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

Imprint

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For more information please visit the ECMI website: https://ecmi-indmath.org
Print ISSN: 2616-7867
Online ISSN: 2616-7875
Mathematics with industry: driving innovation

Annual Report 2020
Reduction Model Order

Mold Model + Inverse Problem Solver

Heat Flux Estimation

Real-Time Steel-Mold Thermocouples Measurements

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Dear Colleagues,

we all thought that the COVID pandemic would be over by now, but we are still suffering the consequences of this strange situation. ECMI travelling activities requiring a physical presence have been reduced during the past year, giving place to a number of digital and hybrid events. We had online council meetings, a virtual ECMI modelling week, and a whole ECMI conference organised online by the University of Wuppertal. We should be proud that we have been able to keep scientific activities and collaborations alive in spite of the restrictions due to the pandemic. Young researchers deprived of proper social contact with their peers, their young colleagues, and their supervisors, are those who suffered the most. This year the annual report is slightly reduced in size. Nonetheless, we think that now more than ever it is important to showcase what has happened in the ECMI community, and to use the report to keep each other up to date.

We would like to thank all the authors of this issue, and acknowledge the help of Nicola Kirkham, Davide Murari and Matthew Tandy for helping editing this issue of the annual report.

Elena Celledoni, Department of Mathematical Sciences, NTNU
Andreas Münch, Mathematical Institute, University of Oxford
July 2020
Welcome from the President

Dear colleagues,

This is my last welcome message as ECMI President before Nataša Krejic took office. I would like to take the opportunity to thank her and all the other members of the Executive Committee for their support over the past three years, as well as Alessandra Micheletti for accepting to be Vice President of ECMI for the next term. I am sure that the new Executive Committee will bring a new energy to ECMI and let us all looking forward to a new and bright future.

The year 2020 was one of the most challenging years for each individual, but also for ECMI as a whole. Like many of you, we quickly had to find ways of adapting to the new reality. Shortly after the COVID-19 outbreak, ECMI turned its activities on-line instead. We organised webinars and a virtual Modelling Week, we launched a special issue of Journal of Mathematics in Industry devoted to collecting articles related to the spread of the SARS-CoV-2 virus, we promoted a student competition among other on-line activities.

These have been difficult times and the recent news about the evolution of the pandemic in Europe does not give hope that the situation will finish in the immediate future. All the plans for physical meetings in 2020 and the first semester of 2021 are affected, in particular the ECMI conference in Limerick. After considerable deliberation, the ECMI Council decided to go for a pure on-line conference that will take place from April 13th to April 15th 2021. This was not an easy decision, but we are confident that it will be an excellent event. The Scientific Committee has put together again a high quality, well balanced, scientific programme and the Local Organising Committee in Wuppertal has done amazing work in preparing the programme. I must point out that students from ECMI institutions who have completed a mathematical thesis on an industrial topic are eligible to apply for the Wacker Prize (MSc) or the Anile Prize (PhD). Even without the possibility for the physical contact, I am sure it will be an excellent memorable event and a great opportunity to strengthen collaborations between researchers.
and companies, promoting innovation and enhancing industry-academia links and knowledge sharing.

My final message is to encourage you to make the most of your ECMI membership. In this challenging time, our consortium needs fresh ideas and active nodes. Please continue to follow our blog and to support all ECMI activities. ECMI provides the perfect collaborative working environment for developing the industrial mathematics at European level.

Adérito Araújo University of Coimbra, March 2021
Activities and Initiatives
Modelling, simulation and optimization in a data-rich environment

Modelling, Simulation, and Optimization (MSO) remain the cornerstone for the development of most products in the fields of industry, health, energy, or even finance. Although High Performance Computing, Data Analytics and Artificial Intelligence offer new opportunities, their impact on innovation and the improvement of products and services could remain partial without a massive effort on the axes of modelling, simulation and complex systems optimization. Major opportunities, in particular the establishment of digital twins, rely on the connections at the interface between fields of expertise, domains, businesses, and across the complete lifecycle of products and systems. At the same time, methods have outpaced computational power in terms of capability over the past decades. The MSODE initiative outlined in this article is guided by the certainty that a high level approach on Modelling, Simulation, and Optimization, enriched by data analytics and intensive computing, is a considerable economic asset.

Vision
On the one hand, the future development of industry and society exhibits strongly increasing complexity, and at the same time ever-shorter innovation cycles. On the other hand, digitisation and the internet of things have led to an explosion of data and information. Without novel computational tools and paradigms, we will not be able to manage these challenges. There is a clear need to strengthen a European competitive advantage in industrial innovations, and to start a new initiative to meet the associated societal challenges ahead of us.
For almost all domains of science and engineering, and in almost all industrial sectors, model-based approaches are well established. A multitude of commercial and open source software for modelling, simulation, and optimization (MSO) based on mathematical models (“mathware”) is available. At the same time increasingly large amounts of process and product data are available and strong artificial intelligence solutions have been developed to exploit these. All this is fostered by computers becoming more and more powerful. These developments lead to a vision that in the near future holistic approaches can be achieved that combine all these developments. A complete industrial product or process in its whole life cycle can be accompanied by a virtual representation, often called a digital twin, that allows design optimization, process control, lifecycle management, predictive maintenance, risk analysis, and many other features. Digital twins are so important to business today that they were named one of Gartner’s Top 10 Strategic Technology Trends for 2017 [1], as well as in subsequent editions. They are becoming a business imperative, covering the entire lifecycle of an asset or process and forming the foundation for connected products and services. Companies that fail to respond will be left behind.

To establish this vision, or to even come close to it, several new developments that involve multiple scientific communities have to take place, and many obstacles have to be removed. A core need are novel mathematical technologies, to describe, to structure, to integrate, and to interpret across disciplines. Mathematics is the language of digital twins! Mathematics is the language of digital twins!

“Mathematics is the language of digital twins!”

History

NASA was the first to dabble with pairing technology - the precursor to today's digital twin - as far back as the early days of space exploration. How do you operate, maintain, or repair systems when you aren’t within physical proximity to them? That was the challenge NASA’s research department had to face when developing systems that would travel beyond our ability to see or monitor physically.

Figure 1. Concept of a digital twin (picture taken from [?])

Michael Grieves at the University of Michigan first wrote of the concept using the digital twin terminology in 2002 [2]. The digital twin serves as a bridge between the physical and digital world. The components are connected to a cloud-based system or a dedicated hardware that uses sensors to gather data about the real-time status and working conditions. This input is analysed against business and other contextual data. Lessons are learned and opportunities are uncovered within the virtual environment.
that can be applied to the physical world. Digital twins are powerful masterminds to drive innovation and performance. It is predicted the companies that invest in digital twin technology will see a 30 percent improvement in cycle times of critical processes.

**State-of-the-art**
Although first successes are reported [3] and many claims are made [4], neither the classical MSO approaches based on mathematical models and their software implementations, nor the constantly improving techniques for data analysis and machine learning will be enough to achieve this visionary goal [5, 6]. Even the rapid improvements in modern computing hardware, and especially algorithms/software, are not sufficient to achieve this. Currently, due to the high manual human effort, only major companies with large R&D departments can afford to build digital twins, but it would be desirable that companies on all scales can profit from the development. New generations of mathematical paradigms are required to convey today’s highly fragmented approaches in the various disciplines.

