CSQV 2025

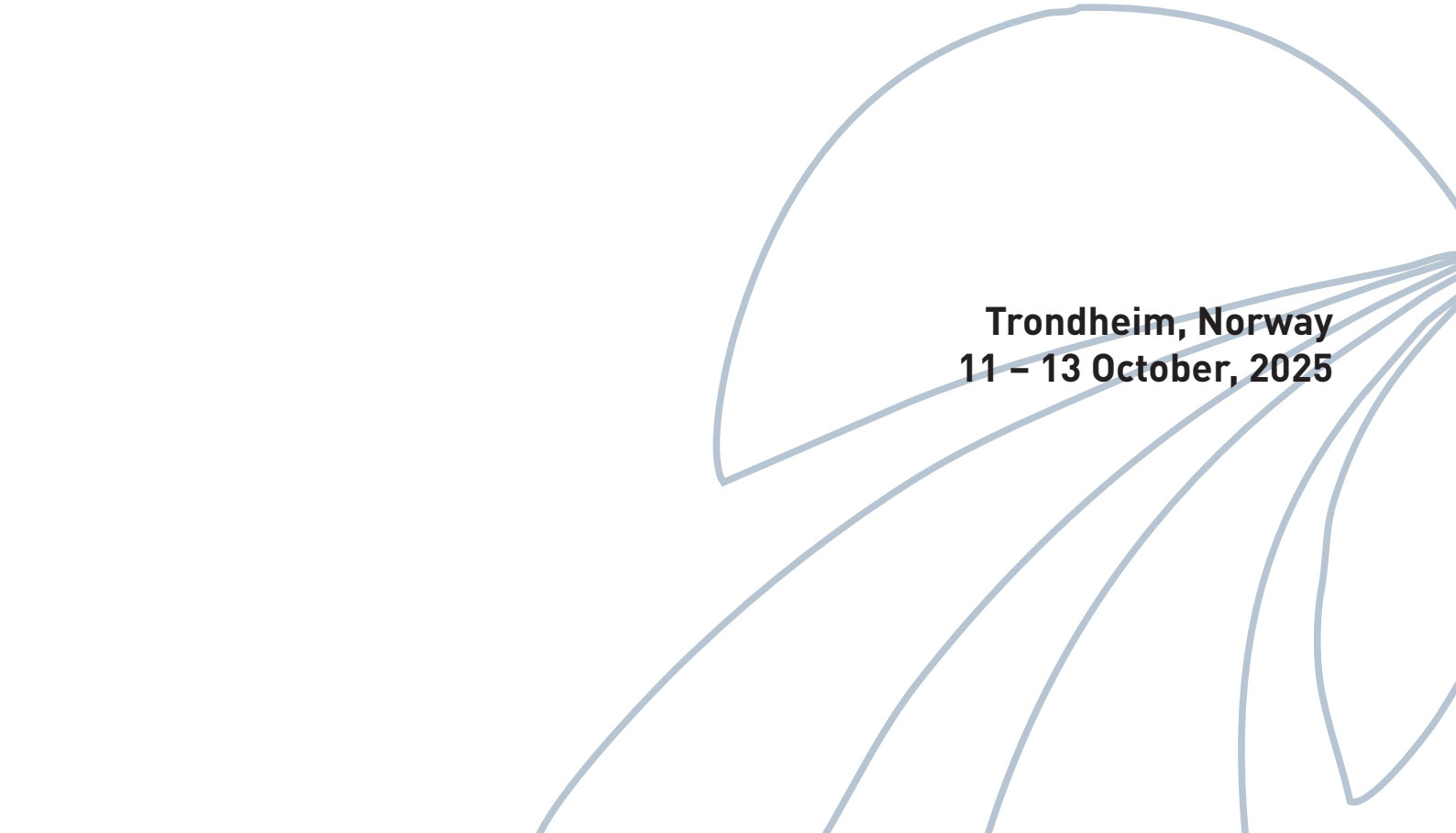
COMPUTATIONAL SCIENCES – QUO VADIS

Trondheim, Norway | 11 - 13 November, 2025

CSQV 2025

Symposium on Computational Sciences - Quo Vadis

Presentations



Trondheim, Norway
11 – 13 October, 2025

Greetings from the Chairs

This volume contains the abstracts of the talks presented at the *Symposium on Computational Science – Quo Vadis (CSQV 2025)*, held at the Britannia Hotel in Trondheim, Norway, on November 11-13, 2025.

