \times (0,T]$, where $\boldsymbol{\eta}$ denotes the outward unit normal to Ω_ℓ on $\Gamma_{\ell,c}$. Here $c_{f,\ell}$ and $c_{f,c}$ represent the drug concentrations in the lens and cornea, respectively, and $A_{\ell,c}$ (m/s) denotes the partition coefficient on $\Gamma_{\ell,c}$.
- Interface between the cornea and anterior chamber:

$$\begin{cases} \mathbf{D}_{f,c} \nabla c_{f,c} \cdot \boldsymbol{\eta} = \mathbf{D}_{f,ac} \nabla c_{f,ac} \cdot \boldsymbol{\eta} \\ -\mathbf{D}_{f,c} \nabla c_{f,c} \cdot \boldsymbol{\eta} = A_{c,ac}(c_{f,c} - c_{f,ac}) \end{cases} \tag{6.13}$$

  on $\Gamma_{c,ac} \times (0,T]$, where here $c_{f,ac}$ denotes the drug concentration in the anterior chamber, $\boldsymbol{\eta}$ the outward unit normal to Ω_c on $\Gamma_{\ell,c}$ and $A_{c,ac}$ (m/s) represents the partition coefficient on $\Gamma_{c,ac}$.

Finally, the initial conditions should be imposed to complete the system of partial differential equations (6.1)-(6.4) complemented with the boundary conditions (6.5)-(6.11) and interface conditions (6.12), (6.13). We impose the following

$$c_f(0) = \begin{cases} c_{f,0} \text{ in } \Omega_\ell \\ 0 \text{ in } \Omega_c \cup \Omega_{ac} \end{cases}$$
$$c_b(0) = c_{b,0} \text{ in } \Omega_\ell,$$
$$c_e(0) = c_{e,0} \text{ in } \Omega_\ell,$$

and

$$\mathbf{v}(0) = \mathbf{v}_0 \text{ in } \Omega_{ac},$$

where $c_{f,0}$, $c_{b,0}$, $c_{e,0}$ and $\mathbf{v}_0$ are known functions.

In Figure 3 and 4 we present two typical plots for the drug distribution included before in [20]. Figure 3 illustrates the drug distribution in the anterior chamber when a lens is used where the drug is dispersed in the polymeric structure and entrapped in particles. The results obtained for the drop case are plotted in Figure 4.

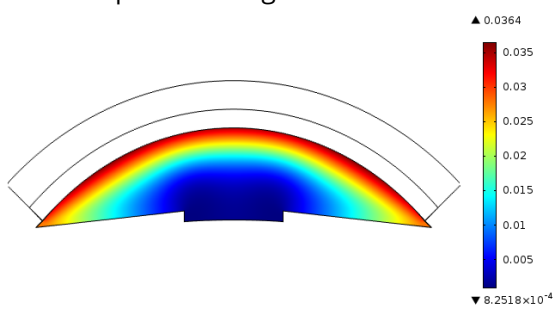


Figure 6.3. *Drug distribution in anterior chamber after 20 minutes for a lens*

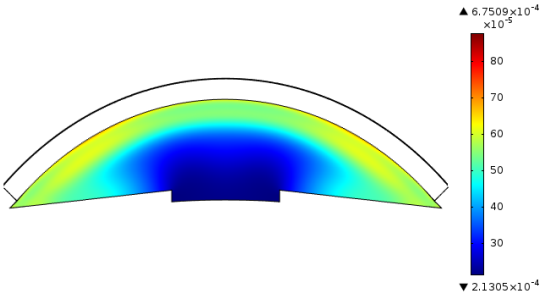


Figure 6.4. *Drug distribution in anterior chamber after 20 minutes for an eye drop*

From the plots we can infer that the amount of drug that reaches the anterior chamber with lens is higher than for drops due to the initial loading. Moreover the drug release from a therapeutic lens is a slower process due to the polymeric barrier for the dispersed and entrapped drugs.

Conclusions

This work aims to contribute to the mathematical modelling of the drug delivery from a drug delivery device - the therapeutic lens - used to decrease IOP in a glaucoma scenario. The model is established under several simplifying assumptions in what concerns the geometry of the spatial domain and the phenomena involved.

Some new models can now be deduced with increasing complexity adding new phenomena and changing the geometry of the spatial domain to include new tissues or organs. For instance the tear turnover can be included requiring the inclusion of a tear film layer in the spatial domain. New equations should be added to the existing set of partial differential equations that describe the drug dynamics in this fluid. Different corneal layers - epithelium, stroma and endothelium - can also be added to the model where the drug presents different diffusion properties. Consequently, the diffusion equation in the cornea should be replaced by three diffusion equations with the correspondent compatibility conditions on the contact surfaces between layers. If the trabecular meshwork is considered (Ω_{tm}) with or without juxtacanalicular tissue, the drug transport is defined by an equation similar to (6.3) where the convective velocity $\mathbf{v}$ is given by Darcy equation (coupled with an incompressibility constraint)

$$\begin{cases} \mathbf{v} = -\dfrac{\mathbf{K}}{\mu\phi}\nabla p \\ \nabla \cdot \mathbf{v} = 0 \end{cases} \tag{6.14}$$

in $\Omega_{tm} \times (0, T]$. In (6.14) $\mathbf{K}$ denotes the permeability tensor and the porosity coefficient is represented by ϕ. It should be stressed that in this case the coupling between the Navier-Stokes equations (6.4) and (6.14) is a challenging topic namely due to the conditions required on the boundary of the trabecular meshwork that is contact with the anterior chamber.

There is a compromise between the complexity of the mathematical model and its utility to predict the IOP evolution in different scenarios. In fact, the number of parameters needed increases with the complexity and some of them are not known.

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Negative selection - a performance measure for algorithmic trading

Algorithmic Trading is the dominant way of trading at electronic stock exchanges. A large number of algorithm is employed, to suit the needs and constraints specified by investors. Performance of different algorithm is measured by the slippage with respect to a chosen benchmark. We propose a new benchmark for algorithmic performance which takes into account the toughness of market conditions for any given trade and results in a objective measurement of the performance.

Algorithmic or automated trading is a dominant way of executing orders at electronic stock markets. Algorithms can be described as the automated execution of trading orders with the goal of meeting a particular benchmark. Slippage to the chosen benchmark is the main quality criteria for a particular algorithm. But the slippage to a benchmark is clearly benchmark-dependent. It is difficult to define one measure for all order executions and all different objectives specified by investors. The purpose of this research has been to propose an objective performance measure, applicable in arbitrary market circumstances and reflecting the quality of trade execution.

This work is being developed at the Department of Mathematics and Informatics, Faculty of Sciences, University of Nov Sad. The project gathered together mathematicians and an expert in algorithmic trading from Nordea Investment Management.

Problem description

Within the variety of available benchmarks the most important are VWAP (Volume Weighted Average Price) and Implementation shortfall (IS). Their properties are the subject of many academic studies and a number of algorithm is developed to minimize the slippage to VWAP or AP, [1, 2, 3, 4]. One of the problems with measuring slippage, whether it is VWAP or IS, is that they either distort the slippage measure or do not reflect the true nature of slippage. The definition of VWAP distorts slippage with increasing order size due to the impact caused by one's own orders and

thus can be flawed for large order size. On the other hand IS, with Arrival Price as the reference price, is unbiased in terms of measuring slippage caused by price drift and market impact, but the reference to a static price (Arrival price) prevents it from capturing the nature of slippage. To understand this flaw better, consider a buy order issued at time t_0. If the price drifts up during the execution, the average execution price will be much higher than the reference price at t_0 and the slippage will be relatively high due to the difficult market conditions. If however the price drifted downwards by the same amount and the entire order quantity was filled on the best bid price, the slippage would remain constant, representing the difference between the best bid price and Arrival Price. Although the slippage in the latter scenario is lower, it does not reflect how much better we *could have done*. In an easy market condition like the case of falling price, intuitively, one may have expected to get negative slippage. However, the IS measure does not reflect this.

A performance measure has to have several important properties. First of all, it should be able to distinguish clearly between filled and partially filled orders as well as between orders filled at different price levels. Furthermore, the performance measure needs to be continuous in the sense that a negligible change in the order size or in the fill price should yield negligible changes in the performance measure. And the most important property of a performance measure is that it should reflect the toughness of market condition at a particular time window and thus allow one to judge the quality of execution.

The term Negative Selection we use deserve a couple of comments. In general one does not want to get filled when the price comes one's way as the price may keep heading in that direction. In this case, it may be better to become more passive and hope to get a better price. Hence one's order being "selected" or "executed" is basically a sub-optimal execution. Negative Selection is an evolved term used to distinguish itself from the original concept in economics, namely adverse selection, referring to skewed and undesirable results due to asymmetry in information held by negotiating parties.

Modeling and challenges

The performance measure which we proposed takes a posteriori view of market conditions and its main characteristic is that it is completely objective. We define the performance measure as the difference between the optimal trading position and the actual execution. The optimal trading position is calculated a posteriori, taking into account all traded quantities within the considered time window. This way, we are capturing the impact caused by our own trading as a cost that affects all trades, including our own and avoid the main problem with VWAP in the case of large trades.