**Technology challenges**
Currently, models, methods, as well as software implementations and data sets are of highly different fidelity requiring many manual interactions. Figure 2 summarizes these interactions in a schematic way (including the interactions with existing initiatives). To meet the future challenges, it is necessary to develop novel MSO paradigms that allow a systematic MSO based approach to build highly automated modularized networks of model hierarchies (from very high fidelity physics based models to very coarse, surrogate, or even purely data based models), and that can deal with multi-physics and multi-scale systems. Key will be a convergence of artificial intelligence methods, and first principle approaches, typically used in MSO by laying down novel mathematical principles as the core language of digital twins. Furthermore, the model hierarchies should

- be able to (automatically) evolve with the availability of new information, data, or even changes in the process,
- allow adaptive models and solutions with seamless choice of accuracy and speed,
- allow real-time and interactive simulation and optimisation,
- be made robust towards inaccuracies in the data and the model,
- be able to quantify the uncertainties and risks that come with the determined solutions,
- lead to the convergence of artificial intelligence and physics-based models,
- exploit new computing architectures, e.g. combined cloud-edge solutions,
- be flexible for new user interaction concepts,
- allow the use of advanced black box solvers MSO software packages.

In the following section, we will go into more detail concerning one of these bullet points, namely the convergence of artificial intelligence and physics-based models, as it leads to great opportunities and many mathematical challenges.
Combining physics-based and data-based models

There is a multitude of opportunities emerging from the combination of physics-based modelling/simulation and data-based machine learning techniques. This is the way forward. On the one hand, we must not ignore the vast amount of fundamental knowledge, built up in many centuries, and only rely on data. On the other hand, we should exploit the increasing availability of data (both measured and computed) and computational resources to analyse these. Hence, we should combine the best of both worlds, make use of the advantages of available techniques in both fields, and thereby creating a breakthrough in the field of modelling and simulation for many scientific and engineering disciplines.

The U.S.A. is a frontrunner in this emerging area. The Department of Energy (DOE) is always very keen on new developments and is one of the biggest sponsors of scientific research. The national laboratories also play a key role in the development of new and emerging technologies. In January 2018 a workshop was held, under the auspices of the DOE, to identify basic research needs for the field of scientific machine learning. This information was then used to examine the opportunities, barriers, and potential for high scientific impact through fundamental advances in its mathematical, statistical, and computational research foundations. The workshop report [7], published early 2019, concludes that scientific machine learning and artificial intelligence will have broad use and transformative effects across all fields of science. The report was followed by a sequence of town hall meetings organised by the Argonne, Oak Ridge, and Berkeley National Laboratories with more than 1000 scientists and engineers participating. The goal of the town hall series was to examine scientific opportunities in the areas of artificial intelligence, Big Data, and high-performance computing (HPC) in the next decade, and to capture the big ideas, grand challenges, and next steps to realising these opportunities. The terminology “AI for Science” was used to broadly represent the next generation of methods and scientific opportunities in computing, including the development and application of AI methods (e.g., machine learning, deep learning, statistical methods, data analytics, automated control, and related areas) to build models from data and to use these models alone or in conjunction with simulation and scalable computing to advance scientific research. An extensive report [8] with conclusions for many scientific and engineering disciplines, ranging from chemistry, materials and nanoscience, biology and life sciences, nuclear and high energy physics to engineering and manufacturing was published at the end of 2019. The main overall conclusion is that “AI will not magically address all opportunities and challenges discussed in the report. Much work will be required within all science disciplines, across science infrastructure, and in the theory, methods, software, and hardware that underpin AI methods. Bringing AI to any specific domain - whether it is nuclear physics or biology and life sciences - will demand significant effort to incorporate domain knowledge into AI systems, quantify uncertainty, accuracy, and appropriately integrate these new mechanisms into state-of-the-art computational and laboratory systems.”

Both reports agree to a large extent with our point of view: exploiting prior information and knowledge to construct combinations of physics-based models and data-based learning machines. One of the fore-runners in this field is George Karniadakis of Brown University [9, 10, 11], who is strongly promoting the field of, what he calls, physics-informed neural networks (PINNs), cf. Figure 3 below being an example of how to combine neural networks with the physics-informed model structure (PDE).
The general aim of Karniadakis’ work is to set the foundations for a new paradigm in modelling and computation that enriches deep learning with the long-standing developments in mathematical physics, or vice versa depending on the angle of view. Methods developed utilise a fully connected neural network (NN) to map a space-time domain to the unknown solution of an initial and boundary-value problem. The NN is inserted into the governing partial differential equation (PDE) or variational principle and symbolically differentiated. This yields another NN, with modified activation functions but identical parameters, a so-called physics-informed NN. No labelled data is required for training. Rather, a combined loss function is minimised. One component is associated with the initial and boundary conditions, the other either with the residual norm or the variational functional of the PDE. The latter component enforces the structure of the physics equation.

Concepts similar to that proposed by Karniadakis are being developed in several places, as more and more researchers are realising that the integration of machine learning and more general artificial intelligence technologies with physical modelling based on first principles will impact scientific computing in science and engineering in fundamental ways. One such development is to embed physics simulation into deep learning. This work is motivated by control engineering, in particular by the development of intelligent reinforcement learning agents. "The end result is that we can embed an entire physical simulation environment as a layer in a deep neural network, enabling agents to both learn the parameters of the environments to match observed behaviour and improve control performance via traditional gradient based learning." [12]. The main ingredient is an adjoint-based solver, which allows efficient backpropagation of gradients and avoids their tedious computation by finite differences. Then, deep convolutional neural networks can be integrated seamlessly with physics-based models in machine learning platforms such as PyTorch and TensorFlow. Another development is in combining field inversion and machine learning (FI[ML] [13]). This method stems from computational fluid dynamics (CFD). For turbulent flows one may either solve Navier-Stokes equations by direct numerical simulation (DNS) or large eddy simulation (LES). This approach is accurate but numerically expensive, since it involves a range of space and time scales. On the other hand, one may use the Reynolds averaged Navier-Stokes (RANS) method, where turbulence effects are accounted for by phenomenological models rather than first principles. This method is much more efficient but less accurate. With the help of FI[ML], both approaches can be combined.

The foregoing clearly demonstrates that we are at a tipping point within scientific and engineering research: first principle-based models will need to be combined with data-based models. Such hybrid modelling combines first principle-based models with data-based models into a joint architecture, and has the potential to improve the Pareto trade-off between simulation accuracy and simulation cost significantly, bringing scientific computing in science and engineering to the next level. Awareness of domain knowledge can enhance domain-agnostic data in terms of accuracy, interpretability, and robustness of models.
Furthermore, incorporating scientific domain knowledge has the potential to dramatically reduce data requirements, as well as to accelerate training and prediction. Domain knowledge is found in many forms, such as physical principles, constraints, symmetries, conservation laws, and other knowledge gained from theoretical or computational studies.