The primary objective of CSQV 2025 is to provide an engaging forum for discussing the future trajectory and evolving role of computational sciences, particularly in light of the transformative potential that artificial intelligence (AI) holds for addressing critical challenges in engineering and science.

Conference presentations will showcase significant advancements made in computational sciences over recent decades and examine anticipated developments for the coming decade. Discussions will especially highlight the rapidly growing fields of data-driven science, machine learning, and artificial intelligence, alongside cutting-edge innovations in computing hardware, emphasizing their interaction with computational science and engineering. Participants will gain valuable insights into the computational methods expected to be central to this exciting evolution. This exceptional event will bring together world-leading experts from diverse disciplines, facilitating stimulating discussions and offering excellent networking opportunities.

During the symposium, we will also celebrate the 60th birthday of Trond Kvamsdal, a highly respected member of our community. Trond has enjoyed a distinguished career at SINTEF and NTNU, making significant contributions to areas such as Adaptivity, Isogeometric Analysis, and Digital Twins. Additionally, Trond is the President-elect of ECCOMAS and will officially begin his term in 2026 at the World Congress in Munich.

Mats Larson, Kjell Magne Mathisen, Knut-Andreas Lie

Chairmen of CSQV

ACKNOWLEDGEMENTS

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NTNU
Norwegian University of Science and Technology

SINTEF
75 år

NOACM
Nordic Association of Computational Mechanics

ECCOMAS

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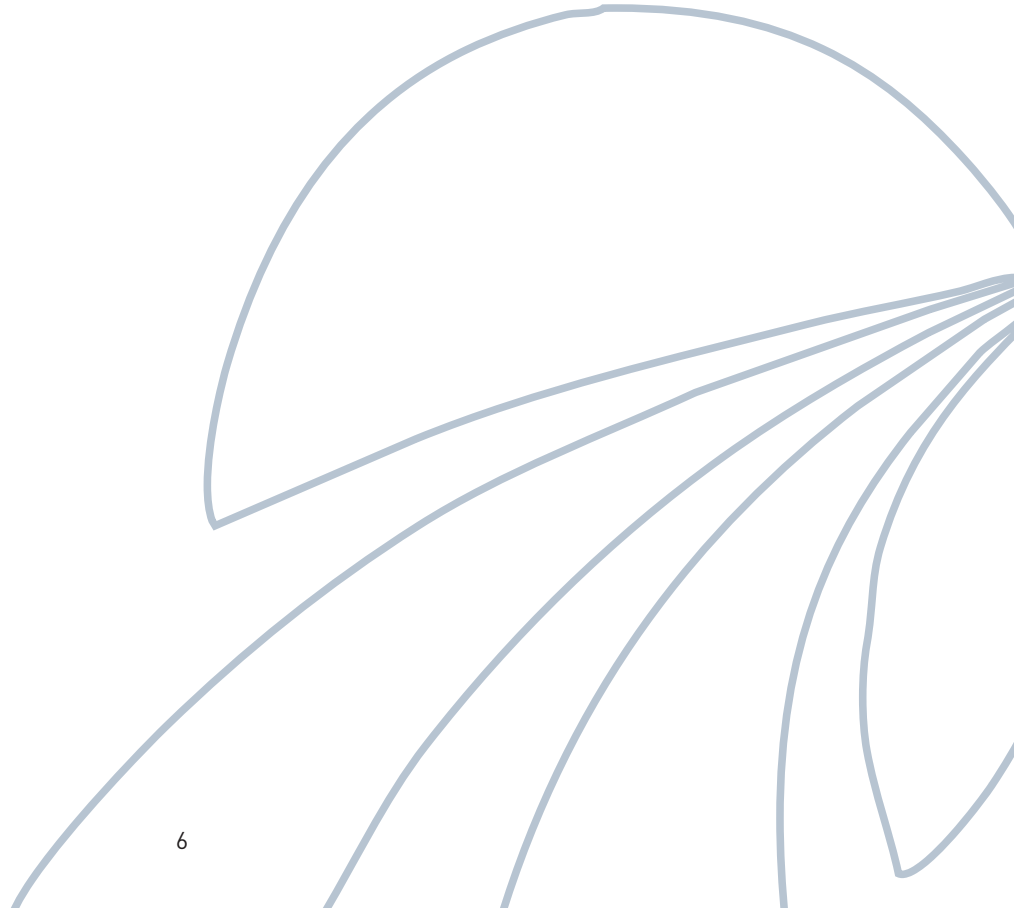