Given a single buy order with a specified quantity Q and a time window $[0, T]$ for the execution, we define the optimal placement of the order as a solution of LP program. The unknowns of the LP are quantities at specific price levels, which add up to Q and would have yielded the lowest possible price during $[0, T]$, if we knew all market conditions during the trading window in advance. Thus the optimal placement is a vector calculated after the trade window $[0, T]$. The Negative Selection is defined as the distance between the actual trade, represented by the vector with a single nonzero component, and the optimal placement.

We consider a market governed by the limit order book implying that the orders are placed in queues by price and arrival time priority. The definition of Negative Selection

is given here assuming that we have to buy Q shares either by placing a market order or taking a passive position at some of the bid levels. For the opposite case, selling Q shares, the definition is completely symmetric. Assume that the buy order of the size Q has to be executed within the time window $[0, T]$. At $t = 0$ the following information is available: the price vector consisting of prices at all bid and ask levels, the volume ahead representing the size of the existing orders in the corresponding bid queues, as well as gain coefficients for all bid levels, defined as the relative difference between the ask 1 price and the bid prices. Also, assume that Q is small enough so it can be traded as a simple order - placed either as the market order or the passive order at a single bid level. Given that the Negative Selection is a posteriori measure, we also use the additional information available at the end of the trading window, $t = T$, like the vector of traded quantities. Therefore we can calculate the available quantities at each trade level as the difference between the volume ahead and the traded quantities.

The optimal placement is now defined as the best position that could have been taken at $t = 0$ if all a posteriori vectors have been available at $t = 0$. In other words, the optimal placement represents the perfect scenario that would have allowed us to execute the order with the lowest possible price. This perfect scenario is a solution of an Linear Programming problem. The objective function of the LP states that we want to minimize the total cost of buying Q shares, while the constraints state that we can only use the available quantities at each price level. A subtle but important point that is not obvious is the following: the optimal placement is not simply buying the available quantities from the lowest bid level upwards until we execute the whole order and the LP is indeed to obtain the optimal placement.

Having the optimal placement as a vector $\mathcal{O}$ representing order sizes at each of the price levels, we define the performance measure as the difference between the optimal placement and the order vector $\mathcal{Q}$, more precisely as the norm of this difference, $\mathcal{N} = \|\mathcal{O} - \mathcal{Q}\|$. For further details see [5]. The following properties of Negative Selection make it a well defined performance measure with desired qualities, objectivity and continuity. First of all, Negative Selection of an optimally placed order is zero. For a completely filled order Negative Selection is nonnegative while for a (partially) unfilled order Negative Selection is negative. If two orders of the same size are placed at different bid levels than Negative Selection of the order on the lower place level is smaller than Negative Selection of the order at higher price level. Finally, if we have two orders of different sizes placed at the same price levels, with $Q_1 > Q_2$, their Negative Selections reflect the difference in the sense that if the larger order is filled then it has larger Negative Selection but if it is unfilled then Negative Selection is negative and hence smaller than Negative Selection of the smaller order.

When placing a buy order, one is faced with the dilemma of being aggressive and cross the spread to buy at the prevailing asking price or take the chance of a better price by bidding at some bid price. In a rising market, a passive order at bid1 will remain unfilled which would lead to chasing the market to get filled, and yield a larger slippage than with crossing the spread. While in a sideways market, one is likely to save the spread cost by being passive. In the case of a falling market, a buyer is considered too aggressive if the entire order is placed at bid1 since one would achieve a better average price by having placed it at an even more passive price level. However, in the latter case, the probability of fill decreases significantly with more passive orders. Therefore, there is a need to split the orders into multiple price levels. Therefore, there is a need to define Negative Selection for an

order distributed across multiple price levels. This can be easily done treating the multiple order as a vector of simple orders and defining Negative Selection as a vector of Negative Selection values for simple orders. Unlike the case of simple order, here exists a certain interaction between the optimal placements for simple orders at different price levels i.e. one must take into account one's own trading.

Empirical results

Good theoretical properties of Negative Selection are verified empirically. The test data consists of 8 moths trade ticks for several stocks at LSE. One of the principal advantages of the NS as a performance measure is that it reflects the toughness of market at any given time. To demonstrate this property we compare the behaviour of NS, VWAP and IS benchmarks in both falling and rising markets. A simple example is considered, [5]. We place an order at bid1 until filled or the time of 10 minutes expires. If the order is not completely filled within 10 minutes, the residual is filled by crossing the spread at the end of given time window. We tested a sequence of orders with increasing sizes, from 0 to 35% of average traded quantity in the selected time window. The 10 minutes windows are chosen randomly. and the relevant trajectories for AZN are shown at Figure 1 and Figure 2. The price trajectories are shown at the left-hand side while the right-hand side shows the slippages with respect to all three benchmarks at both Figures. The horizontal axis shows the traded amount in thousands. The average traded quantity for AZN is 50000 shares in 10 minutes so the simulations are performed for orders of size 1 to 17500 shares with the step size of 500 shares.

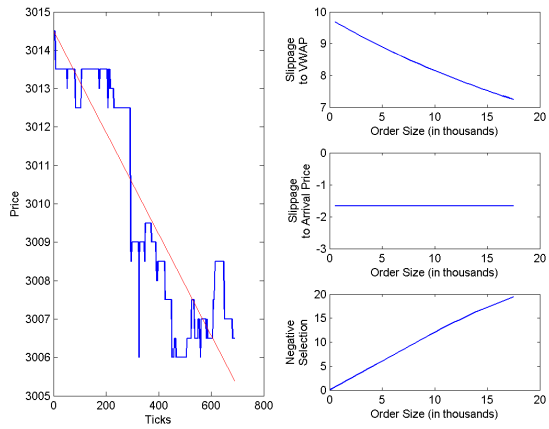

Figure 1: VWAP, Arrival Price and Negative Selection for falling market

In the case of falling market the slippage to VWAP is positive and decreasing with the order size. Figure 1 shows the case of falling market. The slippage to VWAP is positive and decreasing with the increase of order quantity. Clearly, this decrease is a false information as it implies that the trading strategy is good and clearly, in the falling market one should have placed orders at the lower level. Being positive gives the true information of our execution, but the decrease with respect to traded quantity is actually a false information. The slippage to IS is negative and constant. The negative sign here again gives a false information. In the rising market the order placed at bid1 is clearly not filled and results in crossing the spread and paying a higher price. In the case of rising market the slippage to VWAP is positive which is correct, but again we have a false information for larger orders as the decreasing slippage implies that the strategy worked better for larger orders. The slippage to Arrival Price is high and positive. It is constant while there is enough liquidity at $t = T$, but when the order size increases enough - above the quantity available at ask1, the order starts to "walk the book" and the slippage to Arrival Price starts to rise. Whereas, NS is negative and increasing with the order size. Thus the information we get is correct - the execution strategy should have been more aggressive.

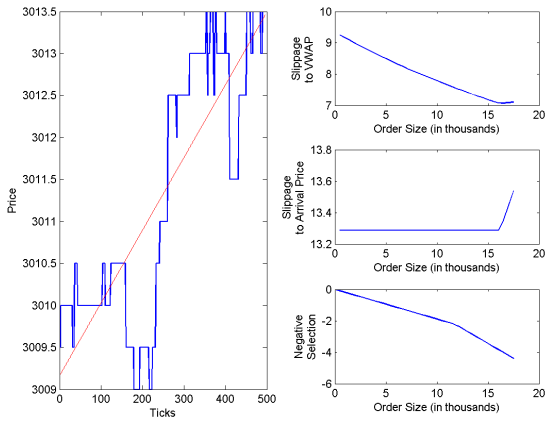

Figure 2: VWAP, Arrival Price and Negative Selection for rising market

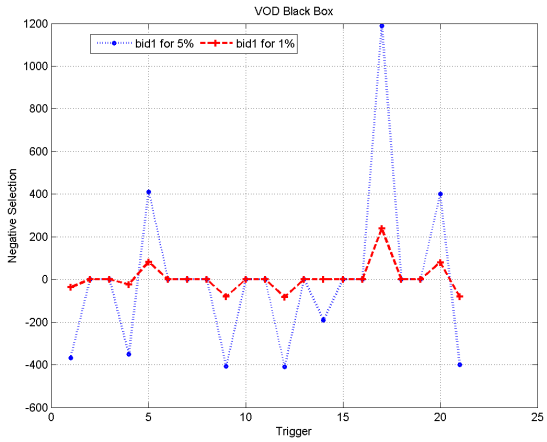

Figure 3: Comparison of Negative Selection by order size for bid/ask1

To demonstrate some properties of NS empirically, we consider a sequence of orders generated by a Black Box (BB) trading strategy with inventory. It is a momentum trading strategy generating signals using a mathematical model. The common parameters of a BB are time execution window, cancel threshold and order size. A combination of the time window width and the cancel threshold are used as the cancellation criterion: an order is canceled if either time expires or the cancellation threshold is reached. Therefore, there are only two possibilities: an order is (partially or completely) filled or canceled within the time window. The algorithm keeps track of open position i.e. all positions are closed with the opposite operation (buy/sell). The BB parameters are selected as follows: the time window is $T = 10$ minutes and the cancel threshold is $45bps$. The tested order sizes vary from 1% and 5% of average traded volume in the time window, which is approximately $40,000$ to $200,000$ shares for Vodafone. Results are shown at Figure 3.