The future needs Computational Science and Engineering, blending data driven and physics-based perspectives

“The future needs Computational Science and Engineering, blending data driven and physics-based perspectives”

Karen Willcox, director Oden Institute for Computational Engineering and Sciences

Scientific domain knowledge can be expressed in many forms, including physical models (e.g., ab initio or first-principles physics), physical constraints (e.g., symmetries, invariances, conservation laws, asymptotic limits), computational simulations, uncertainties, correlations in space and time, and structural forms (e.g., discrete, graph-like, non-smooth data). Looking into more detail, we notice that a large class of models can be decomposed into conservation laws and constitutive laws. The conservation laws are of topological nature and can therefore be discretised easily, leaving little room for data-driven techniques. The situation is different for the constitutive relations, which are of metric nature, and encode phenomenological (material) properties.

Except for simple media (local, linear) there are many potential complications (non-local, hysteretic, non-linear, multi-scale, multi-physics, etc.). Here, data-driven models can be useful, provided that the models fulfil certain admissibility criteria, which can often be expressed in terms of invariance with respect to symmetry groups. It is also clear that the developments of combining real intelligence with artificial intelligence towards hybrid modelling are still in their infancy. Only in the last few years, researchers have started to fully acknowledge the potential of combining first principle-based models with neural networks or other artificial intelligence techniques. The number of publications in the field is growing exponentially (see, for example, Gartner’s assessment [1]). Key high-level challenges, still open and hence to be addressed, are hybrid modelling methodologies that:

- are applicable across a wide range of scientific domains,
- can deal with large-scale and networked systems,
- preserve fundamental system properties, such as stability, structure, dissipativity, etc.,
- strike a superior balance between accuracy and complexity of the resulting models,
- guarantee robustness of model validity, while limiting the amount of measured data needed.

**Conclusion**

We strongly believe that mathematicians should focus their attention on creating novel synergies between physics-based and data-driven approaches, in order to develop a next-generation modelling framework for physical processes and engineering systems. To this end, a detailed mathematical theory needs to be developed to support such a synergetic marriage, leading to models within science and engineering with superior model accuracy,
computational efficiency, robustness to uncertainties and explainability. This field will be full of very nice challenges, and it is hoped that many mathematicians will take up these challenges. Together with industry, this will also lead to true digital twins, needed to bring Europe and its industry forward. These are exciting times!

Wil Schilders¹, Past president of ECMI (2010-2011) and EU-MATHS-IN (2016-2020) ¹ Eindhoven University of Technology

References


A MaGiC experience

Can you imagine a life of waking up early in the morning, doing mathematics with your good friends and colleagues until noon, then taking a long break for skiing in beautiful surroundings, before finishing off the day with some more mathematics?

This is in fact what you do when you attend the MaGiC meeting in the Norwegian mountains. “Manifolds and Geometric Integration Colloquia” is an annual workshop that started back in 1999 by the numerical analysis communities at NTNU and the University of Bergen. The venue has been at different sites in the mountains, and in the early years, with little funding available, it was organised in some primitively equipped cabin where the participants took turns in cooking and doing the house chores, and the lectures were held in a nearby location where a blackboard and a slide projector could be set up. Usually there were about 15-20 participants in total, including PhD students from Trondheim, Bergen, and various European countries. In recent years, the economy has improved and the meeting has been held at places with a little more comfort. But the daily schedule never changed, always lectures from 8:30-11:00, skiing from 11:00-16:00 and lectures again from 16:30-19:00, and finally dinner and card games. The MaGiC meetings have of course also suffered from the pandemic in the last two years. This year it was organised as a hybrid meeting at Ilsetra near the Olympic town of Lillehammer. 7 participants were accommodated in two large apartments, and the living room in one of them was set up as a provisional lecture room with video capabilities. Almost 30 people altogether followed talks over 3 days, some given from the apartment, but most of them from locations around Europe.

Stefan Holzinger’s talk

MaGiC has been adopted as an activity in the ETN project, THREAD\(^1\), and most of the 14 Early stage researchers (ESRs) in THREAD took part. A large portion of them also gave talks about their ongoing PhD work.

\(^1\)https://thread-etn.eu/
The programme was more diverse than usual, varying between theory, applications and software. Munthe-Kaas and Stava discussed algebraic aspects of numerical integrators. The talks by Çokaj, Curry, Holzinger, Leone and Murari were about Lie group integration methods. Then there were geometric integration talks about variational methods and methods with conservative properties by Li, Stavole, Tapley, Tumiotto and Zupan. Additionally, there were some interesting talks with a more applied or software related focus such as the ones by Debeurre, Gustad, Jelusic, Manfredo and Tomec. A complete list of titles and abstracts can be found at https://wiki.math.ntnu.no/thread/start/nwt9/abstracts. Even though only a small number of participants were physically present at Ilsetra, the usual skiing break in the middle of the day was included in the schedule.

Around Europe, the participants in their respective locations were encouraged to go for a walk, a bicycle ride or a run and take photos that were later posted on the conference web page. In this way, some of the spirit of the MaGIC meeting could be shared across several locations.

The MaGIC meeting of 2021 was a great success given the circumstances of the pandemic. But we all agreed that in 2022 we shall meet for real, and hope to have as many ESRs as possible joining us somewhere in the Norwegian mountains to enjoy some math, skiing and card games.

THREAD: Numerical Modelling of Highly Flexible Structures is a European Training Network on mathematical modelling and simulation highly flexible slender structures like yarns, cables, hoses or ropes which are essential parts of high-performance engineering systems. The complex response of such structures in real operational conditions is far beyond the capabilities of current modelling tools that are at the core of modern product development cycles.

Brynjulf Owren, NTNU, Norway
4

Featured People
Interview: Carola-Bibiane Schönlieb

Carola-Bibiane Schönlieb is the chair of the Committee for Applications and Interdisciplinary Relations of the European Mathematical Society (EMS). She is a professor of Applied Mathematics at the Department of Applied Mathematics and Theoretical Physics (DAMTP) at the University of Cambridge, in the UK. Her main area of research is inverse problems for image analysis with variational techniques and partial differential equations. In the last eight years, she has done extensive work in the area of machine learning and deep neural networks for inverse problems in imaging. She is the head of the Cambridge Image Analysis group at DAMTP, at the University of Cambridge, with about twenty PhD students and Post Docs.

Carola can you tell us about the scope of the EMS Committee for Applications and Interdisciplinary Relations that you are the head of?

The EMS Committee for Applications and Interdisciplinary Relations (CAIR) wants to promote Applied Mathematics as a whole through and within EMS. It’s mission is to foster interactions between Mathematics and other disciplines in Sciences, Technology, and Social Sciences and to promote the implications of all areas of Mathematics in this endeavour. In doing so it cooperates with other, sometimes more specialised, societies on the European and global level and with applications-oriented member societies, especially in further improving the public and political awareness about the importance of mathematics to cultural, economic and social development.

In particular, the EMS and ECMI, the European Consortium for Mathematics in Industry, have signed a collaboration agreement since 2012, which at the level of...
the EMS will be carried out by its Committee for Applications and Interdisciplinary Relations (CAIR).

What is your vision as the head of this committee?
I am keen to promote mathematics as a discipline, interactions between different mathematical areas and its sometimes surprising applications to problems in other disciplines and in our everyday life. Together with my co-Chair Josef Malek we have started chairing the committee only in January this year, so are still finding our way. What is clear to us is that mathematical research that is inspired by or indeed resides at the interface with other disciplines and applications is an area of research that we are very passionate about. It is my ambition to convey this excitement and support fruition of such mathematics within Europe and globally. Both from within mathematics as well as to the outside world. Luckily we are supported by the wonderful members of CAIR who are all very dedicated to this cause. Moreover, we are very keen to collaborate with ECMI who have been pioneering industrial mathematics for several years.