Some thoughts starting from Additive Manufacturing

Ferdinando Auricchio

Additive Manufacturing is a technology still growing and reach of challenges in terms of research and application exploitations. After a short the presentation will focus on the following two main aspects.
The presence of different physical, geometrical and temporal scale calls for a multiscale modeling. However, the scale difference is so significative that a more fundamental modeling approach could be extremely valuable. Some idea will be shared in this direction.

The possibility of designing and producing structures with a complex geometry puts a lot of interest toward the solution of topology optimization problems. The presentation will try to interpret in a simple frame some interesting and very well performing algorithms.

Computational Science: An Engineering and Physical Sciences Perspective

Yuri Bazilevs

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ABSTRACT

The talk will make general remarks on the field of computational science (CS) and its importance as a discipline in engineering and physical sciences, drawing mainly from personal experiences. The remarks will be supported by a collection of representative examples/problems computed from contemporary engineering and science applications. The presentation will conclude with some thoughts about the current state of CS education, including that at my institution, and interesting future directions in CS research.

Model and Method Hierarchies for Flow Simulation

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ABSTRACT

Computational analysis and design has achieved a widespread application across all engineering and scientific disciplines. Yet, as the systems being analyzed gain in complexity, the simulation process itself has become complex and fraught with ad hoc solutions and intuition. Continued impact may depend on systematizing the computational practice.

The simulation process may be divided into model, method, and data aspects. Each of the components of this tripod can be seen as a hierarchy of available options, each with certain predictivity (or fidelity) and a certain cost. A rational simulation process should involve selection of a model or models, discretization and numerical methods, and data sets or parameters, with a matched and sufficient predictivity at a minimal cost.

For this vision to become possible, progress needs to be made towards both establishing model and method hierarchies, and gaining insights into their predictivity and cost. On the modeling side, a hierarchy may represent a description of physical phenomena at different levels of abstraction. Examples of biomedical applications relying on varying description of blood constitutive behavior and geometric details are given. The issue of model adaptation, whether global or local, is also discussed.

This is joint work with Anna Ranno, Max Schuster, Fabio Guglietta, Max von Danwitz, Norbert Hosters, and Christoph Susen.

Quo vadis? Romam eo iterum crucifigī

Daniele Boffi

King Abdullah University of Science and Technology (KAUST), Saudi Arabia
and
University of Pavia, Italy

In this provocative talk I will review some of the personal and societal changes induced by the advent of massive AI usage in our everyday life. It goes without saying that by everyday life I mean the typical routine of a university professor, struggling with teaching innovation, meeting deadlines for project proposals, reviewing papers, etc., and - why not if time permits given that a day has 24 hours - writing good papers related to computational sciences.
Disclaimer: no AI tools have been used to write this abstract nor to prepare the presentation. Maybe just some Google searches here and there... it is possible that sometimes instead of Google I received an answer by Gemini... Yes, I have to admit that I've lost control on whether AI has been used or not for this talk.

Structure Preservation and Deep Learning: A Two-Way Path

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ABSTRACT

Deep learning neural networks can be interpreted as discretizations of an optimal control problem subject to an ordinary differential equation constraint.

