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EU-MATHS-IN -- MATHEMATICS FOR INNOVATION: SUCCESS STORIES AND SUPPORT FOR EUROPEAN INDUSTRIES

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ABSTRACT

The European Service Network of Mathematics for Industry and Innovation (EU-MATHS-IN) links 17 national networks across Europe (https://eu-maths-in.eu/). It fosters high-impact collaborations by facilitating communication and information exchange between researchers and industrial partners.

This minisymposium showcases successful technology transfer projects achieved through EU-MATHS-IN. Researchers and industry representatives present real-life examples that demonstrate the power of mathematics to drive innovation.

In addition, we present the EU-MATHS-IN OpenDesk (https://opendesk.eu-maths-in.eu/), an innovative support platform for European companies, start-ups and public administrations. This service provides valuable resources and guidance on how to use mathematics for problem solving and technological progress.

SPEAKERS

1. M.B. Cruz, School of Engineering of the Technical University of Porto, Portugal “EU-MATHS-IN: Connecting Mathematical Excellence with European Industry and Innovation”
2. P. Farrell, WIAS Berlin, Germany, “How Perovskite Solar Cells Degrade and Self-Heal: Insights from Mathematical Reaction-Based Models” (20 minutes)
3. M. Vynnycky, University of Limerick, Ireland, “Mathematics for the extra-terrestrial manufacture of small molecule drugs” (20 minutes)
4. L. Escudero Sartages, Centre de Recerca Matemàtica (CRM), Barcelona, Spain, “Turning Mathematical Models into Engineering Decisions: Optimising Asphalt Solar Collectors for Urban Energy Recovery” (20 minutes)
5. N. Patsalidis IACM, FORTH, Heraklion, Crete, Greece, “From Quantum Chemistry to Large-Scale Molecular Dynamics: Active Learning and Model Selection for Interfacial Force Fields” (20 minutes)

REFERENCES

[1] https://eu-maths-in.eu/success-stories-by-productive-sector/
[2] https://eu-maths-in.eu/about/mso-de-technologies/

1. **M.B. Cruz, School of Engineering of the Technical University of Porto, Porto, Portugal "EU-MATHS-IN: Connecting Mathematical Excellence with European Industry and Innovation" (40 minutes, keynote)**

   Abstract: Mathematical modelling, simulation, optimisation and data-driven methods are increasingly essential for addressing complex scientific, technological and industrial challenges. Their integration with artificial intelligence, high-performance computing and digital twins is also creating new mathematical questions and opportunities for research.

   EU-MATHS-IN, the European Service Network of Mathematics for Industry and Innovation, provides a framework for connecting these challenges with Europe's mathematical research community. Organised as a network of national networks, it brings together researchers and research centres across Europe, facilitating collaboration across disciplines, institutions and countries.

   At the centre of this interaction is OpenDesk, a one-stop shop through which industrial challenges can be identified, translated into mathematical problems and connected with appropriate expertise. The resulting interactions range from exploratory studies and proofs of concept to collaborative R&D, technology transfer, Industrial PhDs and training.

   The impact of this approach is illustrated by the growing collection of EU-MATHS-IN Success Stories, showcasing collaborations between mathematical researchers and companies across a wide range of industrial sectors. These examples demonstrate how advanced mathematical methods can address concrete industrial challenges, while applications themselves stimulate new mathematical questions and research directions.

   EU-MATHS-IN also contributes to identifying longer-term priorities through its Strategic Research Agenda, linking developments in modelling, simulation and optimisation with emerging data-intensive technologies.

   This lecture will present EU-MATHS-IN through its structure, services and selected Success Stories, illustrating a virtuous circle in which industrial challenges stimulate mathematical research, mathematical advances enable innovation, and successful applications reveal new opportunities for mathematics.

2. **P. Farrel, WIAS Berlin, Germany, "How Perovskite Solar Cells Degrade and Self-Heal: Insights from Mathematical Reaction-Based Models" (20 minutes)**

   Abstract: Perovskite solar cells are a promising solution for green energy, but their stability is a major challenge. Surprisingly, unlike silicon-based photovoltaics, perovskite-based solar cells do not simply degrade; they have the unique ability to spontaneously recover their performance in the dark. The mechanisms driving this behavior are not yet fully understood. Existing mathematical models typically study these phenomena separately, focusing either on ion transport or chemical reactions, which fails to capture their coupled effects. To address this, we present a unified reaction-diffusion framework based on non-equilibrium thermodynamics. In this approach, transport fluxes and reaction rates are derived consistently from the same potentials, allowing us to model electrons, holes, and lattice ions within a single mathematical structure. This unified treatment enables a physically accurate description of the system's dynamics. We

demonstrate the utility of this framework by simulating both degradation and recovery processes in perovskite solar cells, offering valuable insights into the factors determining long-term device stability.

The work has been realized in collaboration with Bingjie Li, Paria Forozi, Stefanie Schindler, Annegret Glitzky, Michael O'Donovan, Dilara Abdel, Patrick Jaap, Felix Lang, Dieter Neher, and Jarla Thiesbrummel.