You are an expert of inverse problems and you were a plenary speaker at the ECMI conference 2021, can you tell us what are your current research interests?
I am interested in the interaction between data-driven mathematical models, in particular those based on deep learning (DL), with domain specific knowledge contained in physical-analytical models. My main focus is on solving ill-posed inverse imaging problems that are at the core of many challenging applications in natural sciences, medicine and life sciences, as well as in engineering and industrial applications.

Inverse problems are about the reconstruction of an unknown physical quantity from indirect measurements. In imaging, they appear in a variety of places, from medical imaging, for instance MRI or CT, to remote sensing, for instance Radar, to material sciences and molecular biology, for instance electron microscopy. Here, imaging is a tool for looking inside specimen, resolving structures beyond the scale visible to the naked eye, and to quantify them. It is a mean for diagnosis, prediction and discovery.

Most inverse problems of interest are ill-posed and require appropriate mathematical treatment for recovering meaningful solutions.

Classically, such approaches are derived almost conclusively in a knowledge driven manner, constituting handcrafted mathematical models based on physical-analytical principles. Examples include variational regularization methods with Tikhonov regularization, the total variation and several sparsity-promoting regularizers such as the L1 norm of Wavelet coefficients of the solution.

While such handcrafted approaches deliver mathematically rigorous and computationally robust solutions to inverse problems are about the reconstruction of an unknown physical quantity from indirect measurements. In imaging, they appear in a variety of places, from medical imaging, for instance MRI or CT, to remote sensing, for instance Radar, to material sciences and molecular biology, for instance electron microscopy. Here, imaging is a tool for looking inside specimen, resolving structures beyond the scale visible to the naked eye, and to quantify them. It is a mean for diagnosis, prediction and discovery.

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While such handcrafted approaches deliver mathematically rigorous and computationally robust solutions to inverse

Knowledge driven (total variation regularised) solution to the inverse problem of CT on the left, and a data driven solution (based on deep learning) on the right. Collaboration with Subhadip Mukherjee1.

While such handcrafted approaches deliver mathematically rigorous and computationally robust solutions to inverse

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problems, they are also limited by our ability to model solution properties accurately and to realize these approaches in a computationally efficient manner.

Recently, a new paradigm has been introduced to the solution of inverse problems, which derives solution to inverse problems in a data driven way. Here, the inversion approach is not mathematically modelled in the classical sense, but modelled by highly over-parametrised models, typically deep neural networks, that are adapted to the inverse problems at hand by appropriately selected (and usually plenty of) training data. Current approaches that follow this new paradigm distinguish themselves through solution accuracies paired with computational efficiency that were previously unconceivable. At the same time, the mathematical foundations of these approaches are almost completely missing. Indeed, recent studies have shown that most existing DL solutions for inverse problems are intrinsically unstable as they fail to address the inherent ill-posedness of the underlying physical models. This huge gap between qualitative performance and lack of stability is dangerous and prone to misuse.

Mathematically rigorous foundation for data driven models for inverse problems, in particular those based on DL, by combining them with domain specific knowledge contained in physical-analytical models.

Doing this, I collaborate with mathematicians from various different backgrounds as well as with scientists in other disciplines, to develop demonstrations for these approaches for selected high-impact applications.

You are one of the organisers of the programme in Mathematics of Deep learning at the Isaac Newton Institute of Mathematical Sciences lasting from July to December 2021. What are the objectives of this programme?

The main idea behind this programme is to develop a mathematical foundation of deep learning. We address theoretical questions in two realms:

- Theoretical foundations of deep learning independent of a particular application.
- Theoretical analysis of the potential and the limitations of deep learning for mathematical methodologies, in particular, for inverse problems and partial differential equations.

We are gathering the top experts from various areas of mathematics and of the theory of machine learning, including computer scientists, physicists, and statisticians. The programme is organised with both remote participation and local visitors who are actually present at the Isaac Newton Institute of Mathematical Sciences in Cambridge, and there is a high number of early career researchers.

I am working towards the development of a mathematically rigorous foundation for data driven models for inverse problems, in particular those based on DL, by combining them with domain specific knowledge contained in physical-analytical models.

Which advice would you give to

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3 For more information about the activities of this programme you are welcome to visit the webpage https://www.newton.ac.uk/event/mdl/. #NewtonMDL2021
young people and in particular to young female students passionate for Mathematical research and with ambitions of a brilliant career in applied Mathematics?

Follow your passion and never let anyone try to categorise you - there are many different ways of working and of how mathematics is done, find yours.

Can you tell us about your private life and what you like to do when you are not at work?

A major component of my private life is taken up by my husband, my family, my friends and our dog Sunny. I love hiking and playing with Sunny.

Interviewed by Elena Celledoni, NTNU, Norway
Projects and Case Studies
There is an increasing scientific interest in automatically analysing and understanding human behavior, with particular reference to the evolution of facial expressions and the recognition of the corresponding emotions. In this project we propose a technique based on Functional ANOVA to extract significant patterns of face muscles movements, in order to identify the emotions expressed by actors in recorded videos. This research is part of the BIGMATH project, a European Industrial Doctorate funded by the European Union’s Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie Grant Agreement No 812912.

Here we describe the main mathematical aspects of the work developed by Rongjiao Ji, one of the Early Stage Researchers (ESRs) enrolled in the BIGMATH PhD programme, who is jointly supervised by academic advisors, coming from the universities of Milan and Novi Sad, and by industrial advisors, coming from the company 3Lateral (Serbia, producing virtual reality for entertainment).

Problem description

The study of human facial expressions and emotions never stops in our daily life while we communicate with others. Following the increased interest in automatic facial behavior analysis and understanding, the need of a semantic interpretation of the evolution of facial expressions and of human emotions has become of interest in recent years [1]. In this project, based on a work cooperated with the Serbian company 3Lateral, which has special expertise on building visual styles and designs in animation movies, we want to explore functional statistical instruments to identify the emotions while analyzing the expressions through recorded videos of human faces. The final aim of this research is to use this information to better and more realistically establish virtual digital characters, able to interact autonomously with real humans [2].

The data that we consider are multivariate longitudinal data, showing the evolution in time of different face muscles contraction. Functional Data Analysis (FDA) offers the possibility to analyze the entire expression evolution process over time and to gain detailed and in-depth insight into the analysis of emotion patterns. The basic idea in functional data analysis is that the
measured data are noisy observations coming from a smooth function. Ramsay and Silverman [3] describe the main features of FDA, that can be used to perform exploratory, confirmatory or predictive data analysis.

In our application, Functional ANOVA can be used to determine if there are time-related differences between emotion groups by using a functional F-test [4].

“Our final aim of this research is to use this information to better and more realistically establish virtual digital characters, able to interact autonomously with real humans”

Our study is based on the RAVDESS (Ryerson Audio-Visual Database of Emotional Speech and Song) dataset [5], which contains 24 professional actors (12 female, 12 male) to offer the performance with good quality and natural behavior under the emotions: calm, happy, sad, angry, fearful, disgusted and surprised. Also a neutral performance is available for each actor. The actors are vocalizing one lexically-matched statement in a neutral North American accent (“Kids are talking by the door”).