We discuss briefly the connections between structure preserving algorithms and deep learning trying to describe the advantages on both sides. Some deep neural networks can be designed to have desirable properties such as invertibility and group equivariance or can be adapted to problems of manifold value data. Numerical algorithms with improved performance can be designed using data.

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ABSTRACT

In ongoing work with Ellingsen, Heinrich and Seth, we rediscover a KdV-type equation from simple video recordings of shallow-water solitons. Using two independent data-driven methods — weak-form sparse regression (WSINDy) and a Fourier multiplier approach — we extract the same governing equation, despite noise and lack of control in the experimental setup. This suggests that dynamics are robustly encoded even in rough experimental data.

In this talk I will further reflect on how data-driven techniques can support analysis of PDEs in settings where the underlying dynamics are unknown. I will also describe a separate line of work on numerically exact analysis using interval arithmetic, which rigorously proves existence of waves appearing at very subtle parameter relations. Together, these approaches point toward a future where data, computation and analysis play new and complementary roles in both modelling and mathematical deduction.

More generally I will touch upon the role research mathematics can play in a world where AI has moved beyond today's capabilities.

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The Future of Cardiovascular Mechanics
From a Computational Science Perspective

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Modeling and simulation in cardiovascular mechanics has benefited and continues to benefit from four central pillars: (i) advances in imaging, (ii) refined multiscale modeling, (iii) steadily increasing computing power, and (iv) computational modeling in biomechanics, enhanced by data-driven approaches and machine learning. The synergy of these four pillars also facilitates model validation and testing.

This short communication attempts to analyze future developments in computational cardiovascular mechanics. Machine learning, for example, will offer better opportunities to combine state-of-the-art imaging, multiscale modeling, and experimental and clinical data into systems whose predictive capabilities far exceed the capabilities of classical computational modeling in cardiovascular mechanics. A particularly promising research approach is hybrid architectures that combine machine learning and classical mechanistic modeling to benefit from the strengths of both. This rapidly growing field could represent a turning point, ensuring that the 2020s and 2030s become the decades in which computational biomechanics is fully translated from academic research into clinical practice, becoming a tool that is as ubiquitous in hospitals as finite element simulations are today in industrial engineering companies.

Deep Learning in Computational Mechanics

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ABSTRACT

It is time to sort out the zoo of methods that has emerged in the field of Deep Learning in Computational Mechanics [1,2]. To this end, this talk will provide a very short methodological classification and identify general research directions that have potential.

We will, further, present our own humble discovery by demonstrating an interesting property of neural networks that is not well understood but which enables them to find better local minima in optimization problems [3].

The presentation will finish with an outlook of what might happen when the bubble bursts: Millions of unused graphics cards that can perform matrix vector computations with astonishing efficiency [4].

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Towards Intelligent Variational Multiscale Reduced-Order Modeling for Low-Carbon Energy Systems

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ABSTRACT

Disruptive advances in artificial intelligence, machine learning, and high-performance computing are transforming how we model, simulate, and optimize complex physical systems. In this work, we present a numerical framework that integrates **Variational Multiscale (VMS) stabilized finite element formulation** with **parametric reduced-order modeling (ROM)** to accelerate predictive simulations in **low-carbon energy applications**, including wind turbine wake dynamics, buoyancy-driven flows in thermal systems and hydrokinetic systems. Recent results will be presented and future directions will be discussed.

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Mix Design, Modelling and Analysis of Low Carbon Concrete

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ABSTRACT

Concrete is the most used building material. Mainly Portland cement is used for binding the aggregate. Manufacturing of cement is energy intensive and carbon-dioxide producing process. About 8% of worlds carbon-dioxide is produced by cement industry. Alternative binders, like fly ash and iron slag waste, have been investigated for decades, but only during the last decade the Alcali- Activated Materials (AAM) raised some hopes for more energy saving and ecological concrete production. The chemical durability of the AAM concrete has been investigated quite intensively, but hardly nothing is known of the strength and fatigue behaviour of it.