Figure 4 represents the relative distribution of Negative Selection for bid/ask1 for BB. The distribution of Cancel Time and Fill time for the same sequence of orders is depicted on Figure 5. Cancel Time corresponds to points with negative Negative Selection, while Fill time is on the nonnegative side of the axis. Figure 6 shows the values of Negative Selection for AZN orders placed at different price levels.

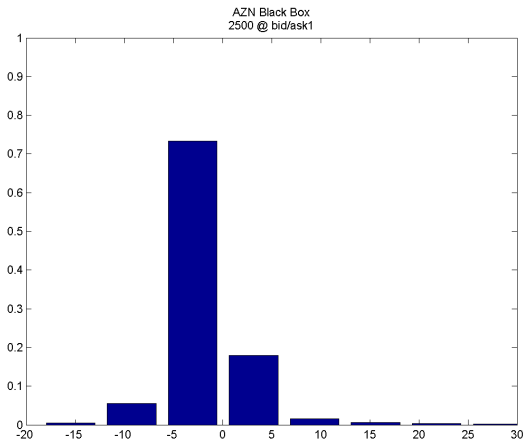

Figure 4: Retaliative frequency histogram of Negative Selection

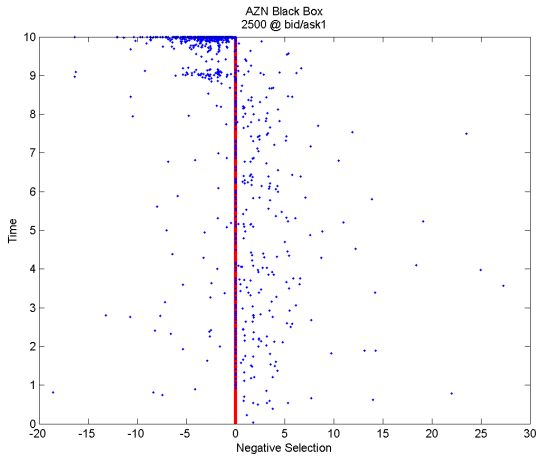

Figure 5:The distribution of Cancel Time and Fill time

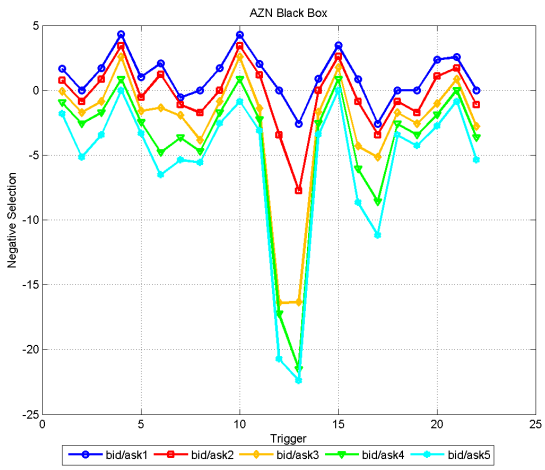

Figure 6: Comparison of Negative Selection for AZN by price levels

Conclusions

We proposed a performance measure that measures quality of automated order execution in objective way, reflective the market conditions during the trade window and thus providing truthful information for each order execution. The performance measure is called Negative Selection to emphasise the situation of sub-optimal order filling which might look good at a glance but is in fact flawed execution in the given market circumstances. The measure is defined as the difference between the actual execution and the optimal placement, calculated a posteriori. The optimal placement is the position one would have taken in the scenario of deterministic future, i.e. knowing all market conditions during the trade window at the beginning of the trade window. This placement is obtained as a solution of a Linear Programming problem and yields the lowest possible price for any particular order within specified time window and under particular market conditions. Therefore, Negative Selections avoids the drawbacks of VWAP and IS. We have demonstrated the properties of Negative Selection both from the theoretical point of view and empirically, using a set of real trade data.

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Modelling, simulating and optimizing the stock of an automotive spare parts wholesaler

This collaboration between mathematics and industry allowed a top player in the Portuguese automotive spare parts market to have an efficient management of their stocks and orders. The project included automatic warning systems, suggested order quantities, and a new system for replacing the traditional ABC leading to considerable gains considering both the quantity in stock as well as the level of service.

Challenge overview

The NORS Group, through their aftermarket spare parts business, identified some needs on developing a mathematical model to support the activities of their operations department. With this purpose, they presented this challenge to LEMA, wondering if industrial mathematics could help them to solve the following problem. Daily, the operations department - group main responsible for the stock management in this business - processes a big amount of data in order to give an efficient response to the company needs in terms of stock. With that purpose, an efficient tool for forecast analysis was needed, as well as a model that allowed some parameterizations in order to accomplish the manager's decisions regarding the quality of service ratio desired. A particular characteristic of this problem is that the references set have very different behaviours regarding the amount of sales per month. Indeed, the same product family may have high rotation references and also very low rotation products leading to the need of applying very different methodologies and forecast techniques.

In the end, industrial and mathematical partners agreed on developing a completely

new tailor-made model, based on updated techniques of forecasting that allows the managers to parameterize the amount of risk they want to take in terms of quality of service parameters. This model returns, an optimal quantity to be ordered regarding each of the references on their portfolio and with respect to a determined objective function developed.

Modelling and implementation challenges

This project was initiated with the Nors manager for the aftermarket department, a statistician and a numerical mathematician from LEMA, who later were joined by an Engineering Mathematics MSc student. In order to find a good balance between accuracy and speed of execution, several meetings were held to discuss intermediate results, allowing Nors management to assess the model's adherence to reality and to use their feedback to adapt the model even more closely to NORS reality. This was made with success, and the first prototype was concluded in 6 months (fig 6.1).

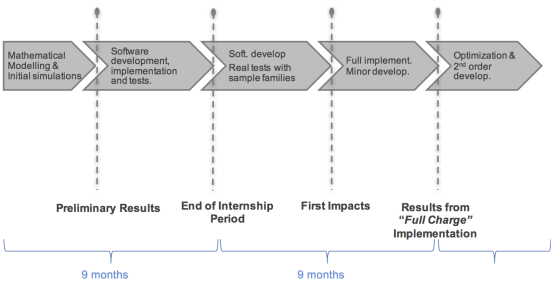


Figure 6.1. *Research, development and implementation timeline.*

There were some main concerns with this challenge: first, the heterogeneity of data (fig 6.2) made very challenge to find a model that fits all the references used by Nors. Second, the scalability and complexity of the model were a concern as there were more than 200.000 references to be analysed and the outputs must be calculated in some acceptable time. Also, the model should adapt easily if the company changes their policy in terms of quality of service, budget or other parameters.

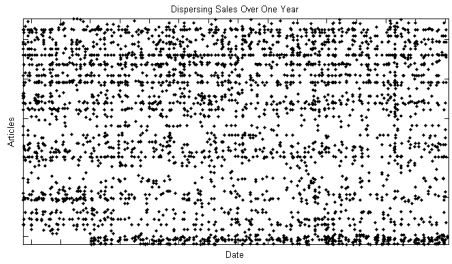


Figure 6.2. *Spy plot on sales of one family references vs time.*

In order to address those challenges, a mathematical model was developed, tailored to the Nors particularities, more efficient, and capable to identify and address the references different rotation types (fig 6.3). With the identification of appropriated forecasting methods, and the definition of appropriated metrics, the challenge of data heterogeneity was tackled.

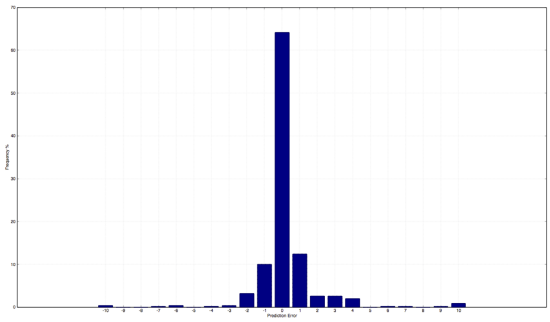


Figure 6.3. *Forecast errors barplot.*

Also, targeting a more efficient stock management, some key performance indicators (KPI) were developed. Implemented on the order management software, developed by this team, they allow a better adjustment to the company needs and, at the same time, to update the user with the current state and trends of the system. Additionally, a set of constrains that takes into account the specific characteristics of each reference was developed, speeding all the process of placing orders. Finally, an optimization

model was coupled to the forecasting process, replacing the ABC methodology with success.