![Emotions represented by the actors in RAVDESS](image)

To avoid being lost in the difference of individual facial appearances, when analyzing the expressions and emotions, researchers mostly focus on the movements of individual facial muscles which are encoded by the Facial Action Coding System (FACS) [6]. FACS is a common standard to systematically categorize the physical expression of emotions, extracting the geometrical features of the faces and then producing temporal profiles of each facial movement. Such movements, corresponding to contraction of specific muscles of the face, are called action units (AUs). As action units are independent of any interpretation, they can be used for any higher-order decision-making process including recognition of basic emotions. Following the FACS rules, OpenFace [7], an open-source software, is capable of recognizing and extracting facial action units from facial images or videos. We applied OpenFace to extract the engagement degrees of action units for the videos in RAVDESS. The extracted action units include 17 functions for each video, taking values in \([0, 5]\), sampled in about 110 time points (which is also the number of frames in each video).

**Methods**

We represent the action units evolution recorded on each video as a multivariate time series

\[ Y(t) = (Y_1(t), \ldots, Y_d(t), \ldots, Y_D(t)), t \in [0, T] \]

containing a set of \(D\) univariate longitudinal functions \((D = 17\) in our case), each defined on the finite interval \([0, T], 0 < T < +\infty\). The observation of \(Y\) on our sample of videos provides the set \(Y_1, \ldots, Y_n\) of multivariate curves, that we represent as multivariate functional data.

First we aligned the action units functions into a common registered internal timeline that follows the same pronunciation speed, to control the influence of the specific pronounced sentence and to detangle it from the influence of the emotions.
we then investigated if there exist patterns which could discriminate the different emotions, using a Functional ANOVA model.

Let $y_{k,g}(t)$ be the evolution of one specific action unit in the video $k \in \{1, \ldots, K\}$ (in our case $K = 48$) for emotion $g \in \{1, \ldots, 7\}$. We can assume that

$$y_{k,g}(t) = \mu_0(t) + \alpha_g(t) + \epsilon_{k,g}(t), \quad (5.1)$$

where $\mu_0(t)$ is the grand mean function due to the pronounced sentence and to the actor, independent from all emotions. The term $\alpha_g(t)$ is the specific effect on the considered action unit of emotion $g$, while $\epsilon_{k,g}(t)$ represents the unexplained zero mean variation, specific of the $k$-th video within emotion group $g$. To be able to identify them uniquely, we require that they satisfy the constraint $\sum_{g=1}^{7} \alpha_g(t) = 0, \forall t$.

By grouping the videos representing the same emotion, we can define a $8K \times 8$ design matrix $Z$ for this model, with suitable 0 and 1 entries, as described in [3, Section 9.2], and rewrite Equation 5.1 in matrix form: $y = Z\beta + \epsilon$, where $\beta = [\mu_0(t), \alpha_1(t), \ldots, \alpha_7(t)]^T$.

To estimate the parameters we used a functional least squares fitting criterion.

In order to investigate which emotions are significantly influencing the change of the action units patterns, for each emotion $g$ and for each action unit we tested the null hypothesis $H_0 : \alpha_g(t) = 0$.

Similarly to the classical univariate ANOVA model, the statistics used to test $H_0$ is

$$FRATIO(t) = \frac{MSR(t)}{MSE(t)}$$

whose distribution under $H_0$ is estimated through a permutation test.

**Preliminary results**

We applied the F-test described in the previous section to detect, for each emotion, which AUs have a mean behaviour significantly different from the neutral performance and in which time period during the videos. In Figure 2 we illustrate the results for emotion angry, as an example.

![Figure 2: The functional coefficients of action units 07 (Lid Tightener), 10 (Upper Lip Raiser) and 26 (Jaw Drop) under neutral and angry emotion and the corresponding F-test results](image)

The first row of Figure 1 illustrates the estimated mean $\mu_0(t)$ (neutral emotion) and the angry emotion effects for three action units. The second row displays the observed F-statistics curves together with the pointwise and maximum 95% quantile for the F-distribution in the dashed and horizontal dotted lines respectively.

Thus when the observed F-statistics are higher than the critical level lines, the emotion has a significant affect on the AU's pattern. We found in general three main situations of influence of one emotion on expression evolution: 1. locally strengthening 2. locally inhibiting 3. globally strengthening. Further, we pointed out the time zones of significant effects due to the angry emotion on the action units in Figure 3, which is beneficial to understand and detect dynamically when and how the facial muscles contractions differ from the baseline.
“We found in general three main situations of influence of one emotion on expression evolution:
1. locally strengthening
2. locally inhibiting
3. globally strengthening”

Table 1 summarizes for each emotion of interest the related action units that show significant changes from the neutral case for our videos dataset. Similarly to the example of angry, we found that for happy and disgust emotions more action units have the globally strengthening effect on a large time range. The Sad emotion sometimes affects the action units to be more constant than in neutral case. Emotion Fearful has more influence on upper half face (brows, eye lids and nose), while emotion calm is more related with the center of the face (Cheek Raiser, Lid Tightener and Lip Corner Puller). The Surprised emotion is the only emotion where AU45 is significantly influenced.

<table>
<thead>
<tr>
<th>Emotions</th>
<th>Related Action Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>Calm</td>
<td>06, 07, 10, 12, 14, 23</td>
</tr>
<tr>
<td>Happy</td>
<td>01, 06, 07, 10, 12, 14, 17, 23, 25, 26</td>
</tr>
<tr>
<td>Sad</td>
<td>04, 06, 10, 14, 17, 20, 23, 25</td>
</tr>
<tr>
<td>Angry</td>
<td>04, 06, 07, 09, 10, 12, 14, 17, 23, 26</td>
</tr>
<tr>
<td>Fearful</td>
<td>04, 09, 10, 12, 14, 15, 17, 23, 25, 26</td>
</tr>
<tr>
<td>Disgust</td>
<td>04, 06, 07, 09, 10, 12, 14, 17, 23, 25, 26</td>
</tr>
<tr>
<td>Surprised</td>
<td>06, 09, 10, 12, 14, 15, 17, 23, 25, 26, 45</td>
</tr>
</tbody>
</table>

Table 1: Emotions with corresponding significant action units

As a conclusion, our results can be joined in a multivariate setting and exploited to build a classifier able to automatically recognize the emotions.
References


ROMSOC - Reduced Order Modelling, Simulation and Optimization of Coupled Systems

ROMSOC is a European Industrial Doctorate (EID) program funded by the European Commission as part of the Marie Skłodowska-Curie Actions within the framework of Horizon 2020. The project brings together 15 international academic institutions and 11 industry partners and supports eleven Early Stage Researchers (ESRs) working on individual research projects in completing their PhD. ROMSOC aims to develop novel modelling, simulation and optimization techniques for multi-disciplinary models with application in different industrial sectors.