The carbonation behaviour of electric arc furnace (EAF) slag and assessed both EAF and basic oxygen furnace (BOF) slags as supplementary cementitious materials (SCMs) have been investigated. Aqueous carbonation of EAF slag proved more effective than slurry carbonation. EAF slag showed delayed alite hydration but enhanced aluminate reactions, leading to higher strength compared to the Portland cement–limestone reference [1].

Compression tests and notched three point bending flexural tensile tests have been performed. The specimens were loaded to different damage levels. Strains were measured using DIC and post-mortem damage pattern characterized by XCT. Algorithms were developed to post-process XCT images to separate air bubbles from cracks. Mesoscale simulations of concrete have been carried out using Abaqus finite element software consisting of aggregates, voids, AAM cement matrix and ITZ as cohesive elements. Rankine tension cutoff model is applied to the cement matrix and the aggregates, with different material parameters. The finite element model is generated from the XCT images and is therefore an exact geometrical representation of the tested specimen. Tensorial continuum damage model has been further developed and analysed [2,3].

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The Computational Scientist in the Age of AI

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ABSTRACT

We explore how artificial intelligence is reshaping computational science. We contrast the *scaling paradigm*—bigger machines and faster algorithms—with a potential *evolution paradigm* driven by AI agents that reason, simulate, and interpret results autonomously. As AI begins to write code, design experiments, and analyze data, the role of the computational scientist may shift from executor to orchestrator. We also present *JutulGPT*, an AI agent integrated with a differentiable reservoir simulator, illustrating both the promise and pitfalls of agentic simulation. Key lessons include the need for hybrid human–AI workflows, better documentation, and transparent validation. Ultimately, the field must confront methodological, educational, and ethical challenges to ensure that computational scientists shape AI's impact—rather than being shaped by it.

Building Digital Twins in the Age of AI

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ABSTRACT

Digital twins, **virtual models mirroring real-world physical systems in real-time**, are transforming how we design, simulate, and operate complex environments before real-world deployment. Building on our work at the Digital Twin Cities Centre (DTCC), I will give an overview of projects such as automatic urban geometry and mesh generation, digital control rooms for construction site management, high-fidelity simulations of wind, pollution, and noise, and the DTCC data platform that underpins AI-driven twins across an entire city.

I will also discuss how **AI can accelerate and enable** each stage of this pipeline: speeding up research exploration and systematic literature studies; co-piloting programming and, where appropriate, generating library code and web interfaces; constructing city-scale 3D models from heterogeneous geospatial data; and learning surrogate models (e.g., neural operators and reduced-order surrogates).

Finally, I will reflect on how stronger AI tools shift the bottleneck from implementation capacity to **attention**. When researchers are amplified, the decisive skill becomes **problem selection**. I'll propose a pragmatic triage—prioritizing by **Impact**, **Tractability**, and **Data Readiness**—to focus effort where it changes practice rather than merely what is easy to do.

Randomized Algorithms in Scientific Computing

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ABSTRACT

The talk will describe how techniques based on randomized methods for dimension reduction have enabled dramatic increases in computational capabilities for fundamental tasks within scientific computing and data science. A prime example concerns randomized methods for approximating matrices and for solving large linear systems. The talk will also describe how these ideas generalize to the case of entire operators such as solution operators for elliptic PDEs, time stepping operators for parabolic problems, and boundary-to-boundary maps such as the Dirichlet-to-Neumann map that form essential building blocks of domain decomposition methods and multi-physics simulations.

Randomized compression techniques can also be used to build accurate but light-weight representations of physical systems for on-the-fly computing in autonomous systems, or in a real-time digital twin of a drone. These are ideal environments where one can afford a one-time expensive computation on a workstation that fully resolves the physics. Randomized compression is then used to build accurate surrogate models that faithfully reproduce the input-to-output map. These models would have small memory footprints and would allow instantaneous evaluation of physical systems where the full model originally involved millions or billions of degrees of freedom.

The ideas presented also provide paths for advances in Scientific Machine Learning. Some paths are straightforward, such as the rapid generation of large training sets, or the fast evaluation and differentiation of objective functions involving global operators. More challenging questions concern how multiresolution representations and randomized compression techniques can be incorporated into compressed models of fully nonlinear operators.