Due to the particularities of the Nors informatics system, an stand-alone module for data analysis was developed. This software interacts smoothly with Nors native system, importing and exporting data in the format required by Nors existing software.

Results and achievements

A new mathematical model for stock management of spare parts was developed. One year after the model being fully implemented on several families of products, the level of service raised 1%, the mean stock value decreased about 18% , in a period where sales increased more than 9%. Additionally, the months of stock KPI, decreased by around 25%, from 5.7 to 4.2 months (fig 6.4).

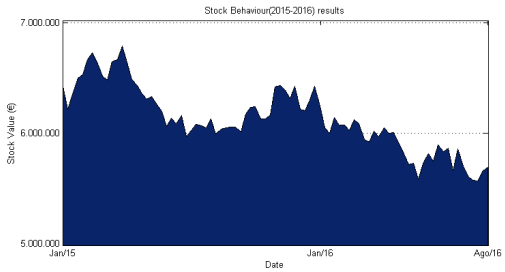


Figure 6.4. *Stock behaviour.*

It was also developed a software tool that implement automatically all the features that NORS asked in the beginning of the project, as well as some upgrades made during the development phase. An easy to use graphical user interface was developed to operate the software (fig 6.5), reducing the order processing times in more than 70%, when compared with NORS native system.

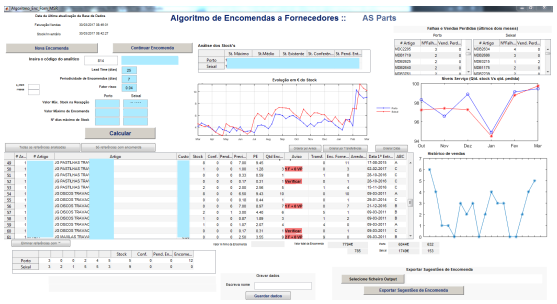


Figure 6.5. *Graphical user interface developed.*

Lessons learned and replicability

The LEMA team who worked on this project found it very challenging as it relies on several mathematical fields. A real team work, mixing the knowledge from different areas, was needed to address the questions posed by the industrial partner. Also, developing the model, seeing the upgrade in the quality of the results and, at the same time, being sure that mathematics was helping a company and their workers daily was fantastic. Finally, being able to complete all the project phases (from modelling to the software development) recurring only to mathematicians and to know that, with this work, they helped to improve the viewing of mathematics in the industrial community was the ultimate reward, in particular when this project opened the first position for a mathematician inside the NORS group.

In the NORS point of view, this was a big challenge because it configured a different approach to one of their most critical issue. The effectiveness of their stock management process is crucial for the parts business success, as they were changing the key drivers of the purchase process and stock management model. This mathematical approach allows them to predict the sales level of each part with accuracy and, at the same time, parameterize the level of risk they want to take, while managing the spare parts business in a optimized way considering the NORS main management guidelines. The implementation of the mathematical model,

provided one significant cost reduction (stock, transport, storing) meanwhile the efficiency increased, as it may be measured by the service level KPI.

The mathematical footprint

The results achieved projected some attentions within the group to the role of industrial mathematics in modern management. In addition, the award of Nors Innovation prize to this project in 2015, lead to other areas in the group to become aware of the goals achieved by industrial mathematics.

Figure 6.6. *Prize awarded to the initial project.*

Since then, new proposals and requests for exploratory studies have been addressed to this team in a regular basis. As consequence a new laboratory, the LAB MI (initials for Industrial Mathematics Laboratory) was created within the Nors aftermarket development section. The initial internship had become into a permanent workplace, and the initial staff of one manager and two external consultors, was reinforced with two more internships. Working in different areas like budget support analysis, vehicle lema/routing, data analysis or waiting queues, this team is working in a daily basis to address new challenges and provide Nors with appropriated mathematical techniques tailored and developed to the singularities of their own business. According to the managing partner, this approach aimed to stablish and reinforce mathematics as an important tool of decision support. It introduces accuracy on the data analysis and transforms the information spread across different systems and between some collaborators into useful and available knowledge with a much wider field of application. This knowledge, made available to everyone, allows Nors to increase the efficiency on their resources management.

R. Costa[1], M. Cruz[2], M. Pina[1], S. Ramos[2]

[1] Aftermarket Development, Nors Group, Portugal
[2] LEMA - Laboratory for Mathematical Engineering, School of Engineering - Polytechnic of Porto, Portugal

7

ECMI Special Interest Groups (SIGs)

Special Interest Groups (SIGs) exist to promote collaborative research on specific topics in Mathematics for Industry within Europe. A particular aim is to enable researchers from both academia and industry with similar interests to get together and submit proposals for funding to the European Union or to other funding bodies. ECMI can act as a catalyst in the formation of such a group by offering advice about the expertise available within Europe, by posting information on the web pages and by circulating information about events to all members.

Math for the Digital Factory

Purpose

The digital factory represents a network of digital models and methods of simulation and 3D visualisation for the holistic planning, realisation, control and ongoing improvement of all factory processes related to a specific product. In the last five or ten years all industrialised countries have launched initiatives to realise this vision, sometimes also referred to as Industry 4.0 (in Europe) or Smart Manufacturing (in the United States).

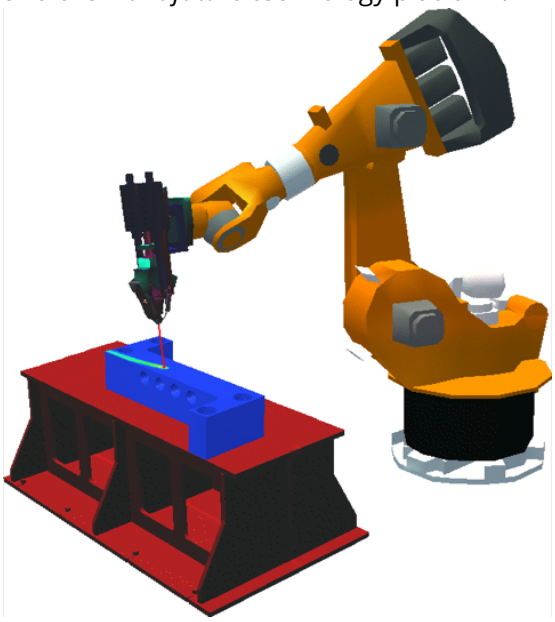
Opportunities

The Special Interest Group MaDiFa (Math for the Digital Factory brings together university mathematicians working in modelling, simulation and optimization related to manufacturing with practitioners from manufacturing industry. The general scientific goal is to develop a holistic mathematical view on digital manufacturing. Topics to be discussed include

- coupling of multibody systems with pde models to describe interactions between machine tool (typically a MBS) and its manufacturing task (typically described by PDEs and ODEs)
- multiscale models of complex manufacturing chains including workflow
- new concepts to model the energy consumption of machine tools and more complex production systems
- optimization strategies for energy and material efficient production

Activities

In 2016 the main focus of attention were activities at the ECMI conference in Santiago di Compostela. We organized a mini - symposium on digital manufacturing and coorganized another one on mathematics in Horizon 2020 and beyond. Here, the main topic related to production was a presentation about Factories of the Future and the *Manufuture* technology platform.



Coupled multibody - PDE simulation of robot guided laser hardening.

We try to foster the organization of joint European research proposals. An European Industrial Doctorate (EID) on “Maths and Materials Science for Steel Production and Manufacturing (MIMESIS)” started in January

2016. Another one related to *Industry 4.0* is in preparation. A multi-author textbook on digital manufacturing will be published later in 2017. The next SIG workshop is planned for March 2018 at the University of Limerick.

Dietmar Hömberg

Weierstraß-Institut and Technische Universität Berlin

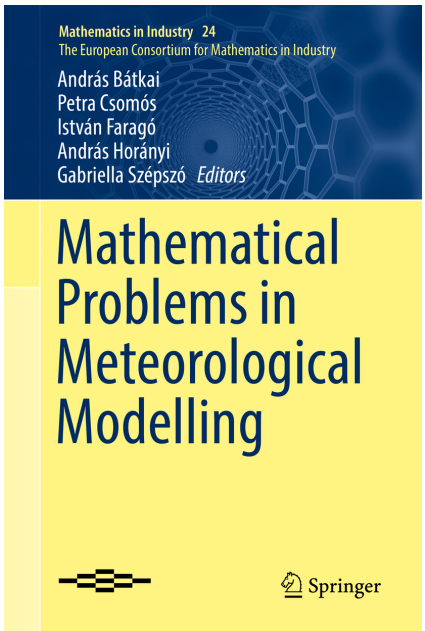
Numerical Weather Prediction

Purpose

Our Special Interest Group focuses on mathematical problems arising from meteorological modelling. The forecast of the state of the atmosphere is based on complicated, nonlinear and stochastic partial differential equations. Since an exact solution is hopeless to be found, one needs to apply certain numerical methods to obtain at least an approximation to it. Our goal is to collect specialists from all over Europe to tackle the actual problems of the modeling and the numerical analysis of various air pollution problems.