Product development today is increasingly based on simulation and optimization of virtual prototypes of products and processes involved therein. Mathematical models serve as digital twins of the real products and processes and are the basis for their optimization, control of design, and improve their functionality. The models must meet very different requirements: very specific mathematical models are required to understand and simulate the needs of each industrial process, while the most general models are the prerequisites to handle the complexity of its control and optimization. To achieve best performance of mathematical modelling, simulation, and optimization (MSO) techniques a complete model's hierarchy should be created. The most efficient way in industrial applications to achieve such a model's hierarchy is to use a sufficiently fine parameterized model and then apply model order reduction (MOR) techniques to tune this fine level to the accuracy, complexity and computational speed needed in simulation and parameter optimization. The main objective of the ROMSOC project is to further develop this common framework and, driven by industrial applications, to lift mathematical MSO and MOR methods to a new level of quality. In particular, the development of high dimensional and coupled systems presents a major challenge for simulation and optimization and requires new MOR techniques.
The doctoral training programme

The ROMSOC doctoral programme trains eleven ESRs to PhD level by means of joint courses and training events on the one hand, and individual collaborative research projects, based on the strengths of the participating academic and industrial partners, on the other hand. The core research programme is defined with respect to three major mathematical methodologies: Coupling methods, Model Reduction methods and Optimization methods, that interact with three main applications fields: Optical and electronic systems, Economic processes, and Materials systems. ROMSOC targets both technological and scientific priorities, their implementation in software and the testing and validation on industrial benchmark problems. The young researchers are supervised by expert tandems, each consisting of an academic and an industrial representative. They spend at least half the time in a company, the rest in a research facility.

The strong demand for synergies between the MSO and MOR methods and the requirements of industrial users is realized through common training schools. The various training activities that took place within the programme comprises the following courses:

- **Multiphysics modelling** organized by the Technological Institute for Industrial Mathematics (ITMATI) in collaboration with the Universidade da Coruña (UDC) and Universidade de Santiago de Compostela (USC)
- **Advanced Programming for Scientific Computing** organized by MOX Politecnico di Milano (PoliMi)
- **Reduced Order Methods for Computational Mechanics** organized by Scuola Internazionale Superiore di Studi Avanzati (SISSA)
- **Mixed integer linear and nonlinear optimization** organized by Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU)
- **PDAE modelling and simulation** organized by the Bergische Universität Wuppertal (BUW)
- **Numerical methods for fluid-structure interaction** organized by MOX Politecnico di Milano (PoliMi)
- **Hierarchical energy based modeling** organized by the Technische Universität Berlin (TUB)
- **Introduction to Information-Based Complexity** organized by the Johann Radon Institute for Computational and Applied Mathematics (RICAM)
- **A Numerical Introduction to Optimal Transport** organized by the Institut national de recherche en informatique et en automatique (INRIA)
- **Deep Learning** organized by the Universität Bremen (U-HB)
- **European Study Groups with Industry (ESGI 139 & ESGI 147) jointly organized by the Technological Institute for Industrial Mathematics (ITMATI) and the Spanish Network for Mathematics & Industry (math-in)
- **Communicating scientific research** organized by MOX Politecnico di Milano (PoliMi)
- **Ethical aspects of the research** organized by the Technische Universität Berlin in cooperation with the Evangelische Hochschule Nürnberg (EVHN)

First Results

Numerical simulations are commonly used to study complex physical systems and in the process of design and optimization. These simulations involve the solution of full order models (FOM) generated by the discretization of partial differential equations (PDEs). The required full order models (FOM) involve coupled multi-physics problems for which the use of standard numerical methods to compute accurate
approximated solutions demands high computational costs and usually fails to provide real-time simulation tools. Hence, considering reduced order models (ROM) at the same time is a necessity for the design of computational tools potentially applicable to real-world industrial problems. Major breakthroughs can be expected when model hierarchies of ROM and MSO software are constructed in such a way that they can automatically adapt to different user needs in accuracy and computational efficiency.

In the following short stories about different industrial problems studied by ROMSOC ESRs are introduced.

**Real-time computing methods for Adaptive Optics control.** The image quality of Extremely Large Telescopes (ELTs) suffers heavily from atmospheric perturbations. In order to correct for the optical distortions in the atmosphere a technique called *Adaptive Optics* is used (cf. Fig. 1, upper part).

![Figure 1: Wavefront sensors (WFS) together with guide stars (GS), deformable mirrors (DMs) and a reconstruction algorithm are utilized to obtain a sharp image. The augmented FEWHA method fulfills the quality as well as the real-time requirements for the ELT.](image)

The goal within ROMSOC is to establish a ROM framework in the atmospheric tomography. In a cooperation of the Johannes Kepler Universität Linz (Austria) and Microgate Srl (Italy) an efficient, iterative solver for the ELT has been developed and implemented on real-time hardware [1, 2]. This method, called *augmented FEWHA*, fulfills the quality as well as the real-time requirements (cf. Fig. 1, lower part).

**Optimal Transportation approach of inverse free-form optical surfaces design.** *Free-form Optics* deals with the problem of designing the reflector of a light source with a given radiation pattern $\mu$ in such a way that the reflected light has a different, desired prescribed pattern $\nu$ (cf. Fig. 2).

![Figure 2: Light source as an interval that emits from each point into a set of directions according to a given radiation pattern $\mu$.](image)

Within the project and in a cooperation of INRIA (France) with Signify N.V. (Netherlands), regularization strategies for computing the desired shape of the reflector were developed and analyzed [3], based on the theory and new fast solvers of the *Optimal Transport Problem*. Also evaluation tools were developed in order to assess the quality of the received radiation pattern. Finally, the regularization and evaluation were combined to design an iterative improvement method for the...
reflector design (cf. Fig. 3).

Desired and RayTraced illumination patterns

*Figure 3: The ray-traced radiation pattern from the developed iterative method converges to the desired prescribed image.*

**Model order reduction for parametric high dimensional models in the analysis of financial risk.** The risk analysis of financial instruments requires the valuation of such instruments under a wide range of future market scenarios. To obtain a ROM, a MOR approach based on the proper orthogonal decomposition (POD) has been developed and implemented [4] in a cooperation of TU Berlin (Germany) and MathConsult GmbH (Austria). Adaptive greedy (AG) sampling is used to overcome the drawbacks of the classical greedy (CG) sampling. The approach, tested for different financial instruments under two prominent models (one-factor and two-factor Hull-White models), provides a significant speedup within an acceptable accuracy over a full model approach (cf. Fig. 4), demonstrating its potential applications in the historical or Monte Carlo value at risk calculations.

*Figure 4: The histogram shows the floater instrument solved for 10000 different scenarios using the ROM. The results are sorted into three categories: the likely return in favorable, moderate, and unfavorable market conditions. The relative error shows that the ROM is an excellent approximation of the FOM. The simulation of the ROM is at least 8-12 times faster than for the FOM.*

**Efficient computational strategies for the control process of continuous casting machines.** In continuous casting of steel, the most critical component is the mold, where the steel begins its solidification. To ensure a proper control of the process, it is necessary to know how the steel is behaving inside the mold. However, it is not possible to make measurements inside the solidifying steel and the only available data are pointwise temperature measurements in the interior of the mold plates. To provide a tool for the proper control of the process, a methodology for the real-time estimation of the heat flux at the steel-mold interface given the temperature measurements has been developed [5] (cf. Fig. 5). With this tool, we allow the caster operator to quickly detect any malfunctioning in the casting, increasing the safety and the productivity of continuous casters. The project is a cooperation of ITMATI (Spain), SISSA (Italy) and Danieli & C. Officine Meccaniche S.p.A. (Italy).