Large-scale crash simulations - Where are the research needs?

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ABSTRACT

Large-scale crash simulations are essential tools in the design and validation of modern vehicles. Over the past decades, major advances in computational mechanics and materials modelling have enabled the development of lighter, more efficient, and safer cars. Today's models encompass thousands of components made of aluminium, steel, polymers, and composites, each represented by constitutive descriptions capable of capturing complex deformation and failure behaviour. Beyond individual materials, the integrity of the structure depends critically on the joining techniques—welding, riveting, adhesive bonding, or hybrids—that connect these components and must sustain severe dynamic loading.

Given this level of maturity, it is natural to ask: where are the next challenges in crash simulation research? While industrial models have reached impressive predictive capabilities, several fundamental challenges remain. These concern, for instance, the accurate modelling of material failure and ductility in recycled materials, the representation of joints that combine disparate materials and scales, and the integration of new energy systems—such as lithium-ion batteries— whose mechanical behaviour under crash or impact remains challenging to predict accurately. Moreover, as vehicle architectures evolve toward electrification and circularity, ensuring structural robustness and crashworthiness while maintaining lightweight design poses additional challenges for both simulation fidelity and computational efficiency.

Reproducibility in reality and computation

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ABSTRACT

Reproducibility is a fundamental tenet of the classical sciences, and is today most commonly encoded in the FAIR principles. Moreover, one may claim that the main reason mathematics has attained the importance it has in science and society, rests on the fact that it is a logical language that encodes the reproducibility observed in reality.

However, the actual real world is not reproducible, and arguably, neither is computational science. Several qualitatively different reasons hinder reproducibility: Some uncertainty may be quantifiable, and be subjected to rigorous analysis, such as fundamental physical uncertainties (Heisenberg), measurement uncertainty, computational uncertainty and errors in data transmission. Other sources of uncertainty are typically impossible to quantify, such as design limitations in experimental or computational studies. Underestimating the importance of unquantifiable undertainty leads to overconfidence bias, which is a major challenge associated with soliciting expert opinions.

In this talk, we will discuss our experience with unquantifiable uncertainty in both experimental and computational science [1,2], and the implications this has for the design and performance of digital twin systems [3].

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Computational Mechanics in the Digital Era.
Challenges and opportunities

Eugenio Oñate

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ABSTRACT

The digital era has revolutionized every field of engineering. As computing power, data availability and digital connectivity expand exponentially, computational engineers now possess unprecedented tools to design, simulate and optimize complex systems. This transformation represents a paradigm shift toward intelligent, data-driven decision-making that reshapes how problems are analyzed and solved across industries.

The presentation presents an overview of some challenges and opportunities that the digital era offers to researchers and practitioners in computational mechanics. Specifically, we will address the following topics.

1. High-Performance and Cloud Computing. The digital age favours the accessibility of high-performance computing and cloud-based simulation platforms. These resources enable engineers to perform massive parallel computations that were once limited to supercomputers.

2. Artificial Intelligence and Machine Learning. The integration of AI and ML with computational engineering creates new methods for modeling, prediction and optimization.

3. Big Data, BIM and Digital Twins. Through data analytics and visualization tools, engineers can gain real-time insights into system performance and reliability. Digital twins and BIM technology allow engineers to simulate and optimize structures, vehicles and networks throughout their life cycle, enabling predictive control, risk assessment and sustainability.

4. Advanced Simulation and Visualization. Modern visualization technologies such as virtual reality (VR), augmented reality (AR), and interactive 3D modeling expand allow engineers can now immerse themselves in complex datasets, interact with multi-physics simulations in real time, and communicate design concepts more effectively.

5. Quantum computing. The integration of GPU-based computing and quantum simulation techniques opens new frontiers in solving highly nonlinear and multi-dimensional problems that were previously unsolvable.

6. IoT and Digital Passport of Products (DDP). The Internet of Things will create a social network of connected products. This will open opportunities for new ways of designing, producing and maintaining industrial products and infrastructures. The DPP will ensure originality and recyclability of all products, and will create new marketing channels.