Activities

- In every semester we organize regular weekly seminars with participation of researchers and students from different scientific fields (mathematics, meteorology, geophysics, astronomy). Subject of the seminars: Selected chapters from the theory of numerical stability, Selected chapters of mathematical modeling
- We have intense collaboration in the supervision of masters- and PhD theses between the Hungarian Meteorological Service and the Mathematical Institute of the Eötvös Loránd University.
- The book "Mathematical Problems in Meteorological Modelling" was published in the ECMI Series of Springer. This book deals with mathematical problems arising in the context of meteorological modelling. It gathers and presents some of the most interesting and important issues from the interaction of mathematics and meteorology. It is unique in that it features contributions on topics like data assimilation, ensemble prediction, numerical methods, and transport modelling, from both mathematical and meteorological perspectives.



The derivation and solution of all kinds of numerical prediction models require the application of results from various mathematical fields. The present volume is divided into three parts, moving from mathematical and numerical problems through air quality modelling, to advanced applications in data assimilation and probabilistic forecasting. The book arose from the workshop “Mathematical Problems in Meteorological Modelling” held in Budapest in May 2014 and organized by the ECMI Special Interest Group on Numerical Weather Prediction. Its main objective is to highlight the beauty of the

development fields discussed, to demonstrate their mathematical complexity and, more importantly, to encourage mathematicians to contribute to the further success of such practical applications as weather forecasting and climate change projections. Written by leading experts in the field, the book provides an attractive and diverse introduction to areas in which mathematicians and modellers from the meteorological community can cooperate and help each other solve the problems that operational weather centres face, now and in the near future.

Readers engaged in meteorological research will become more familiar with the corresponding mathematical background, while mathematicians working in numerical analysis, partial differential equations, or stochastic analysis will be introduced to further application fields of their research area, and will find stimulation and motivation for their future research work.

Coordinator: András Bátkai

Eötvös Loránd University

Sustainable Energies

The ideas for this SIG originated with the "Mathematics in Industry" workshop "Technologies of thin film solar cells", held in Berlin. It was followed by a series of workshops held in the UK and Germany with ever increasing scope from organic photovoltaics, supercapacitors, Lithium-Ion batteries, solar fuels and resulted in the Kick-Off meeting "Nanostructures for Photovoltaics and Energy Storage" for this SIG, which also included electrothermal modelling and simulation of organic materials and devices.

Purpose

We address the challenges posed by the way energy is being generated in the future, with a high demand for sources of sustainable energy and production capabilities and which entails the restructuring of existing as well as the creation of new, smart networks for efficient storage and transport of distributed energy. Mathematics plays a key role in understanding the complex problems that arise in these areas and in exploiting underlying structures and processes.

Opportunities

Researchers and non-academics eg. from industry working in fields such as thermoelectricity, nano-scale optics, organic/polymer electronics such as organic LEDs and storage systems are presently the key stake holders to which this SIG reaches with its activities. Contributions relating to energy distribution and networks are also welcome.

Activities

One of the SIG coordinators co-organised the minisimposium MS25 on "Recrystallization of Si for thin film solar cells: experiments, modelling and numerical simulations" at the ECMI bi-annual conference 2016 in Santiago, jointly with Abou-Ras (Helmholtz-Zentrum Berlin). A Spanish-led initiative focussing on the real-time multiscale simulation of batteries e.g. for electric vehicles was borne out by participants of the ECMI conference, and involved groups in Spain, Germany and the

UK as well as industry participation. These are strong groups working on different aspects of battery modelling and simulation including the effect of stresses in Lithium-Ion batteries arising from the intercalation of Lithium into the electrodes as well as thermodynamically consistent modelling of the electro-chemistry at the micro-level as well as up-scaling to the macro-level. This expertise will be used to assess, model and simulate the long-time behaviour of batteries at various scales as they undergo aging, requiring smart ways of design and management.

Coordinators: Andreas Münch[1] and Barbara Wagner[2],

[1] Mathematical Institute, University of Oxford
[2] Weierstrass Institute Berlin

Computational Finance

The ECMI Special Interest Group Computational Finance was launched at ECMI-2014 in Taormina (June 9–13, 2014) and (together with the ITN STRIKE Project) organized several sessions of a minisymposium in Computational Finance. The aim of the SIG is to extend the network and to build a framework to continue close cooperation in future. It also provides a long term professional contact option for Alumni of ITN-STRIKE.
In 2016 the SIG was active at ECMI-2016 in Santiago de Compostela, Spain. There also was a new Workshop on Financial Risk in Budapest, Hungary.

Purpose

At ECMI-2016 the Special Interest Group on Computational Finance organized a minisymposium *Computational Methods for Finance and Energy Markets*. We brought together again twelve speakers coming from TU Delft and CWI Amsterdam (the Netherlands), DCU Business School (Dublin, Ireland), Universidade da Coruña (Spain), University of St. Gallen (Switzerland), Bergische Universität Wuppertal (Germany) and MathConsult GmbH (Linz, Austria).

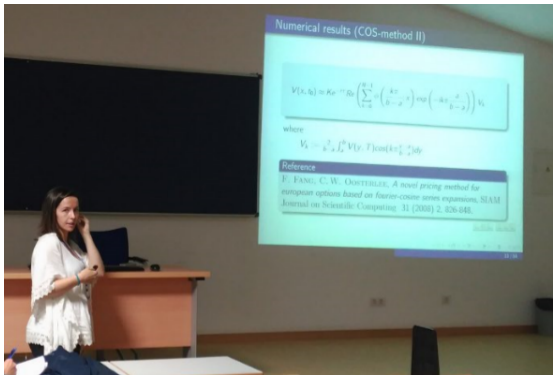
The computational complexity of mathematical models employed in financial mathematics has witnessed a tremendous growth. Advanced numerical techniques are imperative for the most present-day applications in financial industry.

The aim of this minisymposium was to present most recent developments of effective and robust numerical schemes for solving linear and nonlinear problems arising from the mathematical theory of pricing financial derivatives and related financial products. These approaches vary in departing directly from the system of stochastic differential equations (SDEs, involving SABR dynamics) to approaches for the derived partial differential equations (PDEs). The SDE group focusses on fast Monte-Carlo methods involving COS methods and techniques for GPU processors. The PDE group discussed efficient finite difference methods (varying in involving techniques like sparse time integrators by alternating direction methods, or boundary element methods), also combined with pseudospectral methods. Further speakers discussed concisely aspects like Credit Value Adjustment, Counterparty Credit Risk and effects due to uncertainty in parameters.

In the recent years we observe an increasing interest in mathematical methods for energy markets as well. The rapid changes in energy trading within the last two decades have attracted many researchers in academia and industry. Their aim is to adequately model energy prices and typically also to design methods and

guidelines for risk management challenges. Existing modelling tools and numerical methods for this application field face several new kinds of challenges. Coupled with highly inelastic demand and a variety of supply side constraints, the lack of energy storage can result in sudden price spikes and high, time-varying volatility. Mean reversion rates and typical seasonal patterns exhibit a complex multi-scale nature with respect to the time variable. Calibration is an essential ingredient to obtain realistic models. The models need to have a detailed specification with the various quantiles being related to multiple factors through coefficients which have dynamic properties themselves related to some of the exogenous factors.

ECMI-2016: Qiang Feng and Alvaro Leitao from CWI Amsterdam and TU Delft (NL). Recently, both did successfully defend their PhD-Thesis (2017).



ECMI-2016: Maria Suarez Taboada of A Coruña (Spain).

ECMI-2016: Alvaro Leitao (TU Delft) did report on impressive "Efficient one and multiple time-step simulation of the SABR model".

Opportunities

The SIG will look for opportunities for new projects in both directions, Computational Finance and Energy Markets, in the coming years (ETN, EID, and EJD).
The Special Interest Group is open for further participation.

In 2016 the request by colleagues from Eötvös Loránd University, Budapest, Hungary, to start a SIG on Financial Risk, was considered by ECMI's Research and Innovation Committee to become a sub acitivity of the SIG Computational Finance. A *1st Workshop on Understanding the Diversity of Financial Risk – Counterparty Exposure and Robust Risk Modelling in Finance* took place at the Eötvös Loránd University in Budapest on Oct. 21, 2016 (https://valstat.elte.hu/conf2016/).

"Counterparty exposure has become the key element of financial risk management. Unlike the credit risk for a loan, when only the lending banking organization faces the risk of loss, counterparty exposure creates a bilateral risk of loss. The future market value of the exposure and the counterparty's credit quality are uncertain and may vary over time as underlying market factors change. Standard credit risk models cannot explain the observed clustering of default, sometimes described as "credit contagion". Counterparty risk is a potential channel of credit contagion, and its modelling needs complex approaches. Regulators try to mitigate counterparty risk by increasing capital reserve requirements. A more market-conform solution is Credit Valuation Adjustments (CVAs), when the price an investor requires for a product is reduced in the trade with a defaultrisky counterparty as opposed to a default free one. However, various approaches, going beyond CVA also appear in the literature, but they slowly gain acceptance in the financial industry." [citation taken from the website of the Workshop].