*Figure 5: Real-time estimation of the heat flux at the steel-mold interface for given temperature measurements based on the mold model and model hierarchies derived from MOR methods.*
Numerical simulations for the fluid-structure interaction arising in blood pumps based on wave membranes. Numerical simulations of cardiac blood pump systems are integral to the optimization of device design, hydraulic performance and hemocompatibility. In wave membrane blood pumps, blood propulsion arises from the wave propagation along an oscillating immersed membrane, which generates small pockets of fluid that are pushed towards the outlet against an adverse pressure gradient. Within the project, the Fluid-Structure Interaction (FSI) between the oscillating membrane and the blood flow has been studied via three-dimensional simulations using the Extended Finite Element Method [6, 7] (cf. Fig. 6).

![Blood velocity field](image1)

**Figure 6:** The blood velocity field (left) and the flow vorticity field (right) in an innovative blood pump device developed at CorWave SA (France). The progressive wave in the elastic membrane transports blood masses towards the outlet channel (bottom part), resulting in effective outflow generation. In addition, we can check the flow patterns induced by the wave membrane displacement, because some blood adverse events, such as thrombosis, are related to flow vorticity.

In a cooperation of MOX-PoliMi (Italy) and CorWave SA (France), the numerical FSI model has been successfully validated against in-vitro experimental data and employed to predict the hydraulic performance across different pump designs and operating conditions [8].

Other ESR projects that are not covered in detail in this report involve the modelling and numerical simulation of coupled thermo-acoustic multi-layer systems for enabling particle velocity measurements in the presence of airflow (ITMATI (Spain) & Microflown Technologies BV (Netherlands)), the coupling of MOR and Multirate techniques for coupled heterogeneous time-dependent systems (BUW (Germany) & STMicroelectronics SRL (Italy)), the integrated optimization of international transportation networks (FAU (Germany) & DB Cargo Polska S.A. (Poland)), ROM for coupled thermo-hydro-mechanical phenomena arising in blast furnaces (SISSA (Italy), ITMATI (Spain) & Arcelor Mittal S.L. (Spain)) and the optimal shape design of air ducts in combustion engines (WIAS (Germany) & Math.Tec GmbH (Austria)).

**Conclusions**

With its coherent training programme ROMSOC educates the next generation of interdisciplinary researchers to become experts in mathematical MSO and to form a successfully interface between industry and academia. The close involvement of the industrial partners in the research significantly strengthen the societal relevance and quality of the training programme and facilitates the transfer of innovative concepts to industry.

For more information on ROMSOC, see https://www.romsoc.eu/.

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References


Educational Committee
2020 was a difficult year for all of us, and for the activities of the Educational Committee there was no exception.

In the last report regarding our activities in 2019, we started our contribution with the following sentence: 2019 was a great year for the Educational Committee! Unfortunately, in 2020 our lives changed in a rather unexpected and significant way, and the activities of the Educational Committee also needed to change and adapt to the new normal.

But even with many changes in our daily lives, we can be very proud of our achievements!

In February 14th and 15th we had our usual winter meeting, in the beautiful city of Coimbra, hosted by our colleague Marta Pascoal, from University of Coimbra.

During this meeting we had the presentation of 3 Universities that applied to become ECMI Teaching Centers:

- Universität Koblenz Landau (Germany)
- Kaunas University of Technology (Lithuania)
- Bergische Universität Wuppertal (Germany)

and it was decided to

- Recommend the Council to provide the label ECMI teaching center to the University of Szeged (in Hungary)
- Provide the label of provisional ECMI teaching center to Darmstadt (Germany).

The list of teaching centers and candidates is increasing, and this is a signal of the
Another topic that we have discussed was the preparation of the ECMI Modelling Week 2020, that was planned to take place in Saint-Petersburg, in July, organized by our colleague Sergey Lupuleac. We were all very excited about this modelling week, with high expectations not only concerning the impeccable organization of our Russian colleagues, but also looking forward to a stay in a beautiful city, full of history.

To add to the list of events that we were planning was the ECMI Conference, that would take place in Limerick. We had plans some activities, like a mini-symposium, organizing students competitions and the Wacker prize. Needless to say our plans for these activities were either cancelled or changed, with the arrival in Europe of the pandemic situation. Still, we were able to proceed with some of these activities in remote mode. In particular, our colleague Sergey and his colleagues were able to host the Modelling Week, in a virtual mode.

It was our first virtual Modelling Week and the experience was very interesting. The organizers kept as close to traditional ECMI Modelling Weeks as possible, notably in the program: problem presentations on Sunday, group works during the week, and final presentations on Saturday, open to all the members of the Educational Committee. Even some cultural programs were included! Using Google Street View, there was a virtual tour in St. Petersburg focused on the mathematical history of the city. Four projects were proposed:

- Bolted assembly optimization
- Hybrid storage system for peak shifting applications
- Capillary moisture uptake in wood
- Beanstalk (or Stairway to heaven)

All the participants enjoyed the Modelling Week, and it was a success. But of course nothing replaces our traditional meetings, and therefore we are looking forward to next Modelling Week, which hopefully will take place in 2022, in Verona. Meanwhile, we will do our best to cope with the ongoing situation, keeping the interest of Universities, Professors and Students in our ECMI program!

Cláudia Nunes
Chair of the Educational Committee (until July 2020)
ECMI Special Interest Groups (SIGs)
Introduction

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.

Computational Finance and Energy Markets

**Chairs:** Matthias Ehrhardt, University of Wuppertal, Germany, Jan ter Maten, University of Wuppertal, Germany  
**Scope:** The objective of this SIG is to gather specialists from all over Europe to tackle the actual problems of the modelling and the numerical analysis of various problems in computational finance. We aim to create a network of experts in the field to make communication easier, and to enable industrial or governmental organizations to find the right expert for their needs. The network is truly multidisciplinary, combining the power of mathematics, scientific computing, and quantitative finance, for modelling, calibration and simulation.

Implantable devices and drug delivery systems

**Chairs:** Sean McGinty, University of Glasgow, UK, Giuseppe Pontrelli, IAC-CNR, Rome, Italy  
**Scope:** Mathematical modelling is playing an increasingly important role in the field of medicine through the use of models and simulations. These represent a useful tool to complement theoretical and experimental work, and have the potential to inform personalized approaches for treatment. In this SIG we focus on the development of mathematical models and tools to assist with the design and understanding of implantable devices and drug delivery systems.

Liquid Crystals, Elastomers and Biological Applications

**Chairs:** Apala Majumdar, University of Strathclyde, UK, Nigel Mottram, University of Glasgow, UK  
**Scope:** This SIG focuses on the mathematical theories and modelling of soft materials that are intermediate between solids and liquids, with a special emphasis on synergistic links between theory, experiment, simulations, and industrial applications.