7. Sustainability and Global Impact. Computer simulations optimize energy systems, improve materials efficiency and reduce environmental impact. By virtually testing many design scenarios, engineers can identify sustainable solutions without the cost of physical prototypes.

8. Interdisciplinary Collaboration and Automation. The digital era encourages collaboration across disciplines. Automated workflows, enabled by Python scripting, APIs, and integrated modeling environments, allow repetitive or multi-parameter simulations to be executed autonomously. This leads to faster research cycles, reproducibility and continuous improvement in model accuracy.

In summary, the digital era brings a world of opportunities to researchers and practitioners in the field of computational mechanics. The way the new challenges are faced and tackled in academia and industry will be crucial to keep the pace in a global competing world.

Science meets Data: Scientific Computing in the Age of Artificial Intelligence

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ABSTRACT

Computational mechanics, since its inception in the '60s, has tracked developments in both theoretical and applied mechanics, as well as scientific computing. It started with the basics of finite-element development and solvers, with scant attention given to material modeling and physics of solids. However, early in the game a more ambitious plan emerged that encompassed nonlinear material behavior, history dependence and dissipation, coupled thermodynamics and phase transitions, extreme conditions of temperature, pressure and rate of deformation, and generally the full gamut of constitutive behavior of solids. In that way, computational mechanics tracked sweeping trends in the field of solid mechanics, including rational mechanics, micromechanics and multiscale analysis, uncertainty quantification and, more recently, data science and quantum computing. Thus, epochal advances in *ab initio* methods and experimental science have effectively changed solid mechanics from a data-poor and mostly empirical field to an increasingly data-rich and physics-based field.

This paradigm shift raises many fundamental challenges concerned with how best to generate, manage and use material data to enable discovery, prediction and design. Deep mathematical and practical questions arise regarding how to generate data, how to build data into boundary value problems, how to ensure predictive accuracy and convergence of the solutions, and others. Recently, a new potentially game-changing paradigm has arrived in computational mechanics, namely, quantum computing. Quantum computers, operating on entirely different physical principles and abstractions from those of classical digital computers, have the unique ability to simultaneously evolve the state of an entire quantum system, which leads to quantum parallelism and interference. In addition, quantum entanglement enables the representation of systems of enormous dimensionality with a modicum of quantum bits, or qubits. Despite these prospects, opportunities to bring quantum computing to bear on problems of computational mechanics in general and, specifically, on data-driven computational mechanics, remain largely unexplored. Exploratory work to date suggests that quantum computing can indeed accelerate exponentially stubborn long-standing bottlenecks in classical multiscale and data-driven computational mechanics, thus bringing them closer to the realm of feasibility and practicality.

Computational Science in the Age of AI

Alfio Quarteroni

Abstract. In this short presentation, I will revisit the main contributions of artificial intelligence within the field of computational science and outline future perspectives, taking into account emerging computational paradigms.

Reimagining Scientific Discovery Through LLM-Guided Digital Twins

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ABSTRACT

This work presents an end-to-end digital-twin framework that integrates Large Language Models (LLMs) directly into the control loop of a physical asset. By coupling physics-based, data-driven, and hybrid models with natural-language reasoning, the framework bridges human intent, model prediction, and actuation in real time. The asset incorporates physics-based, data-driven, and hybrid predictive models to compare accuracy, generalization, and computational efficiency.

On the control side, three complementary strategies are explored: model predictive control, reinforcement learning trained in the digital twin and deployed on the physical asset, and LLM-based controllers capable of interpreting natural-language objectives. The LLM controllers demonstrate autonomous, explainable control decisions and the ability to handle dynamic operating conditions without manual tuning or explicit domain expertise.

The key message is conceptual: when LLMs are embedded into scientific workflows, they act as cognitive bridges that allow researchers to explore, model, and control systems in fields where they possess little or no prior knowledge. This paradigm redefines scientific practice—transforming experimentation into a conversational, adaptive, and inclusive process. The implications extend far beyond greenhouse control: such frameworks can democratize scientific discovery, accelerate innovation across disciplines, and open entirely new research horizons where human creativity and machine intelligence collaborate seamlessly.