Speakers came from Imperial College (London, UK), Erste Group (Vienna, Austria), University of Évry Val d'Essone (Évry, France), Citibank (London, UK) and Morgan Stanley (Budapest, Hungary), which was the main sponsor of this event. The website still offers video's of the lectures.

Activities

Planned activities for 2017

- Minisymposium *"Recent trends in the analysis and computations of nonlinear partial differential equations and systems"*, at *XVII International Conference Computational & Mathematical Methods in Science and Engineering*, July 4–8, 2017, Rota, Spain, http://cmmse.usal.es/cmmse2017/special-session-and-minisymposiums#ms53.
- Co-organize *ICCF-2017 – International Conference on Computational Finance*, Lisbon, Portugal, Sept. 4–8, 2017, http://cemapre.iseg.ulisboa.pt/iccf2017/.
- Interdisciplinary Workshop *Applied Mathematics Techniques for Energy Markets in Transition*, Sept. 18–22, 2017, Lorentz Center, Leiden, the Netherlands, https://www.lorentzcenter.nl/lc/web/2017/907/info.php3?wsid=907&venue=Oort
- Preparation and submission of EU ETN and EID proposals.

Coordinators: Matthias Ehrhardt and E. Jan W. ter Maten

Bergische Universität Wuppertal

Mathematics for Big Data

Purpose

The availability of huge amounts of data is often considered as the fourth industrial revolution we are living right now. The increase in data accumulation allows us to tackle a wide range of social, economic, industrial and scientific challenges. But extracting meaningful knowledge from the available data is not a trivial task and represents a severe challenge for data analysts. Mathematics plays an important role in the existing algorithms for data processing through techniques of statistical learning, signal analysis, distributed optimization, compress sensing etc.

The amounts of data that are available and that are going to be available in near future call for significant efforts in mathematics. These efforts are needed to make the data useful. The main challenges we plan to consider within this SIG are, roughly speaking, in the area of mathematical optimization and statistics.

Opportunities

Minimization of a cost function, based on large amount of data is a typical problem in all big data areas – from smart agriculture, energy efficiency, computational biology, high tech industries based on simulations, material design, social networks analysis, challenge in policy decisions based on data, risk assessment in finance, security, natural disasters etc. The challenges in these areas, mathematically speaking are design of algorithms that will be able to process huge amounts of data within a reasonable time span and with computer power that is widely available today. Two important issues are distributed optimization and privacy issues. Several EU documents cite privacy of data as an important question that is to be resolved. On the other hand, distributed optimization allows us to employ optimization techniques in parallel, at several different computers placed in networks of different types. On another hand, extraction of meaningful information from data is one of the main tasks of Statistics. In presence of big data the most part of the usual techniques for statistical analysis can not easily been applied, since they are based on the simultaneous processing of the whole dataset. A big effort has been made during these years, mainly by computer scientists, to find fast and scalable procedures that have become popular in presence of distributed architectures (like e.g. the well known MapReduce paradigm). Unfortunately in many situations such procedures can not be applied to solve statistical problems in a distributed way, or they work under too much restrictive and thus unrealistic conditions. The deepening of the mathematical insight in this context may help to better understand the theoretical and applied power of the new algorithms and to extend them to more realistic cases. Sometimes data are “big” because of their high dimensionality and space-time structure (think e.g. to satellite images, signals registered by sensors or antennas, etc.). In such cases suitable mathematical techniques for dimensionality reduction are needed both for data visualization and for their numerical treatment. Functional Statistics, that is a field in which a lot of research is concentrating nowadays, may

help in facing this task. In other contexts data are considered “big” because of their complexity or heterogeneity (e.g. data extracted from social networks with text mining, mixed to socioeconomic data for marketing purposes; or data highly interrelated which may be represented by complex graphs, like atoms and bounds in a protein, relationships between users of a social network, etc.). Sentiment analysis and Topological Data Analysis are new statistical fields of research, still under development, which may help to tackle the problem of analyzing such data.

The aim of this Special Interest Group is to collect people working on the themes described above, coming both from academy and from “industry” (to be intended in a wide sense) to favor scientific collaboration and research, by organizing common activities.

Planned activities for 2017

This is a SIG of new formation.

- A kickoff workshop will be held in Novi Sad (Serbia) on May 31 - June 1, 2017 During the workshop future activities will be discussed and planned.
- The submission of a European project under the MSC-ITN programme is under planning.

For further information see sites.google.com/view/mathbigdata/home

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Coordinators:

Natasa Krejic, University of Novi Sad
Alessandra Micheletti, Università degli Studi di Milano

Liquid Crystals, Elastomers and Biological Applications

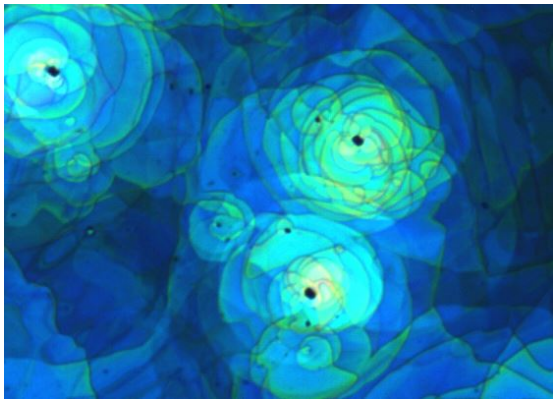
Purpose

The ECMI Special Interest Group in Liquid Crystals, Elastomers and Biological Applications originated with discussions at British Liquid Crystal Society and ECMI meetings, and aims to try and focus the efforts of applied mathematicians to areas of interest concerning anisotropic fluids and solids. The SIG coordinators have since brought together researchers from various fields, and from around the world, at organised workshops and sessions at larger conferences. With new activity planned for the near future, particularly linking to other networks within Europe, the hope is to expand membership over the next year.

Opportunities

From a mathematical point of view, this research area encompasses the analysis of anisotropic materials through continuum mechanics, fluid dynamics, non-equilibrium physics and the analysis of ordinary and partial differential equations.

The intrinsic anisotropic of these materials leads to asymmetries in elasticity and stress which produce interesting couplings between elastic deformation, flow and order. Since these effects are key to a number of existing and burgeoning industries, such as liquid crystal displays, elastomeric materials and active fluids, the greatest opportunity is for mathematicians to interact with industrial researchers within this field.



Microscope image of a nematic liquid crystal as it changes to a twisted grain boundary structure (courtesy of Dr Stephen Cowling, University of York, UK)

Activities

The Group is small at present but plans to expand through collaborations with the British and German Liquid Crystal Society and a number of UK Fluids Networks, which aim to make collaborations within Europe with recent funding for a three year programme of events. Recent meetings have focussed on some of the fundamental theories of orientationally ordered materials as well as the analysis of the resulting differential equations. In 2016, activities and attendance included meetings such as an

Institute for Pure and Applied Mathematics (UCLA) workshop on "Partial Order: Mathematics, Analysis and Simulations" 25th-29th January 2016[1] a Centre de Recherches Mathématiques (Montreal) workshop on "Partial Order in Materials: Analysis, Simulations and Beyond" 21st -30th June 2016[2] and a London Mathematical Society South West and South Wales Regional Workshop on Partially Ordered Materials, University of Bath 21st December 2016[3]. New links have been formed from the SIG to groups around the world through a variety of methods, and links now exist to the University of Malaya (Malaysia), Nanyang Technological University (Singapore), the National Autonomous University of Mexico and the Centro de Investigación en Matemáticas, as well as the Indian Institute of Technology Delhi (India).

Workshop participants from the SIG and Nanyang Technological University

Future activities

The Group is intending to extend participation through frequent meetings as part of ECMI meetings and through funded network meetings such as the Fluids Network groups on "Fluid Dynamics of Liquid Crystalline Materials", co-organised by one of the SIG coordinators, and "Biologically Active Fluids".

Coordinators: Apala Majumdar[1] and Nigel Mottram[2]

[1] University of Bath
[2] University of Strathclyde

[1] http://www.ipam.ucla.edu/programs/workshops/partial-order-mathematics-simulations-and-applications/
[2] http://www.crm.umontreal.ca/2016/Order16/index_e.php
[3] http://people.bath.ac.uk/jlpn20/lms2016.html

Shape and Size in Medicine, Biotechnology and Materials Science

Purpose

Thanks to the development of information technologies, the last decade has seen a considerable growth of interest in the mathematical and statistical theory of shape and its application to many and diverse scientific areas. Often the diagnosis of a pathology, or the description of a biological process mainly depend on the shapes present in images of cells, organs, biological systems, etc., and mathematical models which relate the main features of these shapes with the correct outcome of the diagnosis, or with the main kinetic parameters of a biological system are still not present. In materials science optimisation for quality control, texture description and prediction, etc. require methods of mathematical morphology.