3. **M. Vynnycky, University of Limerick, Ireland, "Mathematics for the extra-terrestrial manufacture of small molecule drugs" (20 minutes)**

   Abstract: Small molecule drugs are low-molecular-weight chemical compounds (typically under 900 g/mol) that form the foundation of traditional pharmaceutical medications, such as aspirin, ibuprofen, and penicillin. Typically, these are manufactured on Earth via a variety of crystallization processes, although the Earth's gravity makes this difficult. However, there is now an increasing interest in being able to manufacture small molecule drugs in microgravity environments, such as onboard low Earth orbit satellites. In this project, carried out in partnership with Varda Space Systems, the world's first in-space pharmaceutical processing and hypersonic Earth re-entry logistics company, we seek to develop experimentally validated, advanced mathematical models for crystallization in microgravity, in particular its effect on polymorphism – the chemical phenomenon whereby a solid substance can exist in more than one crystalline form. Understanding and controlling polymorphism is essential for manufacturing pharmaceuticals, since the crystal structure contributes various characteristics to the material properties of the active ingredient; so, polymorphs of the same molecule can have very different properties, e.g. melting point, hardness, solubility. The modelling work adopts a first-principles approach that considers molecule-specific parameters, the thermodynamics and kinetics that underpin crystallization and multi-phase fluid dynamics.

4. **L. Escudero Sartages, Centre de Recerca Matemàtica (CRM), Barcelona, Spain, "Turning Mathematical Models into Engineering Decisions: Optimising Asphalt Solar Collectors for Urban Energy Recovery" (20 minutes)**

   Abstract: Urban pavements absorb large amounts of solar radiation, raising surface temperatures, intensifying the urban heat island effect and accelerating material degradation. Asphalt solar collectors (ASCs), pipe networks embedded in the pavement, can turn this problem into a resource by recovering heat for nearby buildings. Their deployment, however, faces a key engineering barrier: performance depends on coupled interactions between fluid flow, heat transfer, pavement materials, pipe layout and weather, while testing every design option at full scale is slow, costly and disruptive to road infrastructure.

   Within the ENHANCE Europe project, the Centre de Recerca Matemàtica (CRM) provides the mathematical technology to overcome this barrier: a high-fidelity multiphysics model that reproduces the coupled behaviour of the pavement layers, the embedded pipes and the circulating fluid. Its finite element formulation couples transient heat transfer with incompressible fluid flow, enabling simulations under realistic, time-dependent operating and environmental conditions.

The resulting computational tool translates the collector's physical complexity into quantitative information that directly supports engineering decisions. It predicts temperature fields, recovered thermal energy and hydraulic behaviour, allowing engineers to evaluate and compare collector geometries, material configurations and operating strategies before field implementation.

The simulations are being validated against measurements from four European living labs. This interplay between simulation and experiment paves the way to validated digital tools for monitoring, predicting and optimizing the performance of real installations.

This collaboration illustrates how mathematical modelling and scientific computing turn a promising concept into an engineering solution that can be designed with confidence, supporting cooler, more resilient cities and new local sources of renewable heat.

5. **N. Patsalidis IACM, FORTH, Heraklion, Crete, Greece, "From Quantum Chemistry to Large-Scale Molecular Dynamics: Active Learning and Model Selection for Interfacial Force Fields" (20 minutes)**

Abstract: text Molecular dynamics (MD) simulations provide access to the molecular mechanisms governing the structure, dynamics and properties of liquid/solid and polymer/solid interfaces at length and time scales that are difficult to probe experimentally. Their predictive capability, however, depends critically on the underlying force field: the model of atomic interactions used to calculate energies and forces. Developing accurate interfacial force fields is particularly challenging because adsorption, local coordination and, in chemically active systems, bond rearrangements and charge redistribution arise from quantum-chemical interactions that simple mixing rules or conventional pair potentials may not adequately describe. We present a bottom-up multiscale modelling framework that bridges quantum-chemical calculations and large-scale atomistic MD. A central difficulty is the efficient exploration of the high-dimensional potential energy surface (PES): exhaustive quantum-level sampling is prohibitively expensive, yet an insufficiently diverse training set compromises the reliability and transferability of the resulting model. Our approach combines density functional theory (DFT) reference data with physics-aware potential representations of adjustable complexity, ranging from fitted semi-empirical interactions to models incorporating many-body effects and hybrid physics–AI architectures. To reduce the cost of PES exploration, an iterative active-learning workflow couples model training and configuration generation. Candidate structures are sampled with the current force field, informative or out-of-distribution configurations are selected for new DFT calculations, and the enlarged dataset is used to retrain and validate the model. This strategy concentrates quantum-chemical effort on configurations that improve the description of relevant interfacial environments. Finally, we discuss pathways for scaling up this multiscale procedure through automated validation and model-selection mechanisms that match force-field complexity to interfacial physics and simulation requirements. The central objective is to balance accuracy, computational efficiency and transferability, enabling predictive simulations of increasingly large and diverse interfacial systems.