Should we abandon industrial AI, or can we fix it?

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ABSTRACT

AI can write code, run simulations, interpret results, generate mathematical proofs, and verify their correctness [1-5], but it can still not make your coffee or run a process plant. Hence, only few actors are successfully implementing AI in industrial settings. From an industrial perspective, AI faces significant challenges, including low trustworthiness, immature technology, prohibitive development costs, inadequate validation and verification methods, and a lack of assurance mechanisms. Additionally, the shortage of expertise and limited understanding of emerging regulations further hinder responsible deployment. As a result, its use in critical decision-making remains limited [6]. What is required to make it useful? Is it feasible? And how do we get there?

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Raven - AI based semantic clustering visualizer for scientific abstracts

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Keywords

Semantic clustering; Scientific abstracts; Unsupervised learning; Interactive visualization; Open source.

ABSTRACT

Raven is an AI-based system developed at JAMK University of Applied Sciences (JAMK) for clustering and visual examination of scientific abstracts in large datasets. Instead of relying on traditional keyword-based search or manual classification, Raven infers the semantic proximity between abstracts directly from the text, which enables the examination of tens or even hundreds of thousands of documents as an interactive, content-structured landscape. Because the models are run locally, sensitive or non-public material can be analyzed without the data leaving the organization's infrastructure; this supports privacy-preserving literature reviews and internal foresight/horizon scanning.

We demonstrate Raven with a case study that used abstracts from the ECCOMAS conference held in Lisbon and examined how contributions are distributed across different themes. The resulting maps enable users (i) to grasp the breadth and balance of a research area at a glance, (ii) to discover under-explored sub-areas adjacent to their own interests, and (iii) to rapidly assemble representative document sets for deeper analysis. Raven is open-source software: https://github.com/Technologicat/raven

Raven-visualizer

Multiscale Model Learning in Computational Kinetic Theory

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ABSTRACT

Kinetic theory describes fluid flows in terms of a particle probability distribution in position-velocity dependence. The theory is valid in the dilute/rarefied regime, i.e. if the distance between molecules is large relative to the characteristic length scales in the problem under consideration, but it also encapsulates all conventional macroscopic flow models such as the Navier-Stokes-Fourier equations in the so-called hydrodynamic limit, i.e. if the ratio of the mean free-path between molecules and characteristic length scales passes to zero. Kinetic theory owes this universality to its structural (conservation/dissipation) properties, notably conservation of mass, momentum and energy and entropy dissipation. These properties are also fundamental to stability of the equations.

The details of molecular interactions in kinetic theory are encoded in the so-called collision operator. To enhance the descriptive capabilities of the collision operator, it can be learned from an underlying microscopic model such as molecular dynamics, and encoded in a neural net. The neural net then acts as a multiscale model, bridging between MD and kinetic theory. However, standard learning procedures do not retain the fundamental structural properties, or only do so in an average sense, and thus lead to unstable equations or incorrect limits.

In the presentation I will elaborate how ML can be used in computational kinetic theory (CKT) while upholding the structural properties of the equations. I will also share some personal insights into the role of ML in CKT and CSE in general.

Quo Vadis Computational Mechanics – From the Athenian Agora into the engine room

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ABSTRACT

In this talk, I will attempt to draw a large arc. The plan is to start with some fundamental aspects that I find crucial for our future. I will then try to show that those aspects are not only nice for academic philosophical discussions but are relevant (in a very concrete way) for our field (as well as our daily life and work). The talk will then also cover some more concrete considerations and topics for the future of Computational Science/Mechanics.

Fast physics-based numerical simulations or AI based tools?

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ABSTRACT

While AI tools attract growing attention, their predictive accuracy often relies on large datasets and high computational cost. Fast, physics-based numerical simulations can achieve comparable or better predictions with far greater efficiency and transparency.

This presentation demonstrates how reduced order models and fast implementations enable real-time, reliable predictive modelling. We argue that such physics-driven approaches remain the most effective and trustworthy alternative to purely AI-based methods.

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