Opportunities

From the mathematical point of view, shape analysis uses a variety of mathematical tools from differential geometry, geometric measure theory, stochastic geometry, etc. Quite recently, instruments from algebraic topology have been introduced for shape description, giving rise to a new field of research called Topological Data Analysis. As far as applications are concerned, the members of the SIG emphasize here topics which are relevant in medicine, biotechnology and material sciences. We deal with direct and inverse problems. Among direct problems, spatio-temporal pattern formation deals with the analysis of how patterns are created and developed in biology, medicine and materials science. Modeling, numerical simulation and analyses of the corresponding systems are tasks of paramount importance for direct problems. Among inverse problems, we study various statistical techniques of shape analysis to measure in a quantitative way the random variability of objects; recent methods of image analysis include optical imaging of objects in turbid media, which can be used as a non-invasive technique for the detection of tumors in the body.

Activities

- Minisymposium of the SIG organized at the conference ECMI2016, Santiago de Compostela, June 13-17, 2016. The following talks have been presented during the event:
  - Santiago Velasco-Forero, Ecole des Mines Paris, *Hierarchical analysis of signals on graphs.*
  - Jesus Angulo, Mines ParisTech, *Morphological semigroups and scale-spaces on ultrametric spaces.*
  - Prakash Easwaran, ITWM Kaiserlautern, *Stochastic modeling of 3D fiber systems incorporating*

interaction.

- Alessandra Micheletti, Università degli Studi di Milano, *Statistical properties of the estimators of parameters of a germ-grain model for double phase steel.*

- Marco Longfils, Chalmers University of Technology, *Generalised Eden growth model and random planar trees.*

- Giovanni Naldi, Università degli Studi di Milano, *Some problems related to the image analysis of the vessels remodelling during embryos development.*

- Haisheng Wang, Mines ParisTech, *Modeling of the microstructure of mesoporous alumina constrained by numerical simulation of nitrogen porosimetry.*

Planned activities for 2017

- New workshops or thematic minisymposia in international conferences are being planned and will be announced on the ECMI web pages

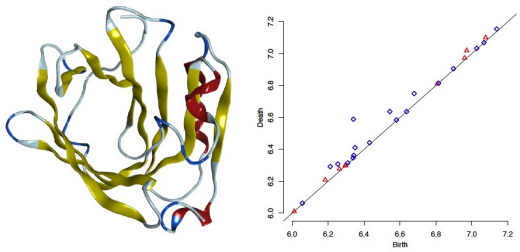


Figure 1: Topological Data Analysis applied to the study of protein binding sites

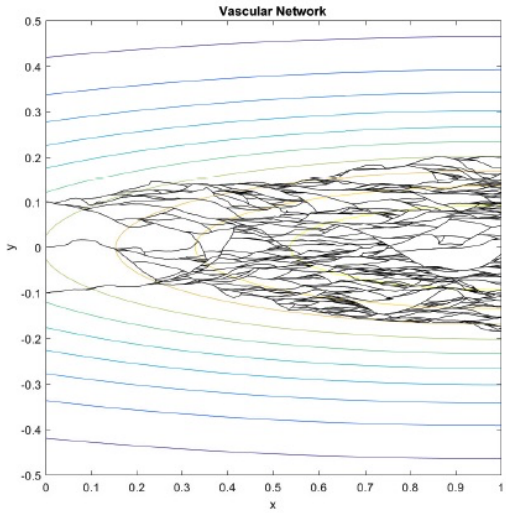


Figure 2: A simulation of a mathematical model for angiogenesis

Coordinator: Alessandra Micheletti,

Università degli Studi di Milano

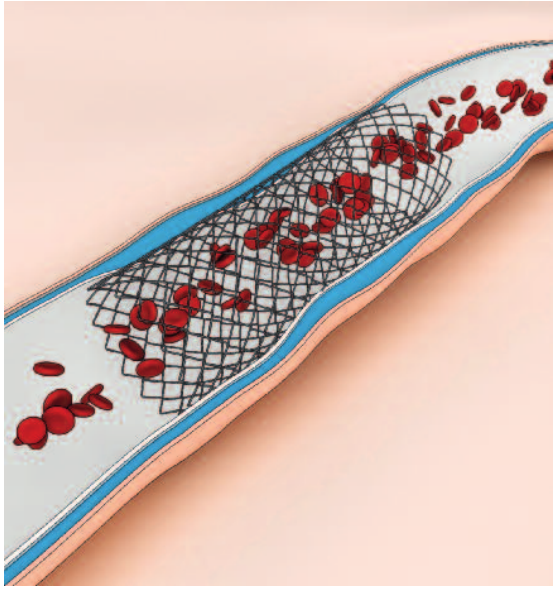
Advancing the Design of Medical Stents

A number of events were organsied over the past year, including the minisymposium "Applied mathematics in stent development" at ECMI 2016 in Santiago de Compostela and the three day workshop "Modelling and experiments in drug delivery systems" at University of Coimbra.

These events brought together in excess of 70 participants including mathematical modellers and experimentalists from several countries including the UK, Ireland, France, Italy, Portugal, Germany, Denmark, Iceland and Spain.

SIG Purpose

Coronary artery disease is a global problem and devising effective treatments is the subject of intense research activity throughout the world. Over the past decade, stents have emerged as one of the most popular treatments. Acting as a supporting scaffold, these small mesh devices are now routinely inserted into arteries where the blood flow has become dangerously restricted. Stents have evolved from bare metal scaffolds to polymer coated drug-delivery vehicles and, more recently, sophisticated fully biodegradable drug delivery configurations. Despite these advances, significant opportunities to improve on arterial stent design remain. In particular, research is focussed on the development of stents which accelerate the healing process to minimise thrombosis risk and which can be used in previously unserved patient groups and lesion types.



This SIG therefore consists of an international network of experts interested in stent research, and provides a platform to co-ordinate research efforts and help expedite the development of novel stent designs and technologies.

Modelling and experiments in drug delivery systems

The Modelling and experiments in drug delivery systems (MEDDS2016) workshop was held at the University of Coimbra in June 2016, under the auspices of the SIG. The workshop achieved its main goal of bringing mathematicians, biologists, physicians and engineers together in an open discussion environment. Whilst there were several talks on stents, the scope of the workshop was wider and included talks on drug delivery in general as well as several specific applications including transdermal delivery and intravitreal implants.

Applied mathematics in stent development

We organised the above titled minisymposium at the 19th European Conference on Mathematics for Industry (ECMI 2016) in Spain. There were five contributed talks from members of the SIG. The talks covered the development of innovative models to help industry optimise and improve stent design, to identify the key parameters governing the behaviour of the system, to simulate the flow of plasma around complex stent geometries, to identify the drug release mechanism, and to help decrease the number of experimental studies, thereby saving time and money. The minisymposium was attended by researchers with expertise in continuum mechanics, physiological flow modelling, structural and soft tissue mechanics, numerical analysis, mathematical biology and multi-objective optimisation, to name but a few. The talks included:

- *The role of mathematics in stent development*, Dr Sean McGinty, University of Glasgow (Scotland).
- *Optimizing the performance of drug-eluting stents: simulations and experiments*, Prof Abdul Barakat, Ecole Polytechnique (France).
- *Mathematical models of drug release from polymer-free drug-eluting stents*, Dr Tuoi Vo, University of Limerick (Ireland).
- *Variable porosity coatings as a means of controlling drug release from stents*, Dr Giuseppe Pontrelli, IAC-CNR, Rome (Italy).
- *Numerical simulation of drug transport in arterial wall under healthy and atherosclerotic conditions*, Javier Escuer, University of Zaragoza (Spain).

SIG Inaugural Committee Meeting

ECMI 2016 also provided the opportunity for us to hold our first SIG Committee meeting, attended by members of the SIG Committee as well as ECMI president Dietmar Hoemberg. It was decided that the SIG seed money would be used to fund a workshop with an Industrial presence (see below). Among the matters raised at the meeting included the possibility of widening the

scope of the SIG in the medium-term to include medical implants and/or drug delivery devices more generally. The idea of submitting a proposal for an EU PhD training network was discussed as well as the possibility of writing a book related to the themes of the SIG which could also act as a teaching resource.

Forthcoming Activities

The SIG intends to submit a minisymposium proposal for the ECMI 2018 conference and additionally plans to use the SIG seed money to partially fund a 3 day workshop in Autumn 2018 in Glasgow, on the theme of "Modelling and experiments in drug delivery systems". A full day of the workshop will be designated as an Industrial workshop, and another full day dedicated to stents research. The attendance of companies, clinicians and experimentalists will only serve to enhance collaboration in this multi-disciplinary area. Those interested in attending should contact Sean McGinty (sean.mcginty@glasgow.ac.uk) or Tuoi Vo (tuoi.vo@ul.ie).

Coordinator: Sean McGinty

University of Glasgow

Slow granular and multiphase flows

Purpose

The flow of granular material is important to manufacturing processes in a wide variety of industries. These include pharmaceutical, chemical, powder metallurgy, food processing and mining sectors. The lack of a fundamental understanding of the mechanisms of granular flows, means the design and control of these processes, which rely on consistent and predictable flow of granular materials, can be expensive and time-intensive. Unfortunately, despite the widespread occurrence of flow of granular materials in industry and the wider environment, a detailed understanding of granular mechanics remains elusive. In continuum models, it is difficult to find accurate models describing the response of granular material to applied stresses and strains. Discrete models, such as the discrete element method are computationally expensive and there is significant difficultly parametrising and validating the proposed particle-particle contact laws. A new interdisciplinary project, based in the University of Limerick with industry partners Johnson & Johnson Automation Centre of Excellence and Rusal Aughinish Alumina, aims to consider granular flow problems arising in an industrial context.

Opportunities

A new industry co-funded project called MOMEnTUM (Modelling of Multi-Phase Transport Processes to Enable Automation in Manufacturing) has recently been established in the University of Limerick (UL). The project brings together engineers and experimentalists from the SSPC (Synthesis and Solid-State Pharmaceutical Centre), industry partners Johnson & Johnson Automation Centre of Excellence and Rusal Aughinish Alumina and applied mathematicians, chiefly based MACSI (Mathematics Applications Consortium for Science and Industry), the ECMI node in Limerick. This collaborative project gives the opportunity to advance the current knowledge base for models of granular flow processes while working on industry relevant projects. The wider group to consider these problems will be composed of applied mathematicians, experimentalists and representatives from industry. Proposed participants are: Geoff Evatt, Nico Gray (Manchester); Mark McGuinness (Wellington); Andrew Fowler, Vincent Cregan, Kevin Moroney, Ekeoma Ijioma (Limerick); John Hinch (Cambridge); Dr. Louise Clune, Rusal Aughinish Alumina Ltd. Askeaton, Co. Limerick, Ireland.

Two key projects have been identified with the industrial partners:

DEM simulation of granular flow on an elliptical bar wobbler feeder: The wobbler feeder is a continuous screening equipment used in the mineral industry for particle size separation of bulk materials. It is important that particles are sorted based on size distributions prior to further processing in a crusher unit. Our modelling

approach uses a Computer-Aided Design (CAD) for accurate representation of the equipment, coupled with a 3D particle-based Discrete Element Method (DEM) to describe the granular flow on the screen of wobbler feeder. Our main objective in this study is to establish key operating conditions that will ensure optimal recovery of fine product, which otherwise could overload the crusher. Thus, the capacity of the crusher is improved by minimising the amount of fine material entering the crusher. The study will investigate the potential of DEM to optimise industrial particle separation processes. A schematic of material flow on the wobbler feeder is shown in Figure 1. A DEM simulation of a wobbler feeder is shown in Figure 2.

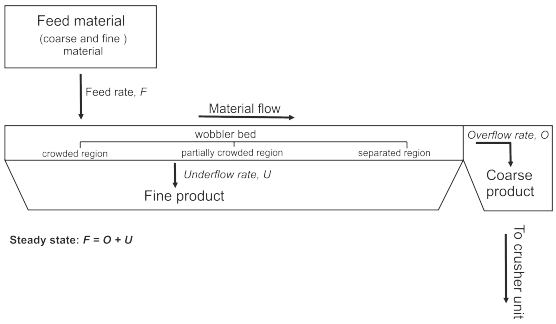


Figure 1: Scheme of the material flow on the wobbler feeder.

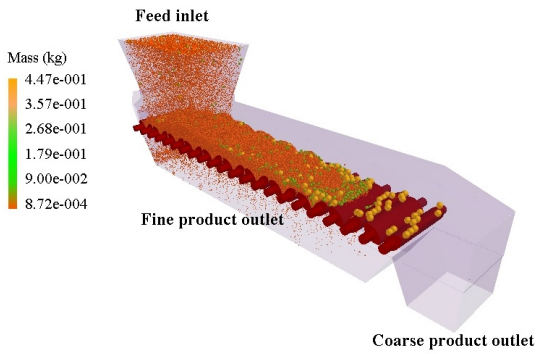


Figure 2: DEM simulation example of the wobbler feeder during a screening operation.

Modelling of granular flow during the manufacture of oral solid dosage forms: An understanding of the underlying physical mechanisms of granular flow is vital to the processing of pharmaceutical powder formulations into tablets (oral solid dosage forms) which are: (i) robust enough to survive subsequent shipping and transport, (ii) have a consistent drug loading and (iii) have the desirable drug release characteristics. There are various processing paths to manufacture tablets, including direct compression, dry granulation via roller compaction and wet granulation. To enable efficient process design and control, accurate models describing fundamental processes such as mixing, milling, granulation, granular flow, segregation and compaction are required. In particular, industry requires an accurate model of the physics of powder compression, which relates the tablet porosity to the applied compaction pressure and includes the dependence on measurable powder parameters and machine settings. This will assist in process control and speed-up the process of scale-up and transfer between equipment. Figure 3 shows a tensile strength testing of a manufactured tablet, one of the key tablet quality indicators.

Figure 3: Tensile strength testing of a manufactured tablet.

Activities

The past year has seen the establishment of the MOMEnTUM project in the University of Limerick. Key activities included:

- Establishment of strong connections with

Johnson & Johnson Automation Centre of Excellence and Rusal Aughinish Alumina. Interaction includes monthly meetings and access to data which can be used to extend and validate proposed models.

- Establishment of working relationships with researchers in the SSPC group. This connection allows access to a suite of laboratory equipment including state of the art powder rheometers to allow characterisation of various material physical and flow properties in order to parametrise granular flow and compaction models.
- Recruitment of postdoctural researchers, Dr. Ekeoma Ijioma and Dr. Kevin Moroney to work on the projects.

Planned activities for 2017

- Further development of connections with interested parties and groups within ECMI, the applied mathematics community and industry.
- The hosting a workshop with industry on industrially relevant granular flow topics. Funds will be leveraged through national and international sources (e.g. MI-NET COST Action).

Ekeoma Ijioma[1], Kevin Moroney[1]

MACSI, University of Limerick

Net Campus for Modeling Education and Industrial Mathematics

The ECMI Special Interest Group Net Campus for Modeling Education and Industrial Mathematics was launched in 2017 following initiatives taken by ECMI's Educational Committee. The aim of the SIG is to coordinate the already ongoing activities at the various ECMI centers in the field of online and digital education and extend them towards joint ECMI online courses.

Purpose

The ECMI educational committee has taken virtual education and web-supported solutions as one of its target areas to complement the other strategic areas like ECMI curriculum development, modeling weeks, mobility of students & staff etc.

The cutting edge knowledge in industrial mathematics is dispersed at small nodes of expertise. Online environments are a viable media to access this knowledge and support innovative processes, training and educational needs, to facilitate distributed consultation processes, etc. The evolution from textbook to interactive cross media environments means a new learning paradigm. Advantages include easy access and portability, flexible updates, dynamic edition, multi–/hypermedia tools from search facilities, quiz–structures to animations, interactive exercises, remote lectures and videoconference etc.

We envisage to build a European digital environment and web–portal for applied and industrial mathematics. More immediate goal is to share information and experience, describe examples of web based courses in applied mathematics and technologies for web publication of interactive documents. Such environment are suitable for students in applied mathematics and engineering programs in advanced BS and MS level as well as for persons who are already in their working life and are looking for continuing education and professional development. The courses should be based on customized content for a special applications area.

Opportunities

A block of online ECMI courses would be seen as a mean to facilitate "virtual mobility". ECMI nodes can use them as added features in their curricula and also as elements attracting interest from abroad to

their local educational program.

Researchers and teaching staff involved in designing and conducting online–based educational activities have a considerable stake in the core fields of this SIG.

Activities

The kick-off meeting initiating this SIG has been held at Koblenz University, Germany (March 23–24, 2017).

Kick–off meeting at Koblenz University, Germany.

As a direct outcome of the meeting we will set–up a first joint online course on Mathematical Modeling as a prototypic example that can be integrated at the final stage of the B.Sc. or at an early stage of the M.Sc. education at various ECMI centers. At the ECMI 2018 conference in Budapest we will organize a minisymposium dedicated to online educational issues.

Recording an online course at the University in Koblenz.

Coordinators: Dietmar Hömberg[1], Thomas Götz[2] and Matti Heiliö[3]

[1] Weierstrass Institute Berlin, Germany
[2] University Koblenz-Landau, Germany
[3] Technical University Lappeenranta, Finland

8

About ECMI

Mission

Mathematics, as the universal language of the sciences, plays a decisive role in technology, economics and the life sciences. European industry is increasingly dependent on mathematical expertise in both research and development to maintain its position as a world leader for high technology and to comply with the EU 2020 agenda for smart, sustainable and inclusive growth. ECMI initiatives in response to these needs may be summarized as follows:

- ECMI advocates the use of mathematical modelling, simulation, and optimization in industry
- ECMI stimulates the education of young scientists and engineers to meet the growing demands of industry
- ECMI promotes European collaboration, interaction and exchange within academia and industry

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May 2016

ECMI EUROPEAN CONSORTIUM FOR MATHEMATICS IN INDUSTRY