Math for the Digital Factory

**Chairs:** Dietmar Hömberg, WIAS, Berlin, Germany, Joachim Linn, ITWM, Kaiserslautern, Germany  
**Scope:** 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 past decade, 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). The SIG 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.
Mathematics for Big Data

**Chairs:** NATASA KREJIC, University of Novi Sad, Serbia, ALESSANDRA MICHELETTI, University of Milan, Italy

**Scope:** Sometimes data are “big” because of their high dimensionality and space-time structure, e.g., satellite images, signals registered by sensors or antennas. 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 with socioeconomic data for marketing purposes; or data highly interrelated which may be represented by complex graphs, like atoms and bounds in a protein, or relationships between users of a social network. Sentiment analysis and Topological Data Analysis are new statistical fields of research, still under development, which may help to tackle the problem of analysing such data. The aim of this SIG 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 favour scientific collaboration and research.

Modelling, Simulation and Optimization in Electrical Engineering (MSOEE)

**Chairs:** OLIVER RAIN, Robert Bosch GmbH, Stuttgart, SEBASTIAN SCHÖPS, TU Darmstadt, Germany

**Scope:** The members of this SIG have agreed on a broad understanding of the application field: it includes circuit simulation, computational electromagnetism (from low to high frequencies, up to optics), electrochemistry, material science with a focus on semiconductors, and plasma physics. Current methodological research is carried out on modelling with differential equations, model order reduction, multiscale and multirate methods, structure preservation, and uncertainty quantification.

Net Campus for Modeling Education and Industrial Mathematics

**Chairs:** MATTI HEILIO, Lappeenranta University of Technology, Finland, ROBERT ROCKENFELLER, University of Koblenz, Germany

**Scope:** This SIG strives to coordinate the activities at the various ECMI centers in the field of online and digital education. The Covid19 pandemic has brought the significance of virtual education and online tools to a new level. There is an acute need to investigate the possibilities of using online courses, webinars, network cooperation in curriculum development and more. The goal of this SIG is to eventually develop a set of courses, a portal, a virtual course portfolio, and an e-learning environment for industrial mathematics, which would be emerging from various ECMI-nodes, authored by colleagues from our SIG.

Shape and Size in Medicine, Biotechnology and Materials Science

**Chairs:** JESUS ANGULO, Mines ParisTech, France, LUIS L. BONILLA, Universidad Carlos III de Madrid, Spain

**Scope:** Often the diagnosis of a pathology, or the description of a biological process, mainly depends on the shapes present in images of cells, organs, biological systems, etc. 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 requires methods of statistical shape analysis. From the mathematical point of view, shape analysis uses a variety of mathematical
tools from differential geometry, geometric measure theory, stochastic geometry, and other areas of research. Quite recently, instruments from algebraic topology have been introduced for shape description, giving rise to a new field of research called Topological Data Analysis.

**Sustainable Energies**

**Chairs:** Andreas Münch, University of Oxford, UK, Barbara Wagner, WIAS, Berlin, Germany  
**Scope:** We address the challenges posed by the way energy will be generated in the future, with a high demand for sources of sustainable energy and production capabilities. It entails the restructuring of existing networks, 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.
The ECMI Special Interest Group Computational Finance and Energy Markets was launched at ECMI-2014 in Taormina (June 9–13, 2014), and (together with the ITN STRIKE Project) organized several sessions of a mini symposium in Computational Finance. Since ECMI-2016 in Santiago de Compostela the focus was extended to also include Energy Markets. The aim of the SIG is to extend the network and to build a framework to continue close cooperation in the future. It also provides a long term professional contact option for Alumni of ITN-STRIKE.

In 2020 the SIG was active at the ALGORITMY 2020 Conference in Podbanske, Slovakia.

Purpose

At ALGORITMY 2020, the international conference on scientific computing, the Special Interest Group on Computational Finance and Energy Markets organized a mini symposium Novel Methods in Computational Finance. We brought together eight speakers from academia that came from the University of A Coruña, Comenius University Bratislava, and University of Wuppertal.

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 mini symposium was to present the 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 commodities and related financial products. These approaches vary from 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 multilevel price estimation of jump diffusion driven assets and multi-step spline schemes for backward stochastic differential equations. Efficiently modelling stochastic correlation is a hot topic. The PDE group discussed efficient finite difference methods (high-order schemes with stochastic volatility and jumps in return). In the recent years we have
observed 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. Typical topics addressed at ECMI-2018 were price modelling for the German secondary balancing power market, gas prices dynamics, the Heston stochastic local volatility model in commodity markets, coupling reserve allocation and renewals, and proxy hedging of bunker fuel.

**Opportunities**

The SIG will look for opportunities for new projects in both directions, Computational Finance and Energy Markets, in the coming years, especially in Marie Skłodowska-Curie Actions in Horizon Europe, 2021–2027 (Training Networks (TN), Industrial Doctorates (ID), and Joint Doctorates (JD)). This also covers the important aspect of modelling Financial Risk and applications of Machine Learning. The Special Interest Group is open for further participation.

"Counterparty exposure has become the key element of financial risk management, highlighted by the bankruptcy of the investment bank Lehman Brothers and failure of other high profile institutions such as Bear Sterns, AIG and Fannie Mae.

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 default risky 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."

**Activities**

- At the regularly-held biennial ICCF Conferences (2015, 2017, 2019, 2022) and at the ECMI Conferences special SIG-Meetings are held.
- The EU-proposal ID CONFIRM involves several SIG-members and will be resubmitted in the Horizon Europe framework.

**Projects**

- Matthias Ehrhardt is leader of the bilateral German - Portuguese Project FRACTAL – FRActional models and CompuTationAL Finance, financed by DAAD (01/2019-12/2021)
- He is member of the bilateral German-Hungarian Project CSITI – Coupled Systems and Innovative Time Integrators, financed by DAAD (01/2019-12/2020)
- He is leader of the bilateral German-Slovakian Project MATTHIAS – Modelling and Approximation Tools and Techniques for Hamilton-Jacobi-Bellman equations in finance and Innovative Approach to their Solution, financed by DAAD (01/2020-12/2021)
Rafał Weron (University of Wrocław, Poland): Investigating Market Microstructure and short-term price forecasting in intraday electricity markets https://www.ii.pwr.edu.pl/~rweron/Grant

Mini-Symposia / Workshops Done

Due to the ongoing COVID19 pandemic the SIG activities were reduced; many events were postponed.


Mini-Symposia / Workshops Planned

- MS Computational Methods for Finance and Energy Markets at ECMI 2021 (virtual) Conference, April 13-15, 2021, hosted by University of Wuppertal, Germany. (this is a replacement of the ECMI 2020 conference, that was planned June 22-26, 2020, Limerick, Ireland and was cancelled due to the pandemic) see https://ecmi2021.uni-wuppertal.de/


- ICCF 2021 – 4th International Conference on Computational Finance, May 24-28, 2021, Wuppertal. This event is planned as face-to-face event and thus it is postponed to June 6-10, 2022, see https://iccf2021.uni-wuppertal.de/ ICCF 2024 is already scheduled for Dublin, Ireland.


Matthias Ehrhardt and E. Jan W. ter Maten
Bergische Universität Wuppertal, Germany
http://www-amna.math.uni-wuppertal.de/ecmi-sig-cf/
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:

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(May 2020)
ECMI Mission

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Guideline for author & templates: https://ecmiindmath.org/annual-reports/
For more information please visit the ECMI website: https://ecmiindmath.org
Print ISSN: 2616-7867
Online ISSN: 2616